NATIONAL TECHNICAL UNIVERSITY OF ATHENS

SCHOOL OF CIVIL ENGINEERING

DEPARTMENT OF WATER RESOURCES AND ENVIRONMENTAL ENGINEERING

Uncertainty-aware simulation-optimization framework for water-energy systems

Thesis submitted for the degree of Doctor of Philosophy

by Georgia Konstantina Sakki

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ΕΘΝΙΚΟ ΜΕΤΣΟΒΙΟ ΠΟΛΥΤΕΧΝΕΙΟ

ΣΧΟΛΗ ΠΟΛΙΤΙΚΩΝ ΜΗΧΑΝΙΚΩΝ

ΤΟΜΕΑΣ ΥΔΑΤΙΚΩΝ ΠΟΡΩΝ ΚΑΙ ΠΕΡΙΒΑΛΛΟΝΤΟΣ

Πλαίσιο προσομοίωσης-βελτιστοποίησης συστημάτων νερού-ενέργειας υπό αβεβαιότητα

Διατριβή για την απόκτηση διδακτορικού διπλώματος από τη

Γεωργία Κωνσταντίνα Σακκή

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To my parents.

Panagiotis and Angeliki

Thank you for keeping the interest rates low

on everything I owe you.

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Dear reader,

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Georgina Sakki
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Abstract

The water-energy nexus plays a crucial role in fostering sustainable growth, since it is the cornerstone for the interconnected and intertwined systems of water and energy supply, consumption, and management. This interrelation is the paramount for achieving sustainable development goals, as both water and energy resources are essential for economic growth, social prosperity, and environmental stewardship. In this respect, this Ph.D. thesis explores, describes and quantifies the complex interdependencies within the water-energy nexus, focusing on the incorporation and management of uncertainty arising from both aleatory and epistemic sources. The research investigates the impacts of climatic variability, social dynamics, and energy market fluctuations on water-energy systems, with a particular emphasis on optimizing system performance under uncertain conditions.

Since, the water-energy nexus is driven by inherently uncertain hydroclimatic processes and multiple human-induced procedures (e.g., legal regulations, strategic management policies, real-time controls, market rules), it is globally recognized that their operation is highly exposed to emerging *climatic*, *anthropogenic*, and *energy-market* pressures and fluctuations. In this respect and to move forward fragmented approaches, we aim at establishing an *uncertainty-aware simulation-optimization framework* that support systems for water planning and management, under the holistic prism of water-energy-society nexus. This shift will require an effective and efficient integration of different theories, i.e., the *triptych of statistics, stochastics and copulas* and tools, i.e., simulation, optimization and agent-based models into a unified methodological framework.

In particular, this framework seeks for the combined effects of the climatic, social and energy market uncertainties within the water-energy nexus, as well as the interplay of their cascades and dependencies that have received considerably less attention to date. For the description of climatic and energy market uncertainty, we are taking advantage of stochastic models, while for the representation of the social dynamics within the technical systems we employ statistical analyses and agent-based models. Through a combination of advanced simulation techniques and optimization procedures, this research identifies uncertainty-aware strategies for adaptive management and decision-making, that affect the system's performance, as quantified in terms of economy, reliability and resilience.

The *uncertainty-aware simulation-optimization framework* for water-energy systems is stress-tested at three scales of interest: (a) the design scale, aiming at the optimal sizing and mixing of small hydropower plants; (b) the long-term management scale, aiming at assessing the policies of water utilities, under changing hydroclimatic and socioeconomic conditions; and (c) the combination of short, mid and long-term scale, aiming at defining their optimal operation policy under changing hydroclimatic and socioeconomic conditions, also dominated by issues of scheduling of energy production under uncertain energy market fluctuations. For the validation of the concepts, methodologies and tools a series of hypothetical and real-world cases are examined covering a wide range of spatial and temporal scales.

Overall, this research contributes to the emerging field of water-energy nexus by addressing the challenges posed by uncertainty and variability across multiple domains. Eventually, the findings offer valuable insights and toolboxes for policymakers, planners, and stakeholders involved in managing and optimizing water and energy resources in a changing and uncertain environment.

Εκτενής ελληνική Περίληψη

Αντικείμενο της έρευνας

Το πλέγμα νερού-ενέργειας παίζει καθοριστικό ρόλο στην προώθηση της βιώσιμης ανάπτυξης, καθώς αποτελεί τον ακρογωνιαίο λίθο για τα διασυνδεδεμένα και αλληλένδετα συστήματα κατανάλωσης και διαχείρισης νερού και ενέργειας. Αυτή η αλληλεξάρτηση είναι υψίστης σημασίας για την επίτευξη των στόχων βιώσιμης ανάπτυξης, καθώς τόσο οι υδατικοί όσο και οι ενεργειακοί πόροι είναι απαραίτητοι για την οικονομική ανάπτυξη, την κοινωνική ευημερία και τη διαχείριση του περιβάλλοντος. Σε αυτό το πλαίσιο, η παρούσα διδακτορική διατριβή εξερευνά, περιγράφει και ποσοτικοποιεί τις πολύπλοκες αλληλεξαρτήσεις εντός του πλέγματος νερού-ενέργειας, εστιάζοντας στην ενσωμάτωση και διαχείριση της αβεβαιότητας που προκύπτει από *αλεατορικές* (aleatory) και *επιστημικές* (epistemic) πηγές. Η έρευνα διερευνά τις επιπτώσεις της κλιματικής μεταβλητότητας, των κοινωνικών δυναμικών και των διακυμάνσεων της ενεργειακής αγοράς στα συστήματα νερού-ενέργειας, με ιδιαίτερη έμφαση στη βελτιστοποίηση της απόδοσης τους υπό συνθήκες αβεβαιότητας.

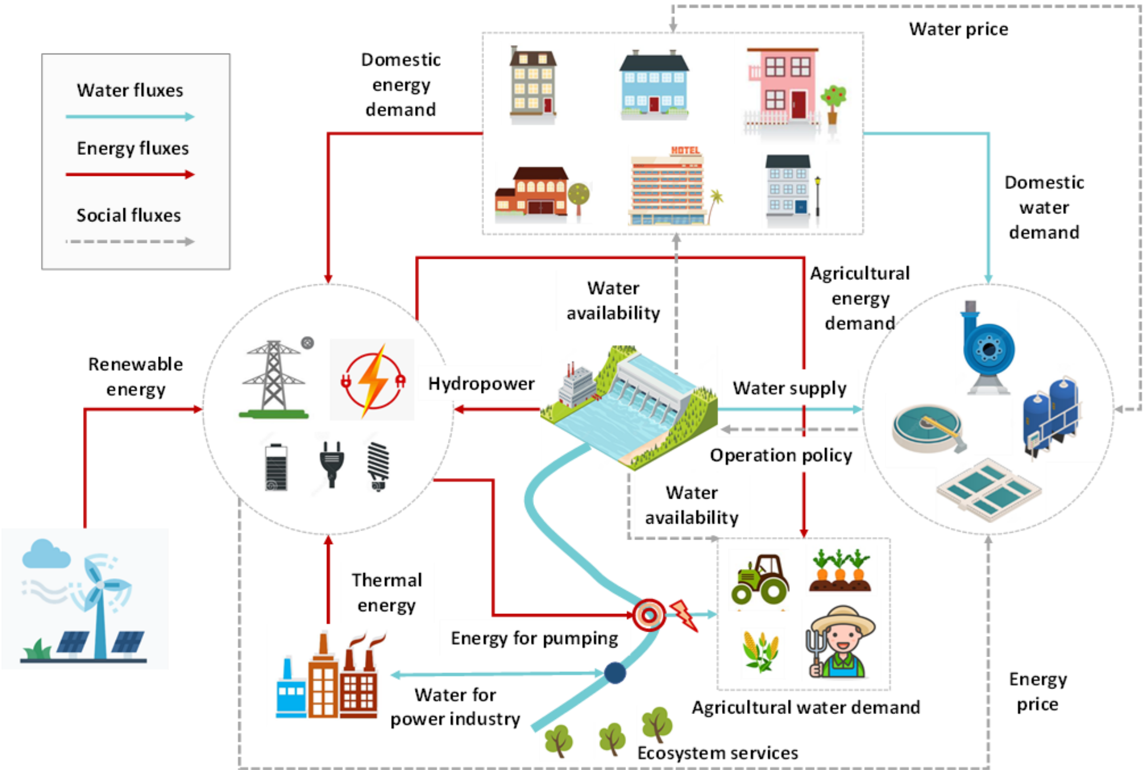
Δεδομένου ότι το πλέγμα νερού-ενέργειας καθοδηγείται από εγγενώς αβέβαιες υδροκλιματικές διεργασίες και πολλαπλές ανθρωπογενείς διαδικασίες (π.χ. νομικές ρυθμίσεις, στρατηγικές πολιτικές διαχείρισης, έλεγχοι σε πραγματικό χρόνο, κανόνες αγοράς), είναι παγκοσμίως αναγνωρισμένο ότι η λειτουργία τους είναι ιδιαίτερα εκτεθειμένη στις αναδυόμενες κλιματικές, ανθρωπογενείς και ενεργειακές πιέσεις και διακυμάνσεις της αγοράς. Προκειμένου να προχωρήσουμε πέρα από τις τυπικές αποσπασματικές προσεγγίσεις, στοχεύουμε στην καθιέρωση ενός πλαισίου προσομοίωσης-βελτιστοποίησης που λαμβάνει υπόψη την αβεβαιότητα και υποστηρίζει τον προγραμματισμό και τη διαχείριση των πόρων, υπό την ολιστική οπτική του πλέγματος *νερού-ενέργειας-κοινωνίας*. Αυτή η μετάβαση απαιτεί την αποτελεσματική και αποδοτική ενσωμάτωση διαφορετικών θεωριών και εργαλείων σε ένα ενιαίο μεθοδολογικό πλαίσιο. Αυτό ενσωματώνει το τρίπτυχο *στατιστική*, *στοχαστική* και *συναρτήσεις σύζευξης* (copulas), εντός των μοντέλων προσομοίωσης και βελτιστοποίησης.

Συγκεκριμένα, αυτό το πλαίσιο επιδιώκει να εξετάσει τις συνδυασμένες επιπτώσεις των κλιματικών και κοινωνικών αβεβαιοτήτων, καθώς και αυτών που προέρχονται από τις ενεργειακές αγορές, και διέπουν το πλέγμα νερού-ενέργειας. Ειδικότερα, δίνεται έμφαση στην αλληλεπίδραση των αλληλουχιών και εξαρτήσεων των παραπάνω πηγών αβεβαιότητας, που έχουν λάβει σχετικά μικρή προσοχή μέχρι σήμερα. Για την περιγραφή της κλιματικής και ενεργειακής αβεβαιότητας, εκμεταλλευόμαστε τα στοχαστικά μοντέλα, ενώ για την αναπαράσταση των κοινωνικών δυναμικών εντός των τεχνικών συστημάτων χρησιμοποιούμε στατιστικές αναλύσεις και μοντέλα ευφυών πρακτόρων. Μέσω ενός συνδυασμού προηγμένων τεχνικών προσομοίωσης και διαδικασιών βελτιστοποίησης, αυτή η έρευνα αναδεικνύει στρατηγικές προσαρμοστικής διαχείρισης και λήψης αποφάσεων με επίγνωση της αβεβαιότητας, οι οποίες επηρεάζουν την απόδοση του συστήματος, όπως ποσοτικοποιείται με όρους οικονομίας, αξιοπιστίας και ανθεκτικότητας.

Το πλαίσιο προσομοίωσης-βελτιστοποίησης υπό αβεβαιότητα για τα συστήματα νερού-ενέργειας δοκιμάζεται σε τρεις κλίμακες ενδιαφέροντος: (α) στην κλίμακα σχεδιασμού, με στόχο τη βέλτιστη διαστασιολόγηση τους, (β) στην κλίμακα μακροχρόνιας διαχείρισης, με στόχο την αξιολόγηση των πολιτικών των υδατικών υπηρεσιών, υπό μεταβαλλόμενες υδροκλιματικές και κοινωνικοοικονομικές συνθήκες, και (γ) στον συνδυασμό βραχυπρόθεσμης, μεσοπρόθεσμης και μακροπρόθεσμης κλίμακας, με στόχο τον καθορισμό της βέλτιστης πολιτικής λειτουργίας τους υπό μεταβαλλόμενες υδροκλιματικές και κοινωνικοοικονομικές συνθήκες, οι οποίες κυριαρχούνται επίσης από ζητήματα προγραμματισμού της παραγωγής ενέργειας υπό αβέβαιες διακυμάνσεις της ενεργειακής αγοράς. Για την ανάδειξη των μεθοδολογιών και των εργαλείων εξετάζονται μια σειρά από υποθετικές και πραγματικές περιπτώσεις που καλύπτουν ένα ευρύ φάσμα χωρικών και χρονικών κλιμάκων.

Στόχοι και προκλήσεις

Όπως προαναφέρθηκε, η παρούσα έρευνα στοχεύει στην απεικόνιση των βασικών στοιχείων του νερού, της ενέργειας και της κοινωνίας ως αλληλοσυνδεόμενων ροών που παρουσιάζουν συνέργειες, αντιθέσεις και συμπληρωματικότητες (**Εικόνα 1**).



Εικόνα 1: Σχηματική αναπαράσταση των ροών νερού, ενέργειας και κοινωνίας ως ενιαίο σύστημα.

Αυτή η προσπάθεια υπόκειται σε έξι βασικούς στόχους, καθένας από τους οποίους εισάγει έναν αριθμό προκλήσεων. Πιο συγκεκριμένα:

(α) Ο πρώτος στόχος περιλαμβάνει την αναθεώρηση των υφιστάμενων σχημάτων προσομοίωσης-βελτιστοποίησης που χρησιμοποιούνται στην μελέτη συστημάτων νερού-ενέργειας, προκειμένου να ενσωματωθούν όλες οι πτυχές της αβεβαιότητας, εξωγενείς και ενδογενείς, που επηρεάζουν τέτοια συστήματα.

(β) Ένας παράλληλος ερευνητικός στόχος προκύπτει από την ανάγκη ενσωμάτωσης της εξαιρετικά αβέβαιης κοινωνικής πτυχής στην τεχνική περιγραφή της διασύνδεσης νερού-ενέργειας, διαμορφώνοντας έτσι μία νέα έννοια, ήτοι *στοχαστικά κοινωνικο-τεχνικά συστημάτα*. Σημαντικός στόχος είναι η μαθηματική τυποποίηση και αναπαράσταση του ανθρώπινου παράγοντα, ακολουθώντας και ερμηνεύοντας την κοινωνική συμπεριφορά, ακολουθώντας δύο προσεγγίσεις «από κάτω προς τα πάνω» (bottom-up) και «από πάνω προς τα κάτω» (top-down). Όσον αφορά την « από κάτω προς τα πάνω» προσέγγιση, η έρευνα αυτή αξιοποιεί και ενισχύει τη θεωρία των ευφυών πρακτόρων (agent-based theory), όπως παρουσιάστηκε από τον Bonabeau (2002), συνδυάζοντας τη με το βέλτιστο σχήμα σχεδιασμού και διαχείρισης νερού-ενέργειας. Αυτή η προσέγγιση θα επιτρέψει στην μελέτη της αλληλεπίδρασης του ανθρώπινου παράγοντα με το τεχνικό σύστημα, ενώ θα μας επιτρέψει την εξαγωγή συμπερασμάτων σε μακροσκοπικό επίπεδο. Από την άλλη πλευρά, η «από άνω προς τα κάτω» προσέγγιση αξιοποιεί ιστορικά δεδομένα και βασίζεται σε αυτά για την περιγραφή του ανθρώπινου παράγοντα και της αντίδρασής του στο τεχνικό σύστημα.

(γ) Ένας ακόμη ερευνητικός άξονας προκύπτει από την αγορά ενέργειας και τις αλληλεπιδράσεις της στη διασύνδεση του πλέγματος νερού-ενέργειας. Αναγνωρίζουμε δύο κρίσιμα ερευνητικά σημεία σχετικά με την αγορά ενέργειας, ήτοι την απεικόνιση της τιμής ηλεκτρικής ενέργειας (π.χ., επιτόκια, τιμή ηλεκτρικής ενέργειας) και τις επιπτώσεις της στη διαχείριση και λειτουργία των συστημάτων νερού-ενέργειας (π.χ. ενεργειακοί στόχοι, κέρδη, λογαριασμοί νερού κ.λπ.).

(δ) Η διαμόρφωση ενός ολοκληρωμένου πλαισίου για τον ανθρώπινο παράγοντα στον άξονα νερού-ενέργειας, υπό μεταβαλλόμενες περιβαλλοντικές και κοινωνικοοικονομικές συνθήκες, θα περιλαμβάνει επίσης απρόβλεπτα και εγγενώς στοχαστικά γεγονότα. Σε αυτό το πλαίσιο, η έρευνα εστιάζει στις επιδράσεις κρίσιμων, επειγουσών και ανώμαλων περιστάσεων, που μπορεί να επηρεάσουν τόσο τη μικρο- όσο και τη μακρο-συμπεριφορά μιας ολόκληρης κοινωνίας μακροπρόθεσμα. Αυτά τα γεγονότα περιλαμβάνουν γεωπολιτικές αλλαγές, οικονομικές κρίσεις και ακραίες υδροκλιματικές συνθήκες (π.χ. επίμονες ξηρασίες), προκαλώντας μακροχρόνιες ελλείψεις νερού και/ή ενέργειας, οι οποίες με τη σειρά τους αντανακλώνται στις αντίστοιχες ζητήσεις, τιμές και πολιτικές. Τονίζουμε ότι στις συνήθεις προσεγγίσεις μοντελοποίησης πόρων νερού και ενέργειας, αυτά τα στοιχεία αντιμετωπίζονται υπό την υπόθεση σταθερής κατάστασης (steady-state approach). Για παράδειγμα, οι ζητήσεις νερού εκφράζονται ως γνωστές εισροές, οι οποίες ακολουθούν προκαθορισμένα εποχικά πρότυπα και μοτίβα, ενώ στην πραγματικότητα εξαρτώνται έντονα από τις κοινωνικές δράσεις ως προς την κατάσταση του συστήματος και στις διάφορες πτυχές των αλλαγών (π.χ. αλλαγές στις υδροκλιματικές συνθήκες και/ή στους λογαριασμούς νερού που μπορεί να μειώσουν την κατανάλωση).

(ε) Καθώς ο άξονας νερού-ενέργειας-κοινωνίας υπόκειται σε πολλαπλές αβεβαιότητες, η αναζήτηση τους, η αναπαράστασή τους, η ποσοτικοποίηση και τελικά η ερμηνεία τους αποτελούν έναν κρίσιμο στόχο της προτεινόμενης έρευνας, ο οποίος θα αντιμετωπιστεί μέσω της διεύρυνσης του στοχαστικού παραδείγματος προσομοίωσης. Σε αυτό το πλαίσιο, η έρευνα στοχεύει στη διεύρυνση της στοχαστικής θεωρίας για την αναπαράσταση κλιματικών, ανθρωπογενών, ενεργειακών και οικονομικών μεταβολών ως τυχαίες διαδικασίες σε διάφορες κλίμακες. Σημειώνουμε ότι τέτοιες προσεγγίσεις συνήθως εφαρμόζονται στη μοντελοποίηση πόρων νερού, μέσω της αναπαράστασης και δημιουργίας συνθετικών δεδομένων βροχής, αναπαράγοντας τα στατιστικά χαρακτηριστικά των αντίστοιχων ιστορικών αρχείων. Από την άλλη πλευρά, οι στόχοι και οι περιορισμοί νερού και ενέργειας, καθώς και οι πολυδιάστατες επιδράσεις από κοινωνικές ομάδες και πιέσεις της αγορά ενέργειας, εκφράζονται συνήθως ως γνωστά, εκ των προτέρων, δεδομένα. Στην πραγματικότητα, όλα αυτά είναι εγγενώς μεταβλητά και απρόβλεπτα. Συνεπώς, οι κρίσιμες πτυχές της αγοράς ενέργειας (π.χ. τιμές ηλεκτρικής ενέργειας), θα αναπαρασταθούν με στοχαστικά μέσα.

(στ) Ο συνολικός ερευνητικός στόχος είναι η σύνθεση όλων των προαναφερθέντων εννοιών και μεθοδολογιών σε ένα ολοκληρωμένο πλαίσιο, υπό το πρίσμα του άξονα νερού-ενέργειας-κοινωνίας. Αυτό το πλαίσιο δύναται να αναλύει τις τρεις διασυνδεδεμένες ροές και τελικά να παρέχει υποστήριξη αποφάσεων για πρακτικά ζητήματα στους υπεύθυνους χάραξης πολιτικών (π.χ. σχεδιασμός, διαχείριση, μακροπρόθεσμη αξιολόγηση, βραχυπρόθεσμος προγραμματισμός, στρατηγική ανάπτυξη, προσαρμογή σε αλλαγές, επιπτώσεις πολιτικών τιμολόγησης κ.λπ.).

Οι κύριες προκλήσεις που συνδέονται με τους έξι ερευνητικούς στόχους είναι, αντίστοιχα:

(α) Η αναπαράσταση του νερού και της ενέργειας ως διασυνδεδεμένο σύστημα συνοδεύεται από σημαντικά μεθοδολογικά και υπολογιστικά ζητήματα. Σε τέτοια συστήματα, πέρα από τις ήδη γνωστές πολυπλοκότητες της μοντελοποίησης υδατικών πόρων (μη γραμμικές δυναμικές, απρόβλεπτες μελλοντικές αλλαγές, μεγάλος αριθμός μεταβλητών και περιορισμών, συγκρουόμενες χρήσεις και κριτήρια κ.λπ.), προκύπτουν πρόσθετες προκλήσεις λόγω της εισαγωγής ενεργειακών συνιστωσών και των συναφών ροών, ορισμένες από τις οποίες είναι παράλληλες με τις ροές του νερού (π.χ. περίπτωση υδροηλεκτρικής ενέργειας). Μια σημαντική δυσκολία αφορά την ανάγκη σύνδεσης δύο διαφορετικών χρονικών κλιμάκων, δεδομένου ότι στη διαχείριση υδατικών πόρων συνήθως υιοθετούνται μεγαλύτερα χρονικά βήματα προσομοίωσης, π.χ. μηνιαία, ενώ για την πιστή και ορθή αποτύπωση της ενεργειακής ισορροπίας (παραγωγή ισχύος έναντι ζήτησης) απαιτείται πολύ λεπτότερη ανάλυση (π.χ. ημερήσια ή ωριαία).

(β) Η ενσωμάτωση του εξαιρετικά περίπλοκου και αβέβαιου κοινωνικού παράγοντα στο τεχνικό σύστημα (δηλαδή στο σύστημα νερού-ενέργειας) αποτελεί εγγενώς μια εξαιρετικά απαιτητική πρόκληση, με πολλά ζητήματα προς αντιμετώπιση. Δεδομένου ότι η προσέγγιση μέσω ευφυών πρακτόρων (agent-based approach), που αποτελεί το βασικό εργαλείο για την αναπαράσταση της ανθρώπινης συμπεριφοράς, ακολουθεί εξ ορισμού μια «από κάτω προς τα πάνω» θεώρηση, μια θεμελιώδης πρόκληση είναι η εξασφάλιση μιας ικανοποιητικής ισορροπίας μεταξύ ακρίβειας και υπολογιστικής αποτελεσματικότητας. Η πρώτη απαίτηση προϋποθέτει μια αντιπροσωπευτική ταξινόμηση των κοινωνικών συνιστωσών (πρακτόρων) και έναν ρεαλιστικό μαθηματικό ορισμό των κανόνων συμπεριφοράς τους, που με τη σειρά του μπορεί να οδηγήσει σε ένα υπερβολικά λεπτομερές μοντέλο. Από την άλλη πλευρά, το μοντέλο αυτό δεν πρέπει να επιβάλλει ανυπέρβλητα εμπόδια στη συνολική υπολογιστική διαδικασία, η οποία περιλαμβάνει επίσης ένα χρονοβόρο μοντέλο προσομοίωσης του τεχνικού συστήματος. Ένα άλλο κρίσιμο σημείο είναι η εξαγωγή μιας σταθερής αλλά και αυτοπροσαρμοζόμενης κοινωνίας, μετά την κλιμάκωση των επιμέρους κοινωνικών συνιστωσών, οι οποίες είναι (και πρέπει να είναι) προκατειλημμένες.

(γ) Επίσης, η αναπαράσταση των πιέσεων της ενεργειακής αγοράς με στοχαστικά μέσα (δηλαδή ως τυχαία μεταβαλλόμενες τιμές ηλεκτρικής ενέργειας) είναι επίσης ιδιαίτερα απαιτητική, καθώς η διαδικασία αυτή παρουσιάζει εντελώς διαφορετικές ιδιομορφίες σε σχέση με τις κλιματικές μεταβλητές, όπως η έντονη μεταβλητότητα και οι αιχμές (Hou et al., 2017), καθώς και διπλή περιοδικότητα, μεταξύ εποχών και εντός του ημερήσιου κύκλου. Περαιτέρω προκλήσεις προκύπτουν από τις περιορισμένες στατιστικές πληροφορίες που παρέχονται από μικρά ιστορικά δείγματα δεδομένων (λίγα χρόνια, ενώ τα υδρομετεωρολογικά αρχεία είναι γενικά διαθέσιμα για αρκετές δεκαετίες), καθώς και από την ανάγκη ενσωμάτωσης στα συνθετικά δεδομένα ανώμαλων αλλά επίμονων μεταβολών στις τιμές της ηλεκτρικής ενέργειας, ώστε να αναπαρασταθούν εξαιρετικά απρόβλεπτα φαινόμενα, όπως η τρέχουσα ενεργειακή κρίση, που αποτελεί μείζονα παράγοντα πίεσης για όλα τα εθνικής κλίμακας συστήματα ηλεκτρικής ενέργειας στην ΕΕ.

(δ) Η αποτελεσματική σύνδεση των κοινωνικών και οικονομικών συνιστωσών στον άξονα νερού-ενέργειας είναι μια απαιτητική εργασία, που αρχικά απαιτεί τον κατάλληλο ορισμό των ορίων, των συνιστωσών και των διαδικασιών του συνολικού κοινωνικο-τεχνικού συστήματος, καθώς και των διεπαφών τους. Σε αυτό το πλαίσιο, το κλειδί είναι η μαθηματική περιγραφή των αυτο- και ετερό-εξαρτήσεων μεταξύ των πόρων νερού και ενέργειας, των υποδομών, των ανθρώπων και των οικοσυστημάτων, καθώς και της δυναμικής φύσης της λήψης αποφάσεων, της αντίδρασης στις αλλαγές και της προσαρμογής σε απρόβλεπτες περιστάσεις που προκαλούνται από παγκόσμιες αλλαγές.

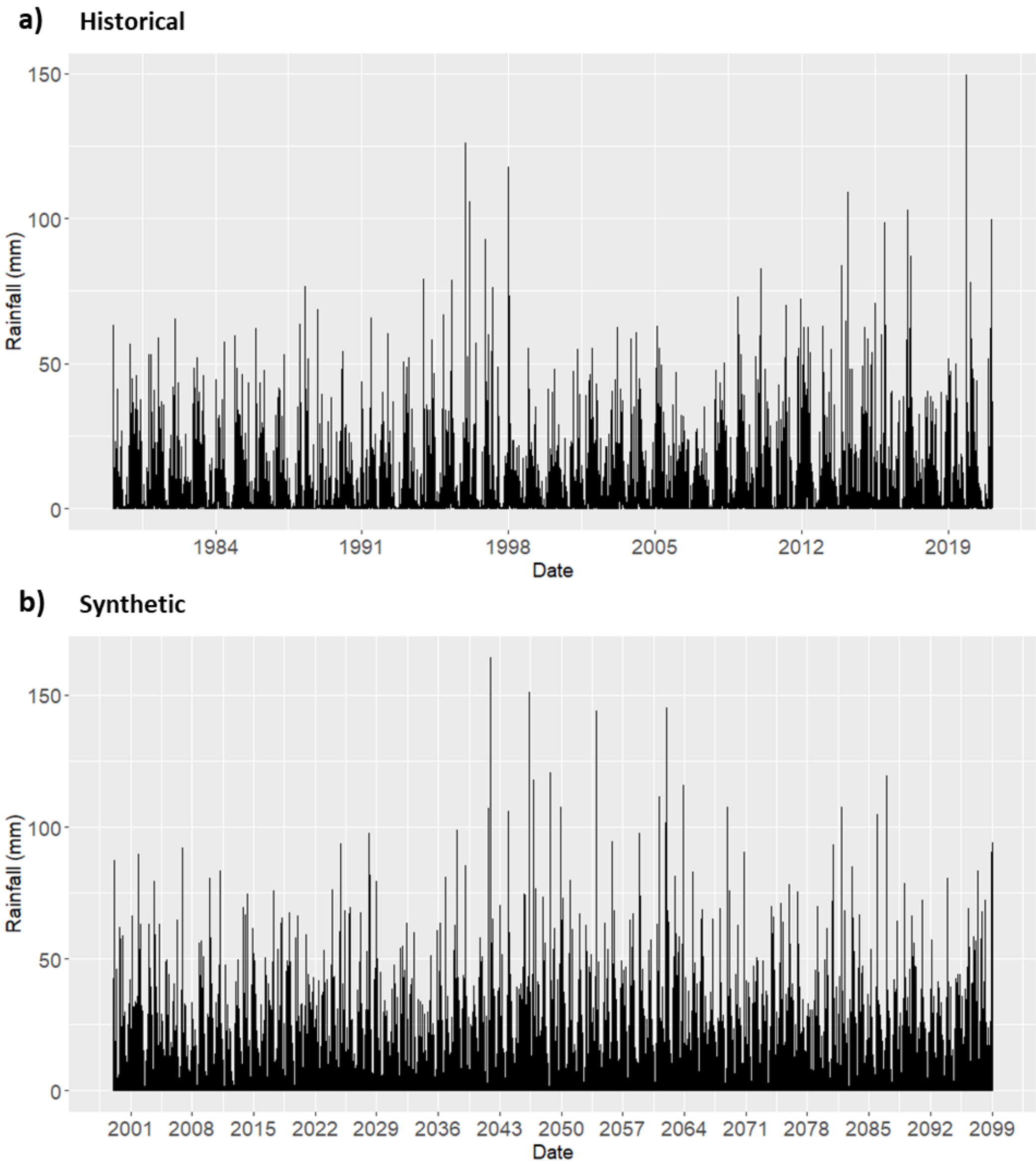
(ε) Η τελική προσπάθεια προσαρμογής του άξονα νερού-ενέργειας-κοινωνίας υπό ένα ενιαίο πλαίσιο εισάγει την ανάγκη διαχείρισης ενός πολύ μεγάλου αριθμού δεδομένων, μεταβλητών ελέγχου, περιορισμών και στόχων, λόγω της ταυτόχρονης μοντελοποίησης των τριών παράλληλων ροών και των αλληλεπιδράσεών τους. Η ερευνητική κοινότητα σε αυτόν τον τομέα παρέχει μάλλον απλοποιημένες διατυπώσεις που αγνοούν σημαντικές συστημικές πολυπλοκότητες και αλληλεξαρτήσεις (Giuliani et al., 2021). Πέρα από αυτή τη δομική πολυπλοκότητα, υπάρχει επίσης μια κρυφή πρόκληση, καθώς η σύνδεση των κοινωνικών και τεχνικών υποσυστημάτων επιβάλλει τη σύζευξη δύο διαφορετικών φιλοσοφιών μοντελοποίησης, δηλαδή των μοντέλων ευφυών πρακτόρων (agent-based models), που ακολουθούν εξ ορισμού μια «από κάτω προς τα πάνω» προσέγγιση, με τα μοντέλα προσομοίωσης νερού-ενέργειας που βασίζονται σε «άνω προς τα κάτω» προσέγγιση. Ωστόσο, το τελικό προϊόν θα πρέπει να είναι γενικό, ευέλικτο, υπολογιστικά αποδοτικό και προσβάσιμο από διαφορετικές ομάδες ενδιαφέροντος και συνολικά ικανό να επιλύει προβλήματα του πραγματικού κόσμου.

Οι παραπάνω προκλήσεις, που έχουν αναγνωριστεί ως καίριας σημασίας στη μοντελοποίηση κοινωνικο-περιβαλλοντικών συστημάτων (Elsawah et al., 2020), προϋποθέτουν την αποτελεσματική σύνδεση διαφορετικών τομέων της επιστήμης, δηλαδή της μηχανικής και της συμπεριφορικής.

Προτεινόμενη «εργαλειοθήκη» για την αναπαράσταση των αβεβαιοτήτων

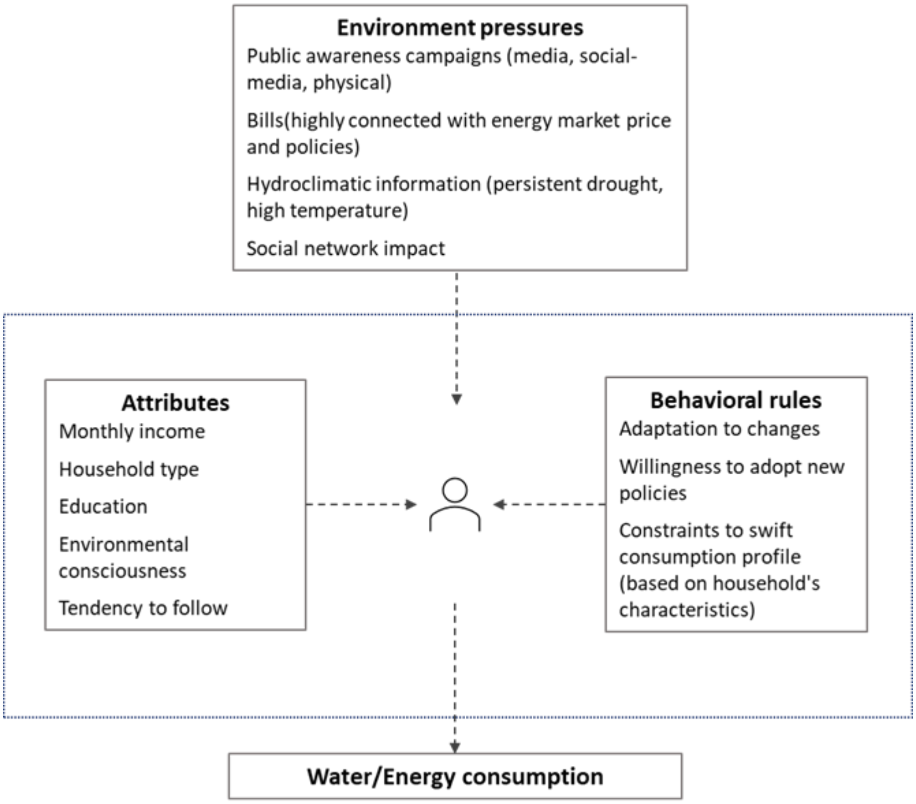
Προκειμένου να εξεταστούν και ποσοτικοποιηθούν οι αβεβαιότητες που πηγάζουν από το κλίμα, την κοινωνία, την ενεργειακή αγορά και από την χρήση των μοντέλων, υιοθετούνται και παρουσιάζονται τα αντίστοιχα εργαλεία, τα οποία συνιστούν μία εργαλειοθήκη.

Συγκεκριμένα, για την αναπαράσταση των κλιματικών μεταβολών, και συγκεκριμένα της βροχής, χρησιμοποιούνται εργαλεία στοχαστικής προσομοίωσης που βασίζονται στο σχήμα SMARTA (Tsoukalas et al., 2018), επιτρέποντας την μοντελοποίηση της διεργασίας ως στάσιμη στην ετήσια κλίμακα και κυκλοστάσιμη στις κατώτερες χρονικές κλίμακες. Σε ετήσιο επίπεδο, η διαδικασία παραγωγής λαμβάνει υπόψη την οριακή κατανομή και τη δομή αυτοσυσχέτισης των ιστορικών δεδομένων, ενσωματώνοντας τη δυναμική Hurst-Kolmogorov, ώστε να αναπαρασταθεί με ακρίβεια το φαινόμενο της εμμονής. Στη **Εικόνα 2** απεικονίζονται η ιστορική χρονοσειρά βροχόπτωσης καθώς και η συνθετική χρονοσειρά σε ημερήσια κλίμακα, ακολουθώντας την προτεινόμενη μεθοδολογία



Εικόνα 2: a) Ιστορική χρονοσειρά βροχόπτωσης. B) Συνθετική χρονοσειρά βροχόπτωσης

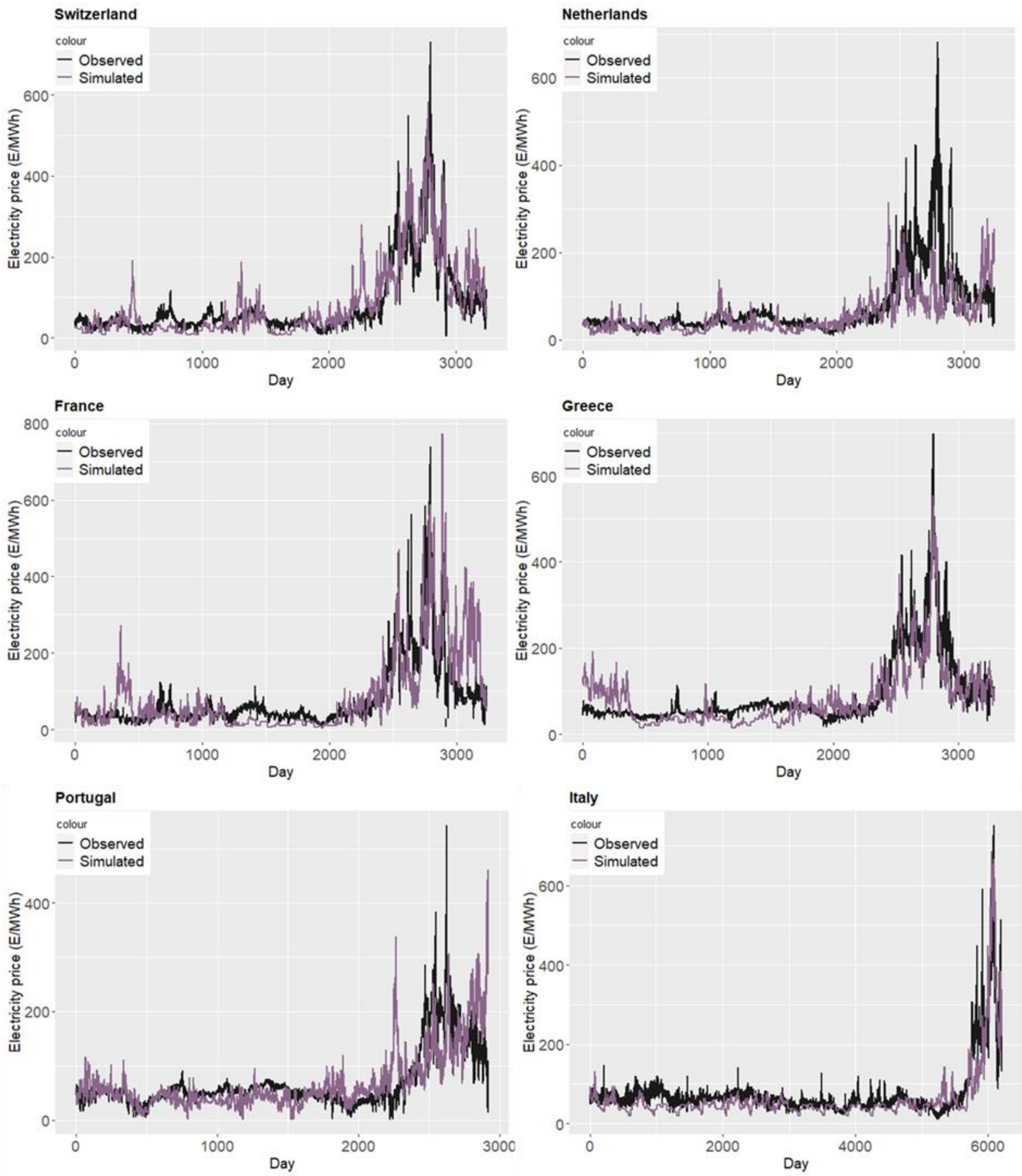
Επιπρόσθετα, για την αναπαράσταση της κοινωνικής συμπεριφοράς των καταναλωτών νερού-ενέργειας, ως εργαλείο προσομοίωσης προτείνεται ένα μοντέλο ευφυών πρακτόρων (agent-based model). Όπως φαίνεται στην **Εικόνα 3**, το μοντέλο ταξινομεί τους καταναλωτές μιας κοινωνίας σε ομάδες, οι οποίοι αντιδρούν στα ερεθίσματα ώστε να μεταβάλλουν την ζήτηση τους για νερό ή/και ενέργεια.



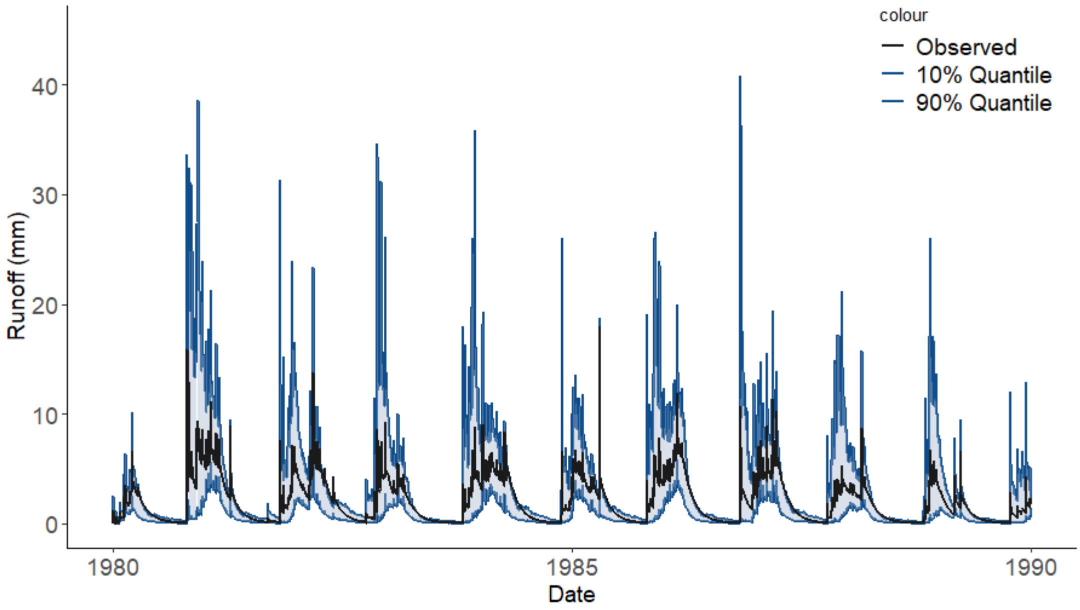
Εικόνα 3: Σχηματική απεικόνιση της συμπεριφοράς των καταναλωτών σε σχέση με εξωτερικές πιέσεις και ερεθίσματα.

Ακόμα, για την αναπαράσταση της αβεβαιότητας της αγοράς ενέργειας, και συγκεκριμένα την παραγωγή συνθετικών δεδομένων τιμών ηλεκτρικής ενέργειας, ακολουθείται η μεθοδολογία SMARTA. Πιο λεπτομερώς, χρησιμοποιούνται δύο επίπεδα ανάλυσης της τιμής ηλεκτρικής ενέργειας, ήτοι ημερήσια και ωριαία κλίμακα. Τονίζεται ότι η συγκεκριμένη διεργασία χαρακτηρίζεται από α) διατήρηση αυτοσυσχέτισης στην ημερήσια κλίμακα, β) διπλή περιοδικότητα (μήνα-μήνα και ώρα-ώρα) και γ) ύπαρξη αρνητικών τιμών. Στην **Εικόνα 3** παρουσιάζονται οι ιστορικές τιμές ηλεκτρικής ενέργειας αντιπαραβάλλοντας τες με ένα δείγμα των συνθετικών σε έξι Ευρωπαϊκές χώρες (Γαλλία, Ελβετία, Ελλάδα, Ιταλία, Πορτογαλία και Ολλανδία).

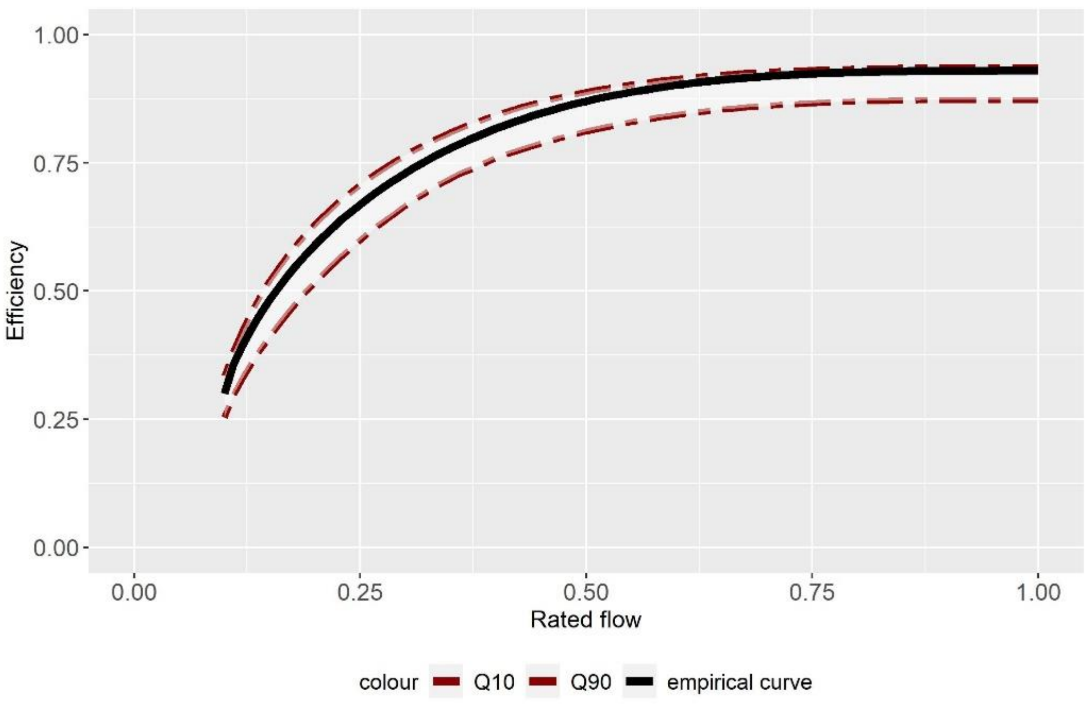
Τέλος, για την αναπαράσταση της επιστημικής αβεβαιότητας, προτείνονται τρεις μεθοδολογίες για τη μοντελοποίηση των παραμέτρων, τη μοντελοποίηση της δομής και των παραμέτρων και την βαθμονόμηση των μοντέλων. Κάθε μεθοδολογία εξετάζεται στα διαφορετικά πεδία εφαρμογής. Για παράδειγμα, η μοντελοποίηση των παραμέτρων χρησιμοποιείται στην εκτίμηση της αβεβαιότητας του βαθμού απόδοσης των στροβίλων (**Εικόνα 4**), ενώ οι άλλες δύο στην ποσοτικοποίησης των αποκλίσεων των μοντέλων βροχής-απορροής (**Εικόνα 5**).



Εικόνα 3: Ιστορικές τιμές ηλεκτρικής ενέργειας αντιπαραβάλλοντας τες με ένα δείγμα των συνθετικών σε έξι Ευρωπαϊκές χώρες (Γαλλία, Ελβετία, Ελλάδα, Ιταλία, Πορτογαλία και Ολλανδία).



Εικόνα 4: 80% περιθώρια αβεβαιότητας της συνθετικής χρονοσειράς απορροής συγκρινόμενα με την παρατηρημένη.



Εικόνα 5: Ισοπίθανες καμπύλες απόδοσης, γύρω από την εργαστηριακή καμπύλη απόδοσης υδροστροβίλου

Πεδία εφαρμογής της προτεινόμενης εργαλειοθήκης

Όπως εξηγήθηκε η προαναφερθείσα εργαλειοθήκη εξετάστηκε σε μία σειρά από πραγματικά πεδία εφαρμογής, ήτοι για α) την εξέταση της Ευρωπαϊκής αγοράς ενέργειας και πρόγνωση τιμών ενέργειας σε διάφορες κλιμακες, β) τον σχεδιασμό και την μακροπρόθεσμη αξιολόγηση συστημάτων ανανεώσιμων πηγών ενέργειας, γ) την αξιολόγηση των μακροπρόθεσμων πολιτικών διαχείρισης συστημάτων νερού υπό το πρίσμα του πλέγματος νερού-ενέργειας-κοινωνίας και δ) την αξιολόγηση και βελτιστοποίηση των μακροπρόθεσμων πολιτικών διαχείρισης σε ταμιευτήρες πολλαπλού σκοπού.

Συγκεκριμένα, εφαρμόζοντας την εργαλειοθήκη επέτρεψε την ολιστική προσέγγιση μοντελοποίησης των αβεβαιοτήτων σε όλα τα προβλήματα μηχανικού που εξετάστηκαν, ήτοι:

- στην πρόβλεψη των τιμών ηλεκτρικής ενέργειας, όπου αποδείχθηκε ότι η χρήση κατάλληλων στοχαστικών εργαλείων επιτρέπει την αναπαραγωγή της εξαιρετικά πολύπλοκης συμπεριφοράς των ενεργειακών αγορών, και των έντονων μεταβλητοτήτων τους σε όλες τις χρονικές κλίμακες
- τον σχεδιασμό ενεργειακών έργων, με ενδελεχή ανάλυση του προβλήματος βελτιστοποίησης του μίγματος στροβίλων μικρών υδροηλεκτρικών σταθμών υπό πολλαπλές πηγές αβεβαιότητας, ήτοι της δίαιτας της βροχόπτωσης στην ανάντη λεκάνη απορροής, του μετασχηματισμού βροχής-απορροής, του βαθμού απόδοσης των υδροστροβίλων, και της επενδυτικού ευκαιρίας.
- στη μακροπρόθεσμη διαχείριση συστημάτων υδατικών πόρων, καίρια συνιστώσα των οποίων είναι το ενεργειακό κόστος, που με τη σειρά του επηρεάζει την τιμή του νερού, άρα και την κατανάλωση, με εφαρμογή στο ιδιαίτερα πολύπλοκο υδροδοτικό σύστημα της Αθήνας, που για πρώτη φορά αντιμετωπίστηκε υπό το πρίσμα ενός στοχαστικού τεχνικο-κοινωνικού συστήματος.
- στον βέλτιστο προγραμματισμό των απολήψεων και της υδροηλεκτρικός παραγωγής ταμιευτήρων πολλαπλού σκοπού, με εφαρμογή στο υδροσύστημα του Πλαστήρα, χαρακτηριστικό του οποίου είναι η έντονη ανταγωνιστικότητα των διαφορετικών χρήσεων νερού.

Ο Πίνακας 1 παρουσιάζει την λίστα των πεδίων εφαρμογών, ξεκινώντας από ένα μεμονωμένο (ήτοι την αγορά ενέργειας και έργα ανανεώσιμης ενέργειας) καταλήγοντας στην ολιστική προσέγγιση του συστήματος νερού-ενέργειας-κοινωνίας, που χρησιμοποιούνται στην παρούσα Διδακτορική Διατριβή, περιλαμβάνοντας τις πηγές αβεβαιότητας που εξετάστηκαν.

Συνοψίζοντας, αυτή η έρευνα συμβάλλει στο αναδυόμενο πεδίο του πλέγματος νερού-ενέργειας αντιμετωπίζοντας τις προκλήσεις που θέτει η αβεβαιότητα και η μεταβλητότητα σε πολλαπλούς τομείς.

Εν κατακλείδι, η παρούσα διδακτορική διατριβή προσφέρει εργαλεία υποστήριξης αποφάσεων προσαρμοσμένα σε πραγματικές εφαρμογές, επιτρέποντας στους υπεύθυνους χάραξης πολιτικής και τους εμπλεκόμενους φορείς να λαμβάνουν τεκμηριωμένες αποφάσεις. Μέσω της προσομοίωσης και βελτιστοποίησης πολλαπλών σεναρίων υπό συνθήκες αβεβαιότητας, το πλαίσιο παρέχει σημαντικές πληροφορίες, όπως η εκτίμηση των αναμενόμενων κερδών και των επιπέδων κινδύνου για μελλοντικές συνθήκες, που επηρεάζονται από κλιματικές, κοινωνικές και οικονομικές αλλαγές.

Αυτή η διατριβή θέτει νέα πρότυπα στις μεθοδολογίες προσομοίωσης-βελτιστοποίησης στα συστήματα νερού-ενέργειας, ενώ τα ερευνητικά της αποτελέσματα καταδεικνύουν ότι μπορούν να συνεισφέρουν σημαντικά στην υποστήριξη του στρατηγικού σχεδιασμού, της διαχείρισης ρίσκου και του σχεδιασμού ανθεκτικών συστημάτων νερού-ενέργειας, με έμφαση στην αντιμετώπιση των μελλοντικών αβεβαιοτήτων.

Πίνακας 1: Λίστα των πεδίων εφαρμογής (τίτλοι κεφαλαίων) και οι αντίστοιχες πηγές αβεβαιότητας που λήφθηκαν υπόψη.

Πεδίο εφαρμογής/ Αβεβαιότητα	Κλιματική	Κοινωνική	Αγορά ενέργειας	Επιστημική
Από τη μακροπρόθεσμη προσομοίωση έως την πρόβλεψη της αγοράς ηλεκτρικής ενέργειας της Ε.Ε.			X	
Σχεδιασμός και αξιολόγηση έργων ανανεώσιμων πηγών ενέργειας υπό το πρίσμα της αβεβαιότητας	X		X	X
Συστήματα ύδρευσης υπό το πρίσμα του πλέγματος νερό-ενέργεια-κοινωνία	X	X	X	
Αντιμετώπιση των συγκρούσεων του πλέγματος νερού-ενέργειας: η περίπτωση των ταμιευτήρων πολλαπλών χρήσεων	X	X	X	X

1 Introduction

1.1 Setting the scene

Water resources development and management should follow the global goal of sustainability. This requires an integrated viewpoint, which also takes into consideration natural resources protection and energy transition concerns, along with economic growth, environmental improvement and social prosperity. In this scene, it is recognized that the concept of water-energy nexus is a critical turning point for the route to sustainability, and the means to enhance water and energy security (Scanlon et al., 2017).

Water and energy are subject to complex interactions with uncertain physical processes, and human-induced procedures (e.g., legal regulation, management policies, market rules). However, the physical and social interrelation in practice is rather fragmented. In fact, conventional modelling approaches for water-energy problems misuse, if not ignore, the complex and dynamic anthropogenic behavior and its multiple interactions and feedback loops with the technical system components (water and energy fluxes, and related infrastructures).

To move forward this monomeric approach, we aim at establishing a paradigm shift, thus introducing an *uncertainty-aware simulation-optimization framework* for water planning and management, under the holistic prism of water-energy-society nexus. This shift requires an effective and efficient integration and modelling of three parallel fluxes, i.e., water, energy and social (Figure 1.1). Also, it is needed to embed different theories and tools (including simulation, optimization, stochastics, and agent-based models) into a unified methodological framework. We remark that the key components of Figure 1.1 will be progressively built, following the structure of the thesis to eventually conclude to the holistic *uncertainty-aware simulation-optimization framework tailored for the water-energy nexus.*

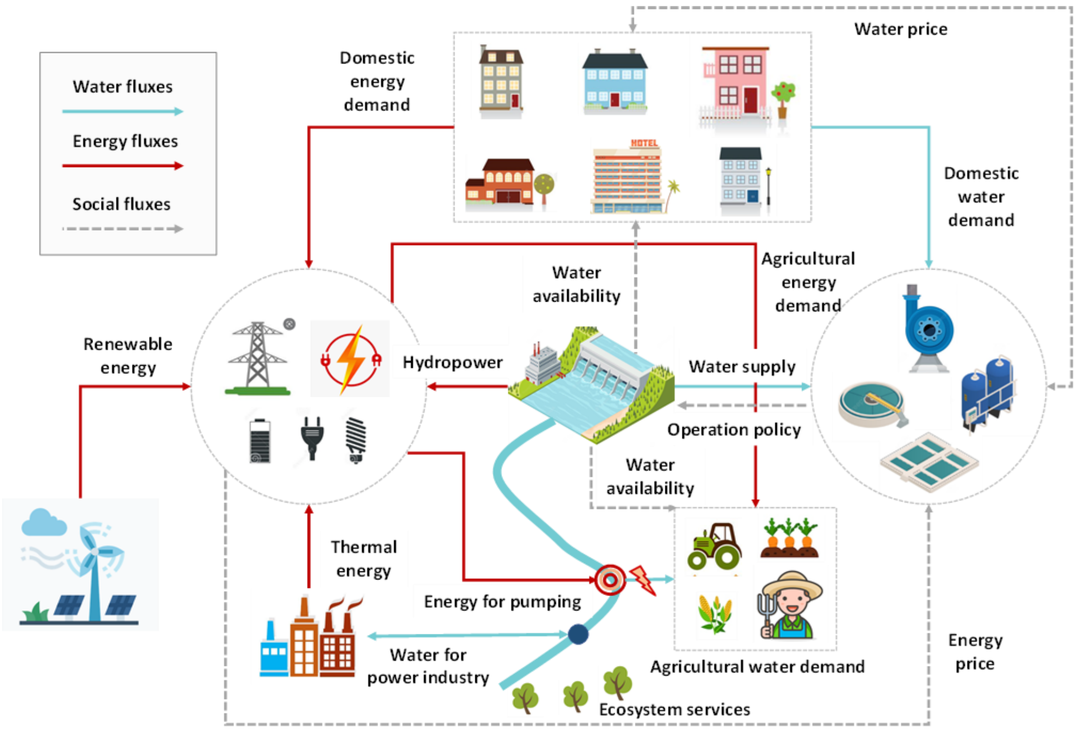


Figure 1.1: Schematic representation of water, energy and social fluxes as a nexus.

1.1 Research objectives and challenges

This research aims at representing the building blocks of water, energy and society, as a nexus of interconnected fluxes that have synergies, antitheses and complementarities. This task is subject to *six key objectives*, each one revealing a number of challenges. More specifically:

(a) The first objective involves the revision of running simulation-optimization schemes that are tailored for water-energy, in order to incorporate all facets of uncertainty, exogenous and endogenous, that drive such systems.

(b) A parallel research goal originates from the need to account for the highly uncertain social feature within the technical description of the water-energy nexus, thus formatting the novel concept of stochastic sociotechnical systems. Key objective is the integration of the mathematical formalization of the human factor, both from bottom-up and top-down perspectives. Regarding the bottom-up approach, this research is taking advantage of adjusting and enchasing the so-called agent-based theory, launched by Bonabeau (2002), and couple it with water-energy planning and management schemes. The adaptation of a bottom-up approach, to study the agent interactions both with the technical (i.e., water-energy) system and among each other, at the micro level, will allow to draw conclusions about the system's (emergent) behavior at the macro level. On the other hand, the top-down approach leverages the historical data and builds upon this to describe the human factor and its response within the technical system.

(c) Another aspect of research originates from the energy market and its interactions within the water-energy nexus. We recognize two crucial research points regarding the energy market, i.e., the representation of the electricity price and its effects in the management and operation of water-energy systems. In this respect, key objectives are the mathematical description of the market-related components (e.g., interest rates, electricity price) and the exploration of the associated effects (e.g., energy target, profits, water bills etc.)

(d) The establishment of a comprehensive context of the human agency within the water-energy nexus, under inherently varying environmental and socioeconomic drivers, will also include disruptive and unpredictable events. In this vein, this research is also focus on the effects of crucial, urgent and abnormal circumstances, which may affect both the micro- and macro-behavior of an entire society over the longer term. These may include geopolitical shifts, economic crises and extreme hydroclimatic conditions (e.g., persistent droughts), causing long-term water and/or energy shortages, which are in turn reflected to the associated demands, prices and operation policies. We highlight that in common approaches for water and energy resources modelling, these elements are handled under the steady-state hypothesis. For instance, the demands are expressed as known inputs, which follow a priori specified seasonal patterns, while in fact they are strongly depended on the social actions and reactions against the system's state and its various aspects of change (e.g., changes in hydroclimatic conditions and/or water bills that may reduce consumption).

(e) Since the water-energy-society nexus is subject to multiple uncertainties, their identification, representation, quantification, and eventually interpretation is a crucial objective of the proposed research, to be handled by extending the stochastic simulation paradigm. In this respect, this research aims at extending the stochastic simulation paradigm to represent climatic, anthropogenic and energy market threats as random processes across scales. We remark that such approaches are quite usually applied in water resources modelling, as the means to provide long synthetic data for reservoir inflows that reproduce the statistical characteristics of the corresponding historical records. On the other hand, water and energy targets and constraints, as well as the multidimensional effects by social group and energy market stresses, are typically expressed as a priori known inputs. In fact, all these are inherently varying and unpredictable. Similarly, key facets of the energy market (e.g., electricity prices), will be represented in stochastic means.

(f) The overall research target is the synthesis of all aforementioned concepts and methodologies into a holistic framework, under the view of water-energy-society nexus. This framework will be able to analyze the three interconnected fluxes, and eventually provide decision support for practical issues across the technical system (e.g., planning, management, long-term assessment, short-term scheduling, strategic development, adaptation to changes, impacts of pricing policies, etc.).

The *main challenges* across the six research objectives are, respectively:

(a) The representation of water and energy as an integrated system is subject to a number of challenging methodological and computational issues. In such systems, apart from the well-known complexities of water resources modelling (nonlinear dynamics, unpredictable future inflows, large number of variables and constraints, conflicting uses and criteria, etc.), additional challenges arise due to the introduction of energy components and associated fluxes, some of which are parallel to water fluxes (e.g., case of hydropower). A major difficulty is the need for coupling two different temporal scales, given that in water resources management, coarser simulation time steps are typically adopted, i.e., monthly, yet for a faithful accounting of the energy balance (i.e., power production vs. demand) a much finer resolution (e.g., daily or hourly) is required.

(b) The incorporation of the extremely complex and uncertain social factor within the technical (i.e., water-energy) system is inherently a highly challenging task, with numerous issues to address. Since the agent-based approach, which is the core tool for representing the human behavior, follows by definition a bottom-up perspective, a fundamental challenge is ensuring a satisfactory equilibrium between accuracy and computational effectiveness. The first requirement presupposes a representative classification of the society's components (agents) and a realistic mathematical description of their behavioral rules, which in turn may result to an over-detailed model. On the other hand, this model should not impose formidable barriers to the overall computational procedure, which also includes a time-demanding simulation model of the technical system. Another crucial point is the derivation of a stable and self-adaptive society, after upscaling the individual social components, which are (and should be) biased.

(c) Also, the representation of the energy market stresses in stochastic means (i.e., as randomly varying electricity prices), is also very challenging, since this process exhibits quite different peculiarities with respect to climatic variables, such as volatility and spikes (Hou et al., 2017), as well as double periodicity, across seasons and within the intraday cycle. Further challenges are induced by the limited statistical information provided by the small historical data samples (few years, while hydrometeorological records are generally available for several decades), and the need to implement within the synthetic data abnormal yet persistent shifts to the electricity prices, in order to represent "black swan" phenomena, such as the running energy crisis, that has been a major stressing factor for all national-scale power systems over the EU.

(d) The effective coupling of the social and economic components across the water-energy nexus is a challenging task, which initially requires a proper definition of the boundaries, components and processes of the entire socio-technical system, as well as their interfaces. In this vein, the key is to describe in mathematical terms the auto- and cross-dependencies among water and energy resources, infrastructures, humans and ecosystems, and the dynamic nature of decision-making, adaptation, reaction to influences, and adjustment to unexpected circumstances, induced by global changes.

(e) The ultimate attempt to customize the water-energy-society nexus under a unified framework introduces the need to handle a very large number of inputs, control variables, constraints and objectives, due to the simultaneous modelling of the three parallel fluxes and their interactions. Past research in this area has only provided rather simplified problem formulations that misrepresent important systemic complexities and intersectoral interactions (M. Giuliani et al., 2021). Apart from this structural complexity, there is also a hidden challenge, since the link of the social and technical sub-systems imposes coupling of two different modelling philosophies, i.e., ABMs, following by construction a bottom-up approach, with top-down models for water-energy simulations. Nevertheless, the final product should be generic, flexible, computationally efficient and accessible by different groups of interest, and overall able to solve real-world problems.

The aforementioned challenges, which have been recognized as of key importance in socio-environmental systems modelling (Elsawah et al., 2020), presuppose the effective coupling of different domains of science, i.e., engineering and behavioral, as explained herein.

1.2 Thesis overview and contribution

The primary objective of this thesis is to develop and demonstrate an uncertainty-aware simulation-optimization framework for water-energy nexus. The scope of this research spans over three levels of interest: (a) the design scale, aiming at the optimal siting, sizing and mixing of energy sources; (b) the long-term management scale, aiming at defining their optimal operation policy under changing hydroclimatic, environmental and socioeconomic conditions; and (c) the short-term scale, dominated by issues of scheduling of energy production under the uncertain energy market evolution. For the validation of the concepts, methodologies and tools a series of hypothetical and real-world cases will be examined covering a wide range of spatial and temporal scales.

This thesis is divided into nine chapters and an appendix.

Chapter 1 introduces a preamble to the subject, the motivation of this work and the research objectives, as well as the challenges.

Chapter 2 provides an extensive literature review on a) the topic of uncertainty in general, from its historical roots to the application of various scientific fields, b) the concept of water-energy nexus, and c) the incorporation of uncertainty within the water energy nexus.

Chapter 3 conducts a thorough literature review on the key sources of uncertainty that drive the water-energy nexus. A section for each source of uncertainty is dedicated, including the definitions, the common modelling approaches and eventually our approach to deal with. Specifically, for the hydrometeorological processes we are taking advantage of stochastics, while for the social uncertainty an agent-based model is developed tailored for water-energy systems. Eventually, to account for the energy market fluctuations, we also employ the stochastic theory, by introducing a novel approach for simulating the electricity prices.

Chapter 4 includes two different analyses across the energy market, the first refers to the simulation of electricity prices and the second to their forecasting across different scales of interest. The first approach is applied to six European Energy Market by following the associated framework of **Chapter 3**, while the second one is stress-test to the Greek Energy Market by introducing a copula-based tool.

Chapter 5 proposes a *generic stochastic simulation-optimization framework*, that will be employed to renewable energy systems (RES), able to address the multiple facets of uncertainty, external and internal, as introduced in **Chapter 3.** These categorized into aleatory and epistemic, exogenous and endogenous, and refer to the climatic processes, the system states, and the broader socioeconomic environment. All expressed in probabilistic terms through a novel coupling of the triptych statistics, stochastics and copulas. Since the most widespread sources (wind, solar, hydro) exhibit several common characteristics, we first introduce the formulation of the overall modelling context under uncertainty, and then offer uncertainty quantification tools to put in practice the plethora of simulated outcomes and resulting performance metrics (investment costs, energy production, revenues). The proposed framework is applied to two indicative case studies, namely the design of a small hydropower plant (particularly, the optimal mixing of its hydro-turbines), and the long-term assessment of a planned wind power plant. Both cases reveal that the ignorance or underestimation of uncertainty may hide a significant perception about the actual operation and performance of RES. In contrast, the stochastic simulation-optimization context allows for assessing their technoeconomic effectiveness against a wide range of uncertainties, and as such provides a critical tool for decision making, towards the deployment of sustainable and financially viable RES.

Chapter 6 focuses on mitigating this emerging paradigm in the modelling of water supply systems. In this vein, this sets the specifications for an adjustable framework that couples four modelling subsystems, i.e., physical, technical, economic, and social. The overall frameworks is employed to the highly extended raw water supply system of Athens, Greece, to reveal the multiple methodological and computational challenges of this implementation in practice. This consists of: (a) a simplified simulation of water-energy processes and associated infrastructures (reservoirs, aqueducts, pumps, etc.), in order to fulfill given water demands, under already optimized operational rules for the long run; (b) a water price model that accounts for simulated energy consumption, electricity prices, and net present fixed costs, and (c) an agent-based context that represents water consumer groups, whose behavior is influenced by water bills, water-saving campaigns, and their social network, as is described in **section 3.2.3**. Since the external drivers of the water-energy-society nexus (hydrometeorological processes and energy price) are expressed in stochastic terms, the water supply is sketched as a sociotechnical system under uncertainty.

Chapter 7 deals with the optimization of management policy across multipurpose hydropower reservoirs. In particular, this chapter proposes an uncertainty-aware optimization methodology that supports operators in accounting for the cascade effects of three main uncertain drivers, i.e., rainfall, water demands, and energy scheduling. To describe climatic and energy-market uncertainties stochastic approaches are followed, as described in **sections 3.1.3** and **3.3.3**, to generate synthetic rainfall and electricity price data, respectively. On the other hand, for the human-oriented procedures, i.e., water and energy targets, we employ statistical analyses of historical abstractions to fit copula-based relationships, in which the desirable releases for energy production depend on day-ahead electricity prices. Eventually, a toolbox is established that offers insights for decision-making regarding the estimated profits, their expected changes and the associated risk due to climate or market-oriented shifts. This approach is demonstrated in a multipurpose reservoir in Greece, Plastiras, which is affected by highly increasing socioeconomic conflicts.

Finally, there is the overarching conclusions and future research suggestions **Chapter 8**, to complete the thesis main body. There also two smaller chapters as **Appendices:**

Appendix 10.1 provides supplementary material and information of **Chapter 4.**

Appendix 10.2 provides supplementary material and information of **section 5.3.4**

1.3 List of Publications

The research objectives are addressed with the following journal and conference publications within the timeframe of the PhD:

Publications related to Thesis:

Publications in peer-reviewed journals:

1. **Sakki, G. K**., Castelletti, A., Makropoulos, C., and Efstratiadis, A.: Unwrapping the triptych of climatic, social and energy-market uncertainties across multipurpose hydropower reservoirs, Journal of Hydrology, Volume 648, 2025, doi: 10.1016/j.jhydrol.2024.132416
2. **Sakki, G. K**. and Efstratiadis, A.: Water supply systems under the sociotechnical context driven by the energy market, 2024
3. A. Zisos, **G.-K. Sakki**, and A. Efstratiadis, Mixing renewable energy with pumped hydropower storage: Design optimization under uncertainty and other challenges, Sustainability, 15 (18), 13313, doi:10.3390/su151813313, 2023.
4. G. Moraitis, **G.-K. Sakki**, G. Karavokiros, D. Nikolopoulos, P. Kossieris, I. Tsoukalas, and C. Makropoulos, Exploring the cyber-physical threat landscape of water systems: A socio-technical modelling approach, Water, 15 (9), 1687, doi:10.3390/w15091687, 2023.
5. A. Efstratiadis, and **G.-K. Sakki**, Revisiting the management of water–energy systems under the umbrella of resilience optimization, Environmental Sciences Proceedings, 21 (1), 72, doi:10.3390/environsciproc2022021072, 2022.
6. **Sakki, G. K**., I. Tsoukalas, P. Kossieris, C. Makropoulos, and A. Efstratiadis, Stochastic simulation-optimisation framework for the design and assessment of renewable energy systems under uncertainty, Renewable and Sustainable Energy Reviews, 168, 112886, doi:10.1016/j.rser.2022.112886, 2022.
7. K.-K. Drakaki, **G.-K. Sakki**, I. Tsoukalas, P. Kossieris, and A. Efstratiadis, Day-ahead energy production in small hydropower plants: uncertainty-aware forecasts through effective coupling of knowledge and data, Advances in Geosciences, 56, 155–162, doi:10.5194/adgeo-56-155-2022, 2022.
8. **Sakki**, **G.-K** ,I. Tsoukalas, and A. Efstratiadis, A reverse engineering approach across small hydropower plants: a hidden treasure of hydrological data?, Hydrological Sciences Journal, 67 (1), 94–106, doi:10.1080/02626667.2021.2000992, 2022.

Book chapters :

1. A. Efstratiadis, and G.-K. **Sakki**, The water-energy nexus as sociotechnical system under uncertainty, Elgar Encyclopedia of Water Policy, Economics and Management, edited by P. Kountouri and A. Alamanos, Chapter 64, 279–283, doi:10.4337/9781802202946.00071, 2024.

Conference Publications**:**

1. **Sakki, G. K**., Castelletti, A., Makropoulos, C., and Efstratiadis, A.: Trade-offs in hydropower reservoir operation under the chain of uncertainty, EGU General Assembly 2024, Vienna, Austria, 14–19 Apr 2024, EGU24-3487, https://doi.org/10.5194/egusphere-egu24-3487, 2024.
2. Efstratiadis, A. and **Sakki, G.-K**.: Driving energy systems with synthetic electricity prices, EGU General Assembly 2024, Vienna, Austria, 14–19 Apr 2024, EGU24-3165, https://doi.org/10.5194/egusphere-egu24-3165, 2024.

3. **G.-K. Sakki**, A. Efstratiadis, and C. Makropoulos, Stress-testing for water-energy systems by coupling agent-based models, Proceedings of 7th IAHR Europe Congress "Innovative Water Management in a Changing Climate", Athens, 402–403, International Association for Hydro-Environment Engineering and Research (IAHR), 2022.
4. V.-E. K. Sarantopoulou, G. J. Tsekouras, A. D. Salis, D. E. Papantonis, V. Riziotis, G. Caralis, K.-K. Drakaki, **G.-K. Sakki**, A. Efstratiadis, and K. X. Soulis, Optimal operation of a run-of-river small hydropower plant with two hydro-turbines, 2022 7th International Conference on Mathematics and Computers in Sciences and Industry (MCSI), Marathon Beach, Athens, 80–88, doi:10.1109/MCSI55933.2022.00020, 2022.
5. A. Efstratiadis, and **G.-K. Sakki**, Revisiting the management of water-energy systems under the umbrella of resilience optimization, e-Proceedings of the 5th EWaS International Conference, Naples, 596–603, 2022.
6. P. Pagotelis, K. Tsilipiras, A. Lyras, A. Koutsovitis, **G.-K. Sakki**, and A. Efstratiadis, Design of small hydropower plants under uncertainty: from the hydrological cycle to energy conversion, European Geosciences Union General Assembly 2023, Vienna, Austria & Online, EGU23-15407, doi:10.5194/egusphere-egu23-15407, 2023.

Publications within wider research field:

Publications in peer-reviewed journals:

1. E. Dimitriou, A. Efstratiadis, I. Zotou, A. Papadopoulos, T. Iliopoulou, **G.-K. Sakki**, K. Mazi, E. Rozos, A. Koukouvinos, A. D. Koussis, N. Mamassis, and D. Koutsoyiannis, Post-analysis of Daniel extreme flood event in Thessaly, Central Greece: Practical lessons and the value of state-of-the-art water monitoring networks, *Water*, 16 (7), 980, doi:10.3390/w16070980, 2024.
2. A. Roxani, A. Zisos, **G.-K. Sakki**, and A. Efstratiadis, Multidimensional role of agrovoltaics in era of EU Green Deal: Current status and analysis of water-energy-food-land dependencies, Land, 12 (5), 1069, doi:10.3390/land12051069, 2023.
3. A. Efstratiadis, P. Dimas, G. Pouliasis, I. Tsoukalas, P. Kossieris, V. Bellos, **G.-K. Sakki**, C. Makropoulos, and S. Michas, Revisiting flood hazard assessment practices under a hybrid stochastic simulation framework, *Water*, 14 (3), 457, doi:10.3390/w14030457, 2022.
4. K.-K. Drakaki, **G.-K. Sakki**, I. Tsoukalas, P. Kossieris, and A. Efstratiadis, Day-ahead energy production in small hydropower plants: uncertainty-aware forecasts through effective coupling of knowledge and data, *Advances in Geosciences*, 56, 155–162, doi:10.5194/adgeo-56-155-2022, 2022.
5. G.-F. Sargentis, P. Siamparina, **G.-K. Sakki**, A. Efstratiadis, M. Chiotinis, and D. Koutsoyiannis, Agricultural land or photovoltaic parks? The water–energy–food nexus and land development perspectives in the Thessaly plain, Greece, Sustainability, 13 (16), 8935, doi:10.3390/su13168935, 2021.

Conference Publications:

9. C. Ntemiroglou, **G.-K. Sakki**, and A. Efstratiadis, Flood control across hydropower dams: The value of safety, Role of Dams and Reservoirs in a Successful Energy Transition - Proceedings of the 12th ICOLD European Club Symposium 2023, edited by R. Boes, P. Droz, and R. Leroy, 187–198, doi:10.1201/9781003440420-22, International Commission on Large Dams, Interlaken, Switzerland, 2023.
10. P. Dimas, **G.-K. Sakki**, P. Kossieris, I. Tsoukalas, A. Efstratiadis, C. Makropoulos, N. Mamassis, and K. Pipili, Outlining a master plan framework for the design and assessment of flood mitigation infrastructures across large-scale watersheds, 12th

World Congress on Water Resources and Environment (EWRA 2023) "Managing Water-Energy-Land-Food under Climatic, Environmental and Social Instability", 75–76, European Water Resources Association, Thessaloniki, 2023.

11. A. Zisos, M.-E. Pantazi, M. Diamanta, I. Koutsouradi, A. Kontaxopoulou, I. Tsoukalas, **G.-K. Sakki**, and A. Efstratiadis, Towards energy autonomy of small Mediterranean islands: Challenges, perspectives and solutions, EGU General Assembly 2022, Vienna, Austria & Online, EGU22-5468, doi:10.5194/egusphere-egu22-5468, European Geosciences Union, 2022.
12. K.-K. Drakaki, **G.-K. Sakki**, I. Tsoukalas, P. Kossieris, and A. Efstratiadis, Setting the problem of energy production forecasting for small hydropower plants in the Target Model era, EGU General Assembly 2021, online, EGU21-3168, doi:10.5194/egusphere-egu21-3168, European Geosciences Union, 2021.
13. K. Risva, **G.-K. Sakki**, A. Efstratiadis, and N. Mamassis, Hydropower potential assessment made easy via the unit geo-hydro-energy index, EGU General Assembly 2021, online, EGU21-4462, doi:10.5194/egusphere-egu21-4462, European Geosciences Union, 2021.
14. **G.-K. Sakki**, V. Papalamprou, I. Tsoukalas, N. Mamassis, and A. Efstratiadis, Stochastic modelling of hydropower generation from small hydropower plants under limited data availability: from post-assessment to forecasting, European Geosciences Union General Assembly 2020, Geophysical Research Abstracts, Vol. 22, Vienna, EGU2020-8129, doi:10.5194/egusphere-egu2020-8129, 2020.

2 Water-energy nexus under uncertainty

Preamble

This chapter conducts a thorough literature review on uncertainty; from the definition and to its discrimination into several types. Also, this lists the important concepts of water-energy-food nexus and presents its dimensions and the related interconnections among its components. In the last section of this chapter, this presents the important concepts around the uncertainty-aware thinking within the water-energy nexus. The chapter sets the foundations for developing the uncertainty-aware methodology for the water-energy nexus presented in **Chapter 3**. Most of the material here was prepared originally for the thesis, albeit a small part of it is also covered on our publications:

A. Efstratiadis, and **G.-K. Sakki**, The water-energy nexus as sociotechnical system under uncertainty, Elgar Encyclopedia of Water Policy, Economics and Management, edited by P. Kountouri and A. Alamanos, Chapter 64, 279–283, doi:10.4337/9781802202946.00071, 2024.

A. Zisos, **G.-K. Sakki**, and A. Efstratiadis, Mixing renewable energy with pumped hydropower storage: Design optimization under uncertainty and other challenges, *Sustainability*, 15 (18), 13313, doi:10.3390/su151813313, 2023.

G.-K. Sakki, I. Tsoukalas, P. Kossieris, C. Makropoulos, and A. Efstratiadis, Stochastic simulation-optimisation framework for the design and assessment of renewable energy systems under uncertainty, Renewable and Sustainable Energy Reviews, 168, 112886, doi:10.1016/j.rser.2022.112886, 2022.

2.1 Unwrapping uncertainty

"A person is uncertain if he/she lacks confidence about his/her knowledge relating to a concrete question", (Sigel et al., 2010)

Uncertainty refers to a lack of certainty or predictability about a situation, outcome, or future events. It is the state of not fully knowing all the facts, details, variables, circumstances or potential outcomes of a particular situation, thus leading to ambiguity, doubt, or hesitation in decision-making or understanding. Specifically, uncertainty may arise due to several factors, such as insufficient (asymmetry) information, complexity, randomness, or unpredictability. These may be inherent in certain phenomena, processes and systems. Nevertheless, it is a fundamental aspect of life and plays a significant role in fields such as science, economics, business, and everyday decision-making (Bevan, 2022). However, uncertainty is widely referred as anathema or amorphous evil, mainly because this makes decision-making challenging and, in some situations, uncomfortable. Thus, the increasing of anxiety, regarding the future, leads to false perceptions about the uncertainty itself and its opportunities in growth. For instance, the deep knowing and appropriate handling of uncertainty present the opportunities to adaptability and creativity for all decision making. Therefore, while uncertainty might provide difficulties, it can also lead to favorable results if handled and dealt with appropriately.

In this respect, the recognition, description and eventually the disentangling of different aspects and categories of uncertainty is crucial. The unwrapping of uncertainty has been explored from various disciplines, i.e., environmental sciences (López-Gamero et al., 2011; Milliken, 1987), medicine (Kim & Lee, 2018), social sciences (FeldmanHall & Shenhav, 2019), economics (Davidson, 1999) etc. For each discipline, this is defined in various ways. For instance, Brown (2004) defined as uncertainty as "*our inability to resolve a unique, causal, world, either in principle or in practice*", while Walker et al. (2003) noted that this illustrates the starting point of "*any departure from the unachievable ideal of complete determinism*". In addition, Apostolakis (1989) posed the uncertainty in probabilistic terms, giving the definition of "*the distribution for the uncertainty factor is assessed subjectively, using the different predictions of the various models to indicate the possibility range of variation*".

Undoubtedly all these definitions highlight that the description and quantification of uncertainty is a demanding task, since it manifests in numerous forms, depending on the nature of the context. According to the uncertainty's architecture, we can discriminate two kinds, i.e., aleatory and epistemic. The first is also known as "random uncertainty", arises from inherent variability or randomness in a process (Hora, 1996). It is mainly associated with events or outcomes that are inherently unpredictable due to natural variability or chance. On the other hand, epistemic uncertainty refers to the incomplete knowledge or understanding of a system or phenomenon. It stems from limitations in data, information, or scientific understanding (Kiureghian & Ditlevsen, 2009). Another type of uncertainty is called ontological, which can be defined as "*a condition of complete ignorance in the model of a relevant aspect of the system*" (Gansch & Adee, 2020). This term originates from the "ontology", i.e., the study of existence. In this respect, this can be also called as unknown–unknown, introduced by Taleb (2007), which is the state of we do not know that we do not know.

In this scene, Beven (2016) made a more detailed classification of these types and specifically for the epistemic one, regarding the modelling procedure and the associated uncertainties. Specifically, he recognizes four general types, namely aleatory, epistemic, semantic and ontological, while he further discriminates the epistemic to three sub-categories that arises due to system dynamics, forcing and response data and disinformation. The first sub-category refers to the uncertainty that arises from a lack of knowledge about how to represent the system in study in terms of both model structure and parameters, including things that have not yet been perceived as being important but which might result in reduced model performance when surprise events occur. The second category refers to the uncertainty arising from lack of knowledge about the forcing data or the response data with which model outputs can be evaluated. This varies from the latter concept, since the disinformation regards to the known wrong or unreliable data, that are eventually useless. All aforementioned types of uncertainty can often interact and compound each other, making it challenging to fully understand or predict outcomes in complex systems or situations. However, the level of description of its type differs, since the epistemic uncertainty is theoretically reducible, while the aleatory and, even more, the ontological are intrinsically not (Hüllermeier & Waegeman, 2021; Packard & Clark, 2020).

To express and eventually quantify the aleatory uncertainty, tools that originate from the statistical theory are used. Specifically, common instruments are probability distributions and cumulative distribution functions, that provide insights into the range of possible outcomes occurring within a specified range. Besides these simple tools, more advanced techniques are used, namely Monte Carlo simulation (Cox & Siebert, 2006), and probabilistic modeling methods, such as Bayesian networks, Markov chains, and stochastic process. In its simplest setting, Monte Carlo simulation involves randomly sampling values from the probability distributions of uncertain variables and simulating the behavior of the system repeatedly. This technique provides essential insights into the range of potential outcomes and their probabilities, allowing for probabilistic risk assessment and decision-making under uncertainty. On the other hand, a Bayesian network is a mathematical model for representing causal relationships among random variables by using conditional probabilities (Imoto et al., 2006), while Markov chain gives a time dimension, since it is a stochastic model that describes a sequence of possible events in which the probability of each event depends only on the state attained in the previous event (Gagniuc, 2017). In addition, the stochastic processes enable more sophisticated modeling of complex systems with interconnected uncertainties. These are able to capture the dependencies and auto- and cross- correlations between uncertain variables, enhancing the necessary realism and accuracy of aleatory uncertainty modeling.

Similarly with aleatory uncertainty, statistical tools, such as Bayesian statistics, are used to represent and reduce the epistemic uncertainty (Zhou et al., 2022). However, this can also be based on the expert elicitation and judgment (Hester, 2012; Hora, 1996). Specifically, experts in the field of study provide qualitative or quantitative assessments of uncertain structures, parameters or scenarios based on their knowledge and their experience, thus facilitating the identification of key sources of uncertainty, prioritizing research efforts, and improving the robustness of decision-making in the absence of empirical data. Besides this empirical technique, interval theory-based analyses are also used (C. Wang et al., 2018). In particular, these provide bounds in parameter estimates or model predictions within specified confidence levels. Interval methods are particularly useful for handling uncertainty arising from imprecise or incomplete data, measurement errors, or model simplifications.

In contrast with the other two types of uncertainty, the ontological one is unrecognized and unquantifiable. Thus, the expert’s judgment is crucial, since they offer their belief, opinions and insights about the holistic structure or performance of a process and system. In addition, to account for this uncertainty source, scenario analysis have been tested. Specifically, these allow for exploring alternative futures or plausible narratives that reflect different assumptions and conceptual frameworks, thus describing distinct pathways or trajectories of system evolution, incorporating diverse perspectives, uncertainties, and boundary conditions.

Nevertheless, understanding and quantifying all types of uncertainty is essential in fields such as engineering, finance, and risk management, where decisions must be made in the presence of uncertain outcomes and model parameters. In the face of intrinsic unpredictability and randomness, practitioners can more effectively evaluate risks, prepare for contingencies, and make more informed decisions by recognizing and incorporating the multiple facets of uncertainty into models and decision-making processes.

2.2 The concept of water-energy nexus

“Water is the driving force of all nature”, (Leonardo Da Vinci)

Water and energy are the two fundamental resources in the world, and their interdependency is gaining more and more attention from both academics and the general public, since the world’s sustainability is hanged from them. The so-called water-energy nexus refers to the interconnection and interaction between water resources and energy production, consumption and storage. The popularity of the nexus could be dated back to the World Economic Forum in 2008, where the global challenges related to economic development were recognized from the water–energy–food nexus perspective. However, in the literature, there are many definitions and explanations of this concept and its dimensions. In this scene, Albrecht et al. (2018) concluded that its target is to employ effective tradeoffs and synergies between energy, water and food, considering cross-sectoral policies, environmental and social impacts. Focusing on the water-energy linking, Shrivastava and Stevens (2018) support that the “underlying idea behind water-energy nexus is that water is needed for energy generation, e.g., water is the working fluid in power plants where it is used as a heat transfer fluid in power cycles to generate electricity from fossil fuels”. However, the water and energy systems are inextricably mutual effect. We underscore that the “nexus” approach originates from the multidimensional role of water as: (a) energy producer, not only direct, namely for hydropower generation, but also indirect (e.g., irrigation of biofuels, cooling of thermal power plants, PVs' over open water), (b) energy consumer (e.g., pumping, water treatment, desalination), and (c) energy buffer (water stored to hydroelectric reservoirs, energy regulation through pumped-storage systems). Undoubtedly, in the energy system, water is primary for energy production, transportation, and utilization, but it is also a consumer for multiple uses such as water pumping, cleansing, delivering and sea water desalination (Sanders & Webber, 2012).

Nevertheless, the concept of the water-energy-food nexus encompasses a broad range of disciplines and associated research that vary in terms of their focuses. For instance, Walsh et al. (2018) study the water-energy-food nexus, considering the energy component within the electricity and food price. On the other hand, a significant effort has been made in the research of the role of water-energy nexus in the side of water, and specifically in water supply systems (Vakilifard et al., 2018). Specifically, for the last two decade, the long-term management and operation of water supply and distribution systems is based on the water-energy nexus context (Khalkhali et al., 2018; Lee et al., 2017; Sharif et al., 2019; Wu et al., 2020). Focusing on the energy component of this nexus, the synergetic role of renewable energy within this approach receives more attention (Sarkodie & Owusu, 2020). In this respect, a critical question arising, regarding the boundaries of such systems. Expanding the border lines of the water-energy nexus, we can incorporate several dimensions, i.e., social, economic, environmental and political.

Regarding the economic aspect of the water-energy nexus, the focus is given on the energy market, and especially in structure and pricing policy. Specifically, the structure of the electricity market affects substantially the water and energy consumption and efficiency (Zhao et al., 2021). For instance, taking as an example a representative case, i.e., multipurpose hydropower reservoir, its strategy is also the aftereffect of the energy market's operation. From a social perspective, both water and energy are critical for a society to a proper functioning, thus any links between them have a strong social effect. For some segments of society, this effect features more intensively, since they are directly impacted by the nexus. For instance, in the case of multipurpose hydropower reservoirs the farmers are strongly affected of high electricity prices or during periods of drought, since a well-compromised trade-off is difficult to be implemented. Another example originates in the water supply, whereas the distribution of water needs pumping or desalination, and during high electricity price periods the water bills expected to be also high.

In addition, the political dimension is equally important, since it manifests the other components also. Specifically, the policies arising from industry and/or energy-market reconstruction have strong economic and social aspect. Additionally, a potential lack or misleading water and electricity policies, as wells as enforcement of regulation may result in an increase in electricity use, overexploitation of groundwater, and discharge of effluent without proper treatment. In this respect, Wiegleb and Bruns (2018) made a systematic review on the drivers of water-energy-food nexus, concluding that the social scientific perspectives engage with the social, political, and normative elements of the Water-Energy-Food Nexus.

Within the most visible discourse, the environmental dimension of the water energy nexus is the key pillar for itself. By definition, the concept of the nexus created to establish a sustainable environment, preserving the health of natural ecosystems along with economic growth. In this vein, the nexus has synergies, complementariness and conflicts, as well. For instance, in the case of hydropower reservoirs, the incorporation of policies that protect the environment may create water-energy imbalances.

From the above discussion, the aforementioned four pillars of water-energy nexus, i.e., social, economic, environmental and political are inherently interdependent and uncertain. The multiple facets of uncertainty span over all external and internal processes, regarding the system's drivers (environmental and social), the fluxes, as well as their conversions across the water-energy nexus. In this respect, the starting point and simultaneously the cornerstone in study of the water-energy nexus is the exploration, description and incorporation of the uncertain factors.

2.3 Nexus' objectives

As the water-energy nexus is becoming even more important towards the overall goal of sustainable development (Biggs et al., 2015), the concepts of reliability, resilience and effectiveness across these systems is expected to be the key quest for their operation.

2.3.1 The concept of reliability

Reliability within the water-energy nexus stands as a fundamental pillar in ensuring the sustainability of interconnected systems. This concept encapsulates the consistent availability and functionality of water and energy resources to meet societal needs, economic activities, and environmental goals. In this context, reliability can be articulated concerning both duration and magnitude, capturing the average occurrence frequency and volume of deficiencies, respectively (Efstratiadis et al., 2021a). In particular, the time-based reliability is defined as the probability:

$$R_T = 1 - P(\underline{y_t} < \underline{y_t^*}) \tag{2.1}$$

where $\underline{y_t}$ is the actual outflow (e.g., water abstraction, energy release) through the system to fulfil a desirable water or energy demand, $\underline{y_t^*}$. On the other hand, the quantity-based reliability is formulated as:

$$R_v = \frac{E\left[\underline{y_t}\right]}{E\left[\underline{y_t^*}\right]} \tag{2.2}$$

where $E[x]$ denotes the average value of a random process x. We remark that both reliability metrics are crucial, since a technical system should be reliable against pressures both in time and quantity. Besides the pure mathematical expressions, we can discriminate the key components of water and energy reliability, both in quantitative and qualitative terms (Cizelj et al., 2001). In particular, for each source we must ensure the water and energy supply security, quality assurance, continues access and affordability (Gheisi et al., 2016; McCarthy et al., 2007). Specifically, the water and energy supply can be estimated from the above equations, while the quality assurance refers to different notion for each source. For water resources, the quality assurance comprises the maintenance of water quality within acceptable standards to support human health, ecosystem integrity, and industrial processes, while for the energy component regards to ensuring stable power generation from diverse energy sources. Overall, both resources should be equitable accessible to all communities, by means of infrastructure and affordability (Malik, 2002).

Furthermore, the relationship between water and energy underscores the importance of reliability, since the disruptions in one sector have cascading effects on the other, thus amplifying vulnerabilities across the overall system. The interdependencies between water and energy systems introduce complex trade-offs and synergies that influence overall reliability outcomes. For instance, hydropower generation contributes to both energy security and water availability but can also impact aquatic ecosystems and water quality. Similarly, energy-intensive water treatment processes affect both water supply reliability and energy consumption patterns. Understanding these interlinkages is crucial for devising integrated management strategies that optimize reliability across the water-energy nexus while minimizing trade-offs and maximizing co-benefits.

2.3.2 The concept of resilience

Resilience has been deeply investigated across different research fields (e.g., economy, energy, water, agriculture), where the different disciplines involved are addressing this issue from their own perspectives. Overall, resilience is the degree to which a system continues to perform with tolerant reliability under progressively increasing disturbance (Makropoulos et al., 2018). On the other hand, Grafton et al. (2019) poses the resilience management as the planning, adaptation and transformation actions intended to influence the resistance, recovery and robustness (the so-called three Rs) of the social-ecological system under consideration. In the literature, these are defined as follows: a) resistance is a system's ability to actively change, while retaining its identity, or to passively maintain its performance following one or more adverse events; b) recovery is a time measure, where a higher value indicates a shorter recovery time, and c) robustness is the level of pressure that the system can take without failing (Redman, 2014). Finally, Pizzol (2015) highlights that resilience depends on the system's elements and the way these elements are connected. Specifically, a specific architecture and design of a system, which may include less efficient components, can better manage stresses.

The concept of resilience provides the essential background for the assessment and evaluation of an a priori determined design of engineering systems under emerging threats (Nikolopoulos et al., 2020). These may include health and economic crises, population growth, and sudden large-scale changes (also referred to as "black-swan" events), as well as cyber-physical attacks (Moraitis et al., 2020), which is a new type of threat. In the context of water systems that are highly affected by such events, Butler et al. (2017) provides a "roadmap" to sustainability, consisting of a set of basic definitions and concepts of reliability and resilience, and, eventually, an associated evaluation framework.

However, in the water-energy nexus this road is even more challenging, since the complementarities and dependencies of the two components tread a fine line. The first two targets depend both on the structure and the operation of the system, which are outcomes of their design and management, respectively. In particular, the tradeoffs and synergies of the water and energy elements across a well-defined nexus can enrich policy design frameworks, with perspectives from beside and beyond the resilience rationale (Hogeboom et al., 2021).

2.3.1 The concept of effectiveness

Effectiveness within the water-energy nexus embodies the efficiency and success of integrated approaches aimed at optimizing resource utilization, enhancing system performance, and achieving sustainable outcomes (Ahmad et al., 2020). In line with the two aforementioned concepts, i.e., reliability and resilience, effectiveness manifests the ability of interconnected water and energy systems to fulfill societal needs, economic objectives, and environmental goals, while minimizing conflicts and maximizing synergies.

The concept of effectiveness comprises micro and macro-levels of studies, since water-energy nexus regards from the industry scale to the national, even to transboundary one (Dai et al., 2018). In this respect, key components of its concept is the integrated resource management, the technological innovations, the policy interventions, and the stakeholder engagement. In particular, the effective management of water-energy nexus necessitates integrated approaches that recognize the interconnectedness of water and energy systems and mitigate potential conflicts. In addition, innovative solutions, such as smart sensors, data analytics, and automation technologies, enable real-time monitoring, optimization, and management of water and energy resources, thus enhancing the effectiveness (Urban, 2017).

Besides the engineering approaches, the effectiveness of such systems is determined by the engagement of various stakeholder groups and the governance frameworks. In particular, the policy interventions are essential for promoting synergy and coherence within the water-energy nexus, regarding the development of integrated water-energy policies, regulatory mechanisms, and incentive structures that encourage collaboration, innovation, and investment in sustainable solutions (Kaddoura & El Khatib, 2017). In this line, the meaningful engagement of stakeholders fosters ownership, accountability, and social acceptance of water and energy initiatives, thereby contributing to the effectiveness and sustainability of nexus management efforts (Kliskey et al., 2021; Mohtar & Daher, 2016).

2.4 Embedding uncertainty within the water-energy nexus

Heraclitus, the ancient Greek philosopher, recognized that "The only constant thing in life is change". The water-energy nexus, as a key aspect of life, and its associated elements should not be considered as stable, static and steady. Uncertainty in the water-energy nexus can arise from various factors, including hydroclimatic processes, multiple human-induced procedures (e.g., legal regulations, strategic management policies, real-time controls, market rules) and technological innovation .

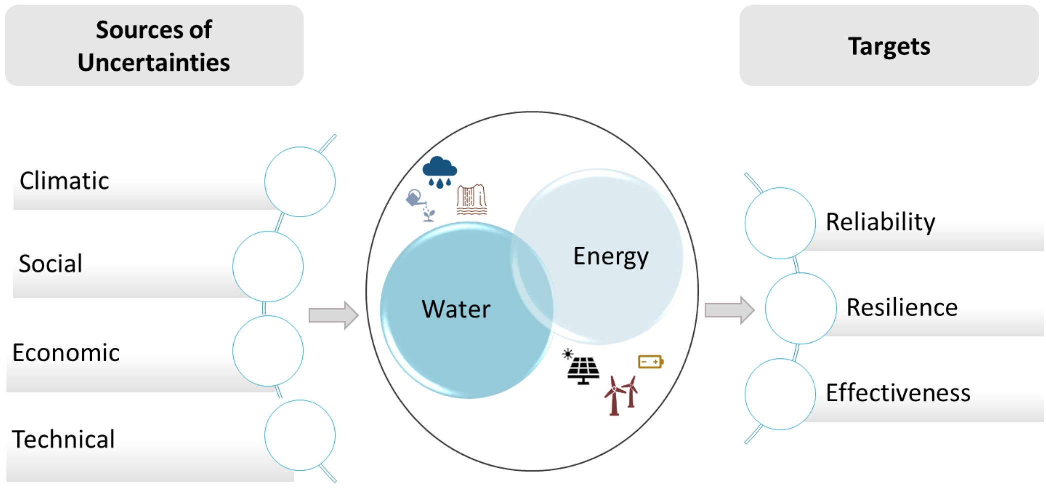


Figure 2.1: Key components of the water-energy nexus and the associated uncertainties.

In this context, and according to the rationale by Sakki et al. (2022), uncertainties can also be identified as exogenous and endogenous, where the first refer to the system's drivers and the second to its internal processes. In particular, the production of water and energy (particularly, renewable energy) is driven by inherently uncertain hydrometeorological processes that exhibit significant peculiarities across scales (e.g., intermittency, intra-day and seasonal periodicity, long-term persistence, complex dependence structures, etc.). However, since these are natural and thus "pristine" processes, their probabilistic regime is, at least partially, explained by the statistical information provided by past observations. In contrast, the human factor is strongly unpredictable, thus displaying emergent properties with respect to highly uncertain environmental, (geo)political and economic drivers, and interactions among different societal groups, as well. On the other hand, the internal uncertainties involve all kinds of spatiotemporal propagations, exchanges, and transformations across the system (e.g., conversion of river flows to hydropower), which are represented through simulation models of all kinds (physically-based, conceptual, empirical, data-driven).

2.4.1 Climatic uncertainty

The different disciplines that are involved in the water-energy nexus address the issue of uncertainty from their own perspectives and methodological means. Environmental sciences have focused on capturing external uncertainties, and specifically those stemming from the highly varying nature of the input hydrometeorological processes. However, it is argued that this source of uncertainty is poorly only reflected when using short historical data within simulations (Bakhtiari et al., 2021). In fact, these data may not be fully representative of the actual hydroclimatic regime of the process of interest, and cannot capture long-term changes, that are of key importance in the assessment of reliability and resilience of such systems. A more comprehensive approach is offered by stochastic synthesis models that are able to reproduce the probabilistic behavior and dependence structure of the hydrometeorological processes.

The use of stochastic models for generating long synthetic data, to be input to deterministic models, is a common practice in water resources and other environmental sciences (Efstratiadis et al., 2014). The literature reports numerous modelling attempts for representing wind, solar and hydrological drivers through statistical and, less often, stochastic approaches (Aguiar & Collares-Pereira, 1992; Katikas et al., 2021; Palma-Behnke et al., 2021; Tsekouras & Koutsoyiannis, 2014). The latter offer a more consistent basis for process description, since they also account for dependencies in time and space, i.e. among correlated processes (Ramírez et al., 2021).

The hydroclimatic uncertainty has been widely studied within water-energy systems, and its applications, also by means of climate change scenarios (Ahmadi et al., 2015; Anghileri et al., 2018; Caceres et al., 2021; Matteo Giuliani et al., 2016; Oyerinde et al., 2016; Park & Kim, 2014; Paseka et al., 2018) or in terms of large synthetic inputs instead of historical records, i.e., by employing stochastic simulation (Bertoni et al., 2019; Ortiz-Partida et al., 2019; G. K. Sakki et al., 2022). Specifically, Suo et al. (2021) enhanced the energy-water nexus model with climate change scenarios for China in order to simulate water availability under changing climate, describing uncertainty derived from long-term planning horizon (2021–2050), and providing optimal schemes for China's energy system management. Similarly, Van Vuuren et al. (2019) introduced a set of model-based scenarios that enable analysis of the relevant relationships and dynamics, as well as the options to formulate response strategies under the changing climate for higher agricultural yields and reduction of food waste purposes.

2.4.2 Social uncertainty

Following the anthropogenic side of the water-energy nexus, it is necessary to investigate the uncertainty in regulatory policies related to water usage, environmental standards, and energy production that affect investment decisions and operational practices in both water and energy sectors. In this respect, Orimoloye (2022) studied the implementation and the associated actions and policies of the water-energy-food nexus over the years and globally. Focusing on the water-energy-food nexus, numerous research attempts have been made, regarding its integration with policy strategies in the presence of partial knowledge and understanding. In this respect, Mercure et al. (2019) proposed a science-policy-law interface to enable the design and implementation of nexus-resilient public policies. Other approaches include the optimization of the system's policy, analyzing of the interconnections and the associated uncertainties, originated from energy prices (Namany et al., 2019), system's (water, energy and crop) cost and environmental constraints (M. Li, Fu, Singh, Ji, et al., 2019; M. Li, Fu, Singh, Liu, et al., 2019) and land competitions (Nie et al., 2019).

Nevertheless, the investigation of the best-compromise trade-offs between physical and social systems and the anthropogenic effects on the natural resources under uncertainty requires the research of all social interactions within the system. In this respect, Vieira *et al.* (2021) developed an economic performance assessment framework, tailored for multipurpose plants, while accounting for demand uncertainty. Additionally, Molajou et al. (2021) introduced a conceptual socio-hydrological-based framework, which aims at investigating the farmer's response under different socio-economic conditions. Similarly, the joint uncertainty, induced by climate and demand dynamics are widely explored. Specifically, Alhazmi et al. (2023) developed a novel analytic for uncertainty-aware day-ahead operation optimization of the interconnected power and water systems, accounting for the wind and water demand forecasts. Giuliani *et al.* (2016) combined climate uncertainty with social one to assess and advance the representation of human behaviors within the feedback between natural and human components.

Thus, for obtaining sustainable and viable outcomes across the water-energy nexus, it is necessary to investigate the socio-climatic tradeoffs among physical and social systems, the anthropogenic impacts on the condition of natural resources and the social externalities of natural resources governance (Bakarji et al., 2017; Biggs et al., 2015). In particular, changes in population growth, urbanization patterns, shifts in lifestyle preferences, industrial activities, and land use practices affect the spatial distribution of water and energy resources, posing challenges for infrastructure planning and resource management. Thus, this structural uncertainty that regards to consumer behavior should be modelled. The modelling approaches of the social factor and the associated uncertainties and constraints will be discussed in section 3.2.

2.4.3 Energy market uncertainty

In contrast to climatic and social uncertainties, the one of the energy market is not broadly investigated in the water-energy-food nexus. However, the fluctuations in energy prices, water tariffs, and financing costs can impact the feasibility of infrastructure projects and the profitability of energy generation facilities. This facet has not been unexplored, since the energy market dynamics is the aftereffect of the recent deregulation and liberalization. Specifically, the variation of energy prices is the indirect effect of social uncertainty since the electricity price process now enables the determination of competitive prices according to supply and demand market forces. The research on this uncertainty mainly focuses on forecasting (Kostrzewski & Kostrzewska, 2019) and market structures (Papavasiliou et al., 2015).

The energy market, as it is operating, has a short history but the fluctuations of the recent energy crises have many effects. In this vein, Bohi (1991) studied the macroeconomic effects of the energy price shock in the 1970s and concluded that in a dataset of four countries there was no correlation between the price shock and the operation of industry. On the contrary, Van de Ven (2017) concluded that the impacts of the energy shocks are correlated with the economic development and the associated circumstances, considering that the economies are dependent on a single source. In the scene, the future of the running energy crisis is unclear. Some economists predict that reshoring will slow the global energy transition as markets fragment (Goldthau & Tagliapietra, 2022), while some researchers disagree. Nevertheless, the water-energy nexus, as an energy related work, are strongly dependent on any energy crises or shocks, and such their design and management should account for these.

In this context and regarding the management of the water-energy systems, the optimal water allocation among users (energy and water demands) relies on the proper economic representation of the effects of alternative allocations using hydro-economic models, which can be the basis for water decision making (Arjoon et al., 2014; Harou et al., 2009). The aforementioned models are based on the concept of opportunity cost, where the objective is to maximize the profits from power sold to the day-ahead market and the profits from water supply and the irrigation, while minimize the penalties of non-fulfilling the water demands. In this scene, the steady-state approach of hydro-economics models should be more advanced in order to account for the fluctuations of the market price, the uncertain human factor and the hydroclimatic variability, as well. All these parameters force the scientific community to consider the issue of uncertainty and embed it in the design and assessment procedures of such projects. In this respect, an effort of representing the drivers of the electricity price fluctuations (K. Li et al., 2019) and the inflation spikes (Ha et al., 2019) has been made, but still are open questions in the modelling and their effects in large-scale systems. The modelling of electricity price process will be further discussed in section 3.3.

2.4.4 Technical uncertainty

Another facet of uncertainty within the water-energy systems relies on its technology. The rapid advancements in water and energy technologies introduce uncertainty regarding the future cost-effectiveness, efficiency, and scalability of different solutions. For instance, emerging technologies such as desalination, water recycling, and renewable energy sources can reshape the water-energy nexus, but their adoption rates and performance characteristics may be uncertain. In this context, Rao et al. (2017) made a review, its relying on the technological and engineering aspects of various connections in the water-energy nexus, and the associated challenges imposed by the technological growth.

In addition, mechanical and electrical engineering sciences have explored the internal uncertainties, which are associated with the system properties (e.g., drop of efficiency due to ageing, maintenance and equipment malfunction), as well as model assumptions and parameters (Giannakoudis et al., 2010; Soroudi & Amraee, 2013; Zisos et al., 2023). In general, such approaches refer to the microscale of the power machine, in order to capture facets of uncertainty across quite complex technical issues, e.g. pitch control to wind turbines (Astolfi, 2019) and hydro turbines (Abbas & Kumar, 2019). In addition, Caputo et al. (2023) proposed an assessment framework that incorporate uncertainties related to components efficiencies values given by the relationships used to design the system. Regarding the “flow-energy” conversions and their associated uncertainties, Pei et al. (2022) focused on the model structures and parameterizations within solar works.

2.4.5 Joint uncertainties

However, the combined effects of internal and external uncertainties, epistemic, aleatory and ontological, as well as the interplay of their cascades and dependencies, have received considerably less attention to date (Mirakyan & De Guio, 2015), although it is accepted that the nonlinearities across the inflow-energy conversions usually amplify the overall uncertainty (Gensler et al., 2018). This leads inevitably to a fragmented approach in planning and management practices for the water-energy nexus, arguably impacting their performance, as quantified in terms of economy and reliability, and the emerging concept of resilience (Efstratiadis et al., 2021b). For instance, in the engineering context, conventional practices often ignore or, at least, underestimate these uncertainties and their dependencies. Yet, it is argued that the ignorance of uncertainty results into fully deterministic outcomes (i.e., a unique optimal design), which eventual leads to risky decisions, regarding critical technical quantities and the economic viability of water-energy nexus of interest across scales.

However, addressing uncertainty in the water-energy nexus is a demanding and multidisciplinary task, since it requires integrated planning, risk management strategies, and adaptive governance approaches. This may involve scenario analysis, stakeholder engagement, robust decision-making frameworks, and the development of flexible infrastructure and policy mechanisms to accommodate changing conditions and mitigate potential risks. Collaboration among policymakers, industry stakeholders, researchers, and communities is essential to address the complex and interconnected challenges posed by uncertainty in the water-energy nexus.

2.5 Conclusions

Uncertainty has been a rather elusive term since its inception, thus making the researchers considering as an amorphous evil or as a challenge. In any cases, uncertainty is key driver of our life, and should incorporated in policy and decision making. There have been numerous proposed definitions, but all finally conclude that this is any deviation from the total determinism, i.e., the unreachable ideal. In general, this is discriminated into aleatory, epistemic and ontological, while a further classification, i.e., exogenous and endogenous, can be made regarding the system's boundaries.

For the water-energy nexus in particular, there exist many schemes that correspond to numerous facets of uncertainty, i.e., climatic, social, energy market and technological. Few approaches are accounting for joint uncertainties in the assessment, design and long-term management, leading to fragmented approaches. What we are identifying as missing, is a generic, flexible and adjustable uncertainty-aware framework tailored for water-energy systems, able to capture, incorporate and quantify joint uncertainties. In this respect, **Chapter 3** focus on the modelling methodologies the aforementioned sources of uncertainty, that will be further considered as inputs in the water-energy nexus.

3 Enclosing uncertainty in a toolbox

Preamble

This chapter conducts a thorough literature review on the key sources of uncertainty (endogenous and exogenous) that drive the water-energy nexus, i.e., climatic, social, energy market and epistemic. A sub-chapter for each source of uncertainty is dedicated, including the definitions, the common modelling approaches and eventually our approach to deal with. Specifically, for the hydrometeorological processes we are taking advantage of stochastics, while for the social uncertainty an agent-based model is developed tailored for water-energy systems. To account for the energy market fluctuations, we also employ the stochastic theory, by introducing a novel approach for simulating the electricity price. In addition, for the epistemic uncertainty, we provide three different approaches, that based on probabilistic and non-probabilistic techniques. Eventually, this chapter provides the information to quantify the uncertainty through copula-based tools. This chapter includes the key modelling approaches that will be further used to the design, long-term management and assessment of the water-energy systems, presented in the next chapters. Most of the material here was prepared originally for the thesis, albeit a small part of it is also covered on our publications:

G.-K. Sakki, I. Tsoukalas, P. Kossieris, C. Makropoulos, and A. Efstratiadis, Stochastic simulation-optimisation framework for the design and assessment of renewable energy systems under uncertainty, Renewable and Sustainable Energy Reviews, 168, 112886, doi:10.1016/j.rser.2022.112886, 2022.

3.1 Climatic uncertainty: modelling the hydrometeorological processes

3.1.1 Definitions

A significant characteristic of the atmospheric processes is their inherent uncertainty. As randomness and predictability coexist and are intrinsic to natural systems, these systems can be treated as deterministic and random at the same time, depending on the time scale. For instance, in the short-run its uncertainty is decreased, while in the long-run this phenomenon is escalated. However, the hydrometeorological processes' uncertainty originates from well-known, but challenging characteristics, e.g., periodicity, intermittency, persistence (auto-dependence), cross-dependence and non-Gaussian probabilistic behavior. In this respect, various modelling approaches have been employed to handle the aforementioned peculiarities. Before describing the simulation schemes it is considered useful to provide some basic definitions and descriptions regarding these main hydrometeorological characteristics.

Periodicity: Periodicity in hydrometeorological processes refers to the variations or patterns in weather and hydrological conditions that occur in a cyclic manner throughout a specific period, i.e., year, month, day. For instance, when the time scale of interest is finer than annual, these processes cannot be regarded as stationary, because of the effects of seasonality to the process mechanisms that are reflected in their statistical properties. However, periodicity can be detected at finer time scales (e.g., hourly) for several atmospheric processes, e.g., wind speed and solar radiation that are driven by the Earth's rotation. According to Koutsoyiannis (2004b) a simple method often used to remove seasonality effects is to standardise the process x_i by using seasonal values of mean, μ_i, and standard deviation, σ_i, i.e. setting $z_i = (x_i - \mu_i)/\sigma_i$, thus assuming that z_i is a stationary process. This simple method fails to catch other statistical properties , e.g., autocorrelation and skewness, due to the assumption of stationarity. In this case, more sophisticated approaches are adopted, assuming a cyclostationary (also known as periodic) process, also accounting for season-to-season correlations coefficients (Tsoukalas et al., 2018b). Understanding, simulating and predicting seasonal patterns in hydrometeorological processes is crucial for various applications, including water resource management, flood forecasting, agriculture, and ecosystem management. It helps stakeholders make informed decisions and implement appropriate measures to mitigate risks associated with seasonal variations in weather and hydrology.

Intermittency: Intermittency in hydrometeorological processes refers to patterns where the underlying atmospheric conditions are not consistently present but rather appear intermittently or in a non-continuous manner. For instance, at fine times scales (e.g., hourly) the precipitation appears as an intermittent processes, as alternates between two states, the dry (zero rainfall) and wet (positive rainfall). In order to reproduce the intermittent behaviour, it is essential to preserve the probability of zero values of the observed time series. In this respect, Koutsoyiannis (2006) offered an extensive review regarding this aspect, presenting the modeling approaches. However, he concluded that it requires more analysis, particularly in their ability to reproduce the rainfall occurrence process and specifically the dry period structure at different scales. One decade later, Schleiss and Smith (2016) proposed two methodologies to address this gap. Recently, Dey (2023) provides an approach to model intermittency, by preserving the temporal structure of the interevent time distribution.

Auto-dependence: A typical characteristic encountered in such processes is auto-dependence, either short or long range (long-term persistence). The short-term dependence (SRD) has been extensively discussed in literature (Song & Fujimura, 2021; Wilson, 2016) and implies an exponential autocorrelation structure that diminishes after few time lags. Regarding the autocorrelation structure, a plethora of theoretical models can be found (Berne et al., 1966; Koutsoyiannis, 2000b; Robertson, 2012; Strey, 2019).

Long-term persistence: Long-term persistence, known also as long-term dependence, or memory, refers to the phenomenon where certain events exhibit perseverance over extended periods of time. Specifically, in hydrology, this behavior is the tendency of wet years to cluster into multiyear wet periods or of dry years to cluster into multiyear drought periods. This characteristics is related also to the Pharaoh's dream of seven sleek and fat cows coming up from the Nile, followed by seven gaunt and lean cows; Joseph interpreted this dream as seven years of plenty followed by seven years of famine and recommended storage. The study of dependence in time has a long history dating back to the study of Hurst (1951), who observed that the annual behavior of the level of the Nile river deviated from that of a purely random process. To account for this hydrological characteristic, also referred to as Hurst-Kolmogorov dynamic (HK) and eventually model this, several methods are employed, e.g., using heavily-tailed autocovariance functions (Barunik & Kristoufek, 2010), climacograms (Dimitriadis & Koutsoyiannis, 2015; Koutsoyiannis, 2010; Koutsoyiannis, 2004a) and least squares correlograms (Young & Jettmar, 1976).

Cross-dependence: Besides the autodependence characteristic of the hydrometeorological processes, it is widely acknowledged that a crucial issue of studying them is the interdependence. Specifically, they exhibit cross-dependencies either to cause-effect relationships (e.g., rainfall-runoff) or to spatial proximity (Drogue & Ben Khediri, 2016; Lebar et al., 2023). In this respect, multivariate stochastic models have been employed to account for both spatial and temporal dependencies (Efstratiadis et al., 2014; Makhnin & McAllister, 2009; Paschalis et al., 2013).

Non-Gaussianity: A crucial characteristic of hydrometeorological processes is asymmetry, which is also due to the aforementioned properties, i.e., intermittency and non-negative values. This implies the use of skewed (i.e., non-Gaussian) distribution functions (Tavares, 1980). This is more intense in the finer timescales, since the annual series may be modeled by linear models with Gaussian inputs, while the daily data often demonstrate nonlinear characteristics and are non-Gaussian as well (Rao & Yu, 1990).

3.1.2 Treatment of uncertainty in common modelling approaches

To handle the aforementioned challenges of hydrometeorological processes in the representation procedure is a demanding task. In general, a reliable model considers the one which offer synthetic realizations that resemble the historical data, in the sense that they reproduce the above characteristics. Thus, a plethora of approaches have been adopted to represent hydrometeorological processes, originating from probabilistic approaches (statistics, stochastics and copulas) or scenario-based ones (e.g., as made by climatic models). Climatic models assume various socio-economic conditions in the long-run, and thus the climatic variability is estimated. However, such models are based on hypotheses and regards to a global scale, thus a downscaling of all these scenarios is needed. In this thesis, the focus is given in stochastic models that are able to represent the statistic information of the past observations and include all possible scenarios. Thus, an overview of the common simulation schemes to generate synthetic timeseries is presented, as classified by Haberlandt et al. (2011). In particular these refer to a) Linear models, b) Point Process Models, c) Disaggregation Models, d) Resampling (non-parametric) Models. Nevertheless, the attention will be given to linear stochastic models, because they have been for years the main tool for stochastic simulation of hydrometeorological processes.

3.1.2.1 Basic probabilistic concepts: Random variables, Distribution functions and moments

All these models originate from the statistical theory. In this respect, the fundamentals definitions of the pivotal probabilistic and stochastic concepts should be presented. Let consider a random variable $\underline{x}$, which is the a function that maps outcomes of experiments from the nonempty set Ω, else called set of elementary events or states, to numbers. The associated cumulative distribution function (CDF) is expressed as:

$$F(x;t) \coloneqq P\{\underline{x}(t) \leq x\} \tag{3.3}$$

while its probability function is:

$$f(x;t) \coloneqq \frac{dF(x;t)}{dx} \tag{3.4}$$

Eq. (3.1) is further expand for n-th order as:

$$F(x_1, x_2, .., x_n; t_1, t_2, .., t_n) \coloneqq P\{\underline{x}(t_1) \leq x_1, \underline{x}(t_2) \leq x_2, \dots, \underline{x}(t_n) \leq x_n\} \tag{3.5}$$

A proper stochastic process is holistically determined, if we know the nth order distribution. Important quantitative measures related with the stochastic process are moments. Our focus is given in following moments, i.e., mean, variance, auto-covariance, auto-correlation, skewness and kyrtosis.

(a) Mean

$$\mu(t) \coloneqq E[\underline{x}(t)] = \int_{-\infty}^{+\infty} x f(x;t)\, dt \tag{3.6}$$

(b) Variance

$$\gamma_o(t) \coloneqq var[\underline{x}(t)] = \int_{-\infty}^{+\infty} (x - \mu(t))^2 f(x;t)\, dt \tag{3.7}$$

(c) Auto-covariance

$$c(t;h) \coloneqq cov\left[\underline{x}(t), \underline{x}(t+h)\ \right] = E\left[(\underline{x}(t) - \mu(t))(\underline{x}(t+h) - \mu(t+h)\right] \tag{3.8}$$

(d) Auto-correlation

$$r(t;h) \coloneqq corr\left[\underline{x}(t), \underline{x}(t+h)\ \right] = \frac{c(t;h)}{[\gamma_o(t)\gamma_o(t+h)]^{1/2}} \tag{3.9}$$

(e) Skewness

$$C_s(t) \coloneqq \frac{\mu_3(t)}{\gamma_o(t)^{3/2}} \tag{3.10}$$

(a) Kyrtosis

$$C_k(t) \coloneqq \frac{\mu_4(t)}{\gamma_o(t)^2} \tag{3.11}$$

Note that $\mu_3(t)$ and $\mu_4(t)$ are the third and fourth central moments of the process, i.e., $\mu_i(t) \coloneqq \int_{-\infty}^{+\infty}(x - \mu(t))^i f(x;t)\,dt$.

3.1.2.2 Linear stochastic models

The stochastic models has a long history dating back to early 20th century, leading to three schools thought, i.e., (a) the Stochastic School, (b) the Time Series School and (c) the Monte Carlo School. (Koutsoyiannis, 2020) The dominant approach in stochastic modelling is to choose and fit a model from a repertoire offered in books on time-series analysis. The most widely known modelling approach is autoregressive models which originated in the researches of Yule (1927) and Walker (1931), that are further earned the stochastic theory following the rationale of Wold (1948) and Whittle (1953).

These models are mostly known by their acronyms, such as $AR(p)$ (for autoregressive of order p), $MA(p)$ (for moving average of order p), $ARMA(p,q)$ (for autoregressive moving average-linear combination of the latter models), $ARIMA(p,d,q)$ (for autoregressive integrated moving average), $ARFIMA(p,d,q)$ (for autoregressive fractionally integrated moving average), able of modelling long-range dependence through the use of a real valued d parameter.

It is noted that all above categories of linear stochastic models are typically employed for the simulation of hydrometeorological processes at the annual and monthly time scales. In the finer scales, these are limited due to their failure to handle intermittency without the use of additional modelling tricks, such as, truncation of negative values to zero, power-transformation functions or latent Gaussian processes.

Despite their large popularity, these models suffer from a number of issues, namely a) definition in discrete time in contrast to the continuous-time evolution of natural systems, b) definition in terms of the autocorrelation structure whose estimation is negatively biased, and c) overparameterization. In this scene and to overcome all these limitations, Koutsoyiannis (2000b) introduced the so-called symmetric moving average (SMA) generating scheme that can be used to generate any kind of stochastic processes with any autocorrelation structure or power spectrum. To advance this, he also developed an alternative parsimonious approach for model identification and fitting based on a generalized form of the autocovariance structure (Koutsoyiannis, 2002), by parametrizing HK processes.

In addition, to overcome the issue of non-Gaussianity, and accept the skewed character of hydrometeorological processes, several modelling approaches have been adopted. Following the rationale by Tsoukalas et al. (2018a) these can be categorized into a) explicit methods, b) transformation-based methods, and c) implicit methods, that treat skewness via employing non-Gaussian white noise for the innovation term. Regarding implicit schemes, Dimitriadis and Koutsoyiannis (2018) provided a model that enables to preserve four moments (up to kurtosis), while a transformation-based approach was followed by Papalexiou (2018), performing the simulation of the dependence structure in the Gaussian domain by using autoregressions and back-transforming to the non-Gaussian domain. A quite similar modelling approach, based on the explicit method, and the Gaussian auxiliary process but combining the SMA model for the generation scheme instead, is developed by Tsoukalas et al. (2018).

3.1.2.3 Point process models

These models are widely used for simulating hydrometeorological processes at finer scales, i.e., sub-hourly, hourly and daily. Rodriguez-Iturbe et al. (1988) introduced the main theory of continuous-type point processes in hydrological sciences. Depending on the type of process that is employed for the cell clustering mechanism, two major models are extensively known, namely the Neyman-Scott (Cowpertwait et al., 1996) and the Bartlett-Lewis processes (Onof & Wheater, 1993). Advantages of the point process models are their physical basis. On the other hand, their main limitations, comparing with the aforementioned linear methods, underlie their inability to preserve significant statistical and stochastic properties the process. Specifically, these are weak to a) reproduce the marginal distribution of the process and b) simulate multivariate processes and season-to-season correlation structures (Kossieris et al., 2018; Onof & Wang, 2020).

3.1.2.4 Disaggregation Models

Disaggregation models were introduced in hydrology by the novel work of Valencia and Schaake (1973). Disaggregation allows simulation in stages for different time steps using each a suitable approach, e.g. modelling daily rainfall with a Markov Chain and then disaggregating it at the hourly scale with a random cascade. However, a major disadvantage of these models regards that all fine time scale rainfall disaggregation techniques summarised above have a common characteristic: they are single-site (Tsoukalas et al., 2019). The problem of multiple site rainfall disaggregation, both for temporal and spatial dimensions, is of significant practical interest but presents significant differences from that of single-site disaggregation, including increased mathematical complexity (Koutsoyiannis, 2003).

3.1.2.5 Resampling Models

An alternative simulation scheme is offered by the so-called *non-parametric* approaches, also referred as bootstrapping techniques, which attempt to replicate the empirical distributions of the observed processes, typically through resampling of historical data (most often using the well-known k-nearest neighbor algorithm) (Huang et al., 2017; Rajagopalan & Lall, 1999). This kind of models are widely used in numerous disciplines, including the environmental sciences, due to their simplicity (Curceac et al., 2019). However, it seems to appear several and crucial limitations, due to the lack of theoretical basis. In this respect, they are not able to reproduce both short- and long-range dependence (i.e., persistence) and cross-correlations among multiple variables. An additional constraint of this technique relies of its inability to reproduce – *extrapolate to* – events beyond the range of the observed data.

3.1.3 Hydrometeorological process generator

The proposed *hydrometeorological process generator*, that will be employed in chapters 5, 6, and 7**,** is based on the stochastic theory, and especially on the linear models, thus providing the ability to account for the uncertainty in modelling natural processes. The crucial driver of the water-energy nexus, related to hydrometeorological processes, is rainfall. In this respect, the description of this generator is dedicated to the rainfall process, but could be applicable to other climatic processes, under a proper configuration.

3.1.3.1 Setting the specifications

As already mentioned, precipitation (more precisely, the areal precipitation over the upstream watershed), as a hydrometeorological process, is characterized by a) long-range dependence in the annual and over-annual scales, also referred to as persistence or Hurst-Kolmogorov dynamics (Koutsoyiannis, 2011), which is more intense in the areal scale with respect to the point one (O'Connell et al., 2023) b) seasonality, and c) intermittency, at the simulation scale, i.e. daily. Thus, precipitation should be handled as a cyclostationary process with marginal distributions and auto-correlation patterns across scales that vary periodically, i.e., from month to month. In this respect, for the generation of synthetic precipitation time series, a *three-level simulation scheme* should be adopted to preserve the probabilistic and dependence properties not only at the time scale of simulation (daily) but also at higher ones (annual, monthly). Furthermore, this should reproduce the long-range dependence attributed to the changing climate.

3.1.3.2 Modelling procedure

The proposed generator is built upon the Symmetric Moving Average (nearly) To Anything (SMARTA) scheme by Tsoukalas et al. (2018), as implemented within the anySim package (Tsoukalas et al., 2020). This allows for simulating stationary processes that exhibit any-range dependence and arbitrary (more precisely, a priori specified by the modeler) marginal distributions. In addition, the Nataf-based Disaggregation to Anything (NDA) is adopted regarding a chain configuration for developing modular simulation schemes that ensure consistent simulations across any sequence of temporal scales (Tsoukalas et al., 2019). In this vein, we consider this process stationary at the annual scale and cyclostationary at the monthly and daily ones. At the annual scale, the generation procedure accounts for the historical data's marginal distribution and autocorrelation structure, also engaging the Hurst-Kolmogorov dynamics.

However, in this modelling procedure, we adopt the Koutsoyiannis's (2000a) approach, formalizing the auto-dependence in stationary means, by embedding an Cauchy-type autocovariance structure within the SMA generation scheme. The mathematical expression of autocovariance function is:

$$\gamma_j = \gamma_0[1 + \kappa\beta j]^{-1/\beta} \tag{3.12}$$

where γ_j is the autocovariance of the stochastic process for lag j, γ_0 is the variance and κ, β are shape and scale parameters, respectively, that are related to the persistence of the target process, $\underline{x}_t$. By adjusting the values of κ and β, one can take a wide range of autocovariance structures. For instance, for $\beta = 0$ we obtain ARMA-type structures, while as β increases, the process becomes more persistent. The relationship between the autocovariance and Hurst-Kolmogorov (HK) dynamics is given by:

$$\gamma_j = \gamma_0\{\frac{1}{2}[(\mathrm{j} - 1)^{2H} + (\mathrm{j} + 1)^{2H} + j^{2H}]\} \tag{3.13}$$

where H is the so-called Hurst coefficient $(0.5 \leq H \leq 1)$.

However, for large time steps this function is well approximated by:

$$\gamma_j = \gamma_0 (1 - \frac{1}{\beta})(1 - \frac{1}{2\beta}) j^{-1/\beta} \tag{3.14}$$

where $\beta = 1 \,/\, ([2(1 - H)]) \geq 1$.

In this respect, the analytical expression of κ follows:

$$\kappa = \kappa_0 := \frac{\kappa}{\beta\left[\left(1 - \frac{1}{\beta}\right)\left(1 - \frac{1}{2\beta}\right)\right]^{\beta}} \tag{3.15}$$

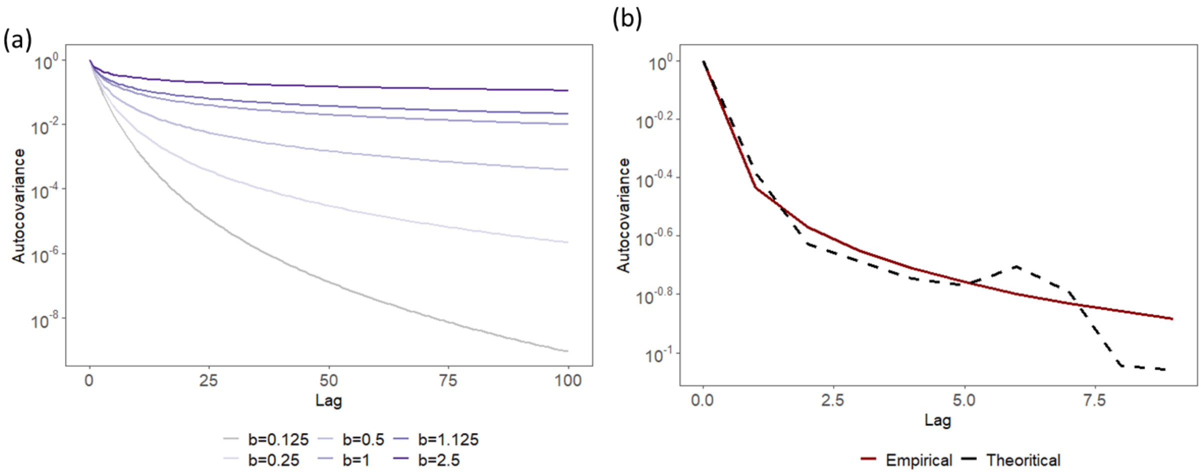


Figure 3.1: (a) Examples of autocovariance sequences of the type for several values of the shape parameter β , (b) Fitting of theoretical autocovariance function to empirical autocovariance, estimated on the basis of annual rainfall.

The obvious estimation of parameters κ and β relies upon adjusting the theoretical autocovariances to the empirical ones, as derived by the observed data. We underline that under the LTP hypothesis, the estimation of empirical autocovariances are subject to significant bias (Dimitriadis & Koutsoyiannis, 2015), while their uncertainty is further amplified when the historical data are not long enough. In this vein, it may be preferable to assign manual parameter values instead of inferring them automatically, i.e., through typical curve-fitting approaches (Efstratiadis et al., 2014). Another option is to force eq. (3.10) to validate the first-order autocovariance term, γ_1, as estimated from the historical data. In this respect, Figure 3.1 demonstrate several autocovariance functions, extracted by using different values of β but keeping the same κ for all cases. In addition, an example of fitting the theoretical autocovariance function to empirical autocovariance, estimated on the basis of annual rainfall in a Greek watershed (Mouzaki, Thessaly), which is next used as a pilot basin for the design of a small hydropower plant under uncertainty (section 5.3.2).

The process of annual rainfall is considered to be stationary and follows a specific cumulative distribution function (CDF), $F_{\underline{x}}$. The overall idea behind SMARTA lies in introducing an auxiliary Gaussian process z_t, simulated through the SMA model, with such parameters that after applying the inverse of their distribution function, results in the target process $\underline{x}_t$ with the desirable correlation structure and marginal distribution.

In this respect, according to the SMA rationale, the auxiliary stochastic process $\underline{z}_i$ is expressed as a weighted sum of a finite number of backward and forward random variables, i.e.:

$$\underline{z}_i = \sum_{j=-q}^{q} a_{|j|}\, \underline{v}_{i+j} = \sum_{j=-q}^{q} a_s \underline{v}_{i-s} + \cdots + a_1 \underline{v}_{i-1} + a_0 \underline{v}_i + a_1 \underline{v}_{i+1} + \cdots + a_s \underline{v}_{i+s} \quad (3.16)$$

where $\underline{v}_i$ are independent identically distributed auxiliary variables (also referred to as noise variables or innovations) that are generated from a Gaussian distribution, and a_j are numerical (i.e., weighting) coefficients that are assumed to be symmetric, and can be analytically determined from the sequence of γ_j. The values of a_j approach zero after some time lag $|j| > q$, where q denotes a large enough positive integer value (the model resembles the theoretical ACF up to q, while it decays to zero after $2q$ time lags). The reader is referred to Koutsoyiannis (2000a), for a detailed description of the algorithmic procedure.

Prior to the estimation of the auxiliary model's parameters (i.e., coefficients a_j), it is essential to identify the equivalent autocorrelations that result to the target ones (i.e., as specified via the theoretical autocovariance function), after the subsequent mapping of the Gaussian auxiliary process, $\underline{z}_i$, to the actual domain, $\underline{x}_t$. For this purpose, the anySim package employs a simple yet efficient Monte Carlo simulation approach, proposed by Tsoukalas et al. (2018b). As already mentioned, the above procedure is applicable to stationary processes that follow given CDFs. In Figure 3.2, an example of fitting for the same annual timeseries is given. As expected, this dataset is well defined by fitting Gamma distribution.

Next, the synthetic annual data is disaggregated by preserving the seasonally varying marginal distributions and the lag-1 month-to-month autocorrelation structures. For this advanced obligation, we are taking advantage of Stochastic Periodic AutoRegressive To Anything (SPARTA) (Tsoukalas, Efstratiadis, et al., 2018a), also included in the anySim package. This scheme is able to simulate cyclostationary processes, by defining the marginal distribution of each month and the establishing s dependence patterns across seasons. In brief, for each process at each season i, a suitable distribution function, $F_i(x)$, is assigned as well as the target coefficients of auto-correlation (month-to-month correlations), i.e., $\rho_{i,i-\tau}$. Also, the autocovariance function is given for each season, in order to preserve the dependence of each process, seasonally based. Next, the estimation of the parameters of the auxiliary PAR model is needed run the model, and eventually generate the auxiliary Gaussian synthetic time series. In Figure 3.3 a comparison of the simulated, as extracted from the disaggregation through SPARTA scheme, and the theoretical cumulative distribution functions of the rainfall process, for each season is demonstrated.

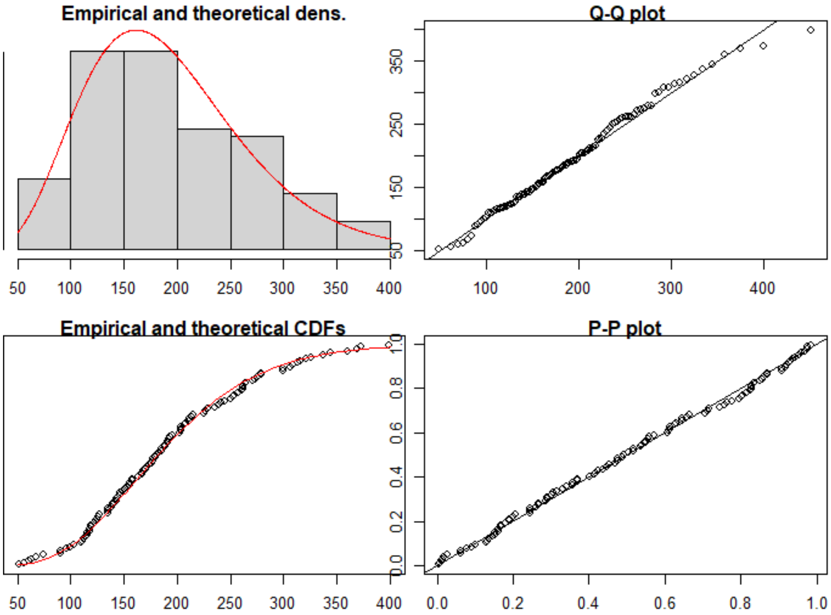


Figure 3.2: Fitting of Gamma distribution function to the historical annual rainfall.

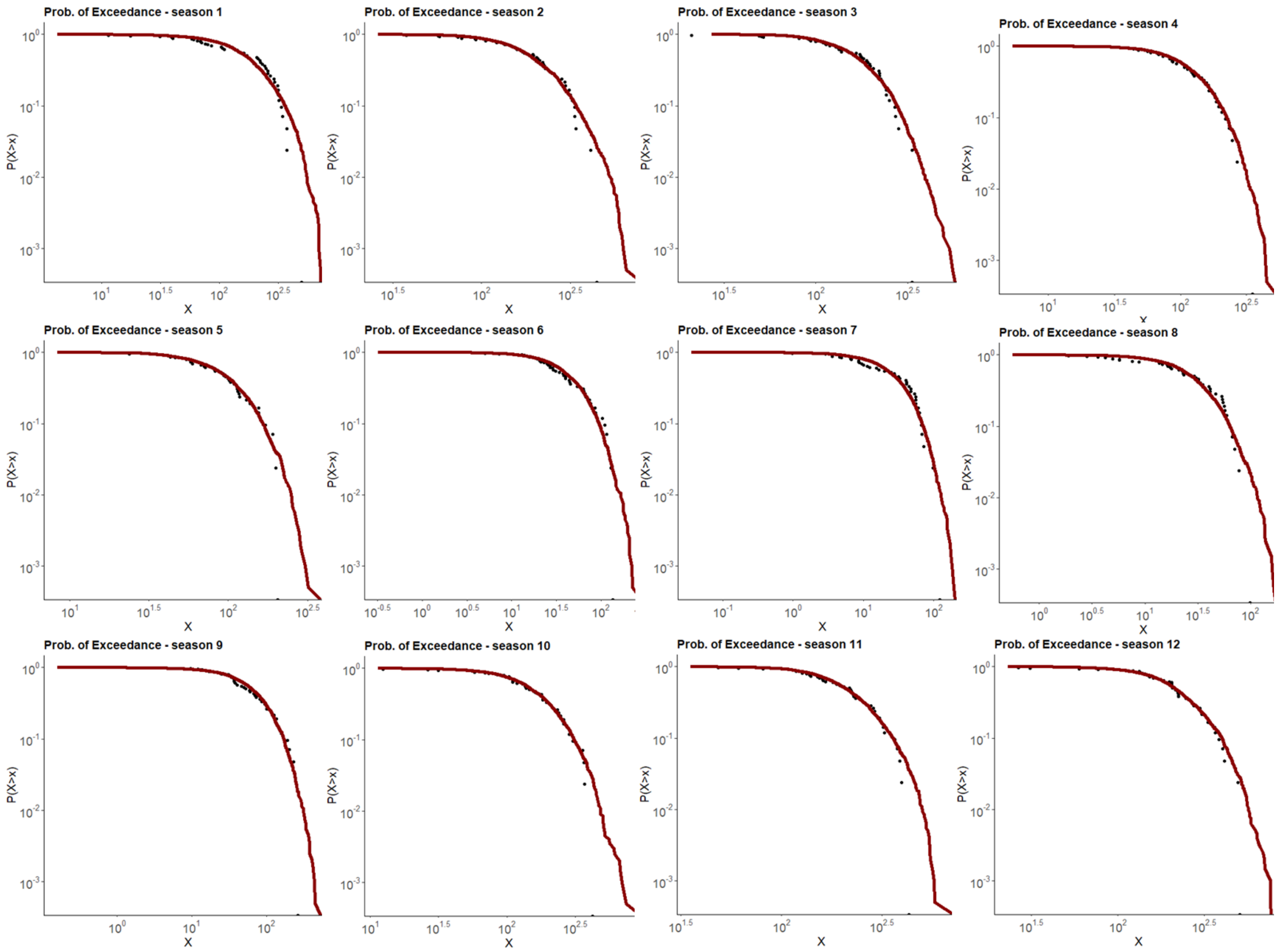


Figure 3.3: Comparison between simulated (SPARTA) and theoretical cumulative distribution functions of the rainfall process.

Finally, at the daily scale, the synthetic monthly values are disaggregated, which, in turn, also accounts for the distribution functions, $F_d(x)$, and the target autocorrelation structures, ρ_d, of the observed daily data for each month. In this case, this process is considered as stationary, thus employing the disaggregation scheme of SMARTA. However, at the daily scale an additional feature is needed, namely the probability dry, $p_d = P(\underline{x} \leq x_d)$. Thus, the distribution followed is zero-inflated, and given by

$$F(x) = \begin{cases} p_d \;\; x \leq 0 \\ p_d + (1 - p_d)G(x) \;\; x > 0 \end{cases} \tag{3.17}$$

where, $G(x)$ is the following distribution for $\underline{x} > x_d$. In Figure 3.4 a snapshot of the historical and the synthetic timeseries is demonstrated.

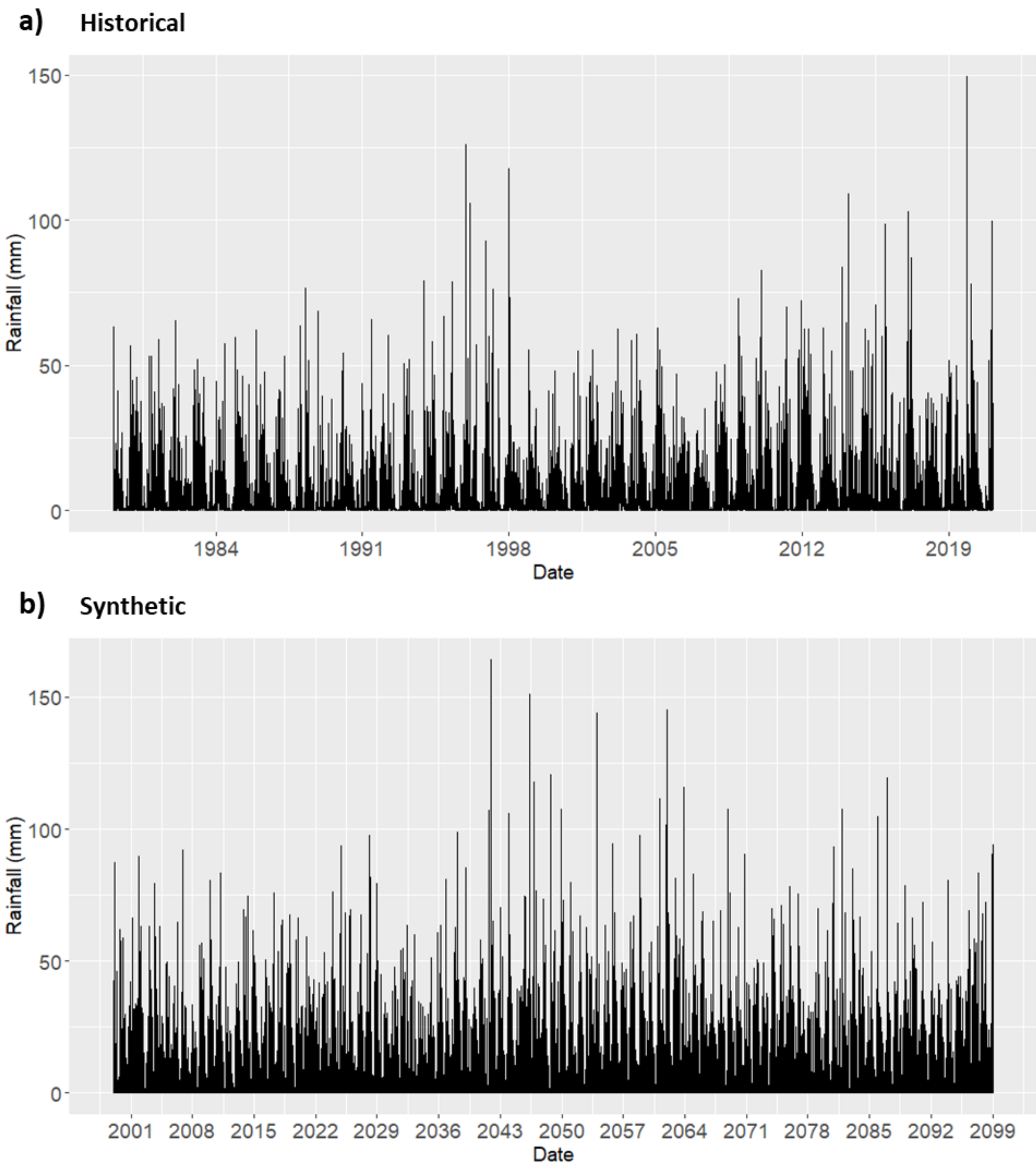


Figure 3.4: a) Historical time series. B) Synthetic time series; randomly selected window of 100 years.

3.2 Social uncertainty

3.2.1 Definitions and specifications

So far, in water-energy systems modelling, the main focus is given to the representation of natural processes (e.g., hydrometeorological) and their conversions across technical infrastructures (e.g., reservoirs, water conveyance and distribution networks, pumping stations, etc.). In contrast, the social factor is only marginally reflected (Di Baldassarre et al., 2019; Elshafei et al., 2014), by means of steady-state water and energy demands that are a priori specified, and thus they cannot be adapted to major social procedures (e.g., legal regulations, management policies, market rules, media, social networks).

In this respect, the establishment of a comprehensive context of the human agency within the water-energy nexus, under inherently varying environmental and socioeconomic drivers, will also include disruptive and unpredictable events. In this vein, a well-established research must focus on the effects of crucial, urgent and abnormal circumstances, which may affect both the micro- and macro-behaviour of an entire society over the longer term. These may include geopolitical shifts, economic crises and extreme hydroclimatic conditions (e.g., persistent droughts), causing long-term water and/or energy shortages, which are in turn reflected to the associated demands, prices and operation policies. We highlight that in common approaches for water and energy (particularly, *renewable energy*) resources modelling, these elements are handled under the steady-state hypothesis. For instance, the demands are expressed as known inputs, which follow *a priori* specified seasonal patterns, while in fact they are strongly depended on the social actions and reactions against the system's state and its various aspects of change (e.g., changes in water bills that may reduce consumption). A similar approach is adopted, regarding the policy making across water-energy systems for long-term management and real-time operation.

However, this steady-state approach, that ignores the social dynamics, by means of decision making, is rather than an obsolete handling. In general, there are two schools of theory for decision making, namely the descriptive decision and the normative one. The first one is concerned with characterizing and explaining regularities in the choices that people are disposed to make, while the latter seeks to provide an account of the choices that people ought to be disposed to make (Kacelnik, 2007; Rapoport, 1994). Nevertheless, all human-induced procedures and decisions are relied on specified behavioural rules that are affected by influences. Koop et al. (2019) distinguished behaviour influencing tactics into three categories, i.e., reflective, semi-reflective and automatic. In the first category, the human attitudes are formed by considering rational arguments, relevant experiences, and knowledge (knowledge transfer and self-efficacy), while in the semi-reflective category the formulation of attitudes focuses on rules of thumb and simple heuristics (social norms, data-driven personal messages etc.). On the other hand, the automatic behaviour influencing tactics are based on emotional shortcuts, priming, and nudging. Nevertheless, the behavioural sculpture also relies on the social network of each human. Hence, the modelling of social networks is a challenging task, since they are highly complex systems because of their size, the interactions among their components (human beings), as well as the interdependency between the individual behaviour and the evolving network structure (Pagan & Dörfler, 2019).

Following the ongoing paradigm shift, regarding the coupling of natural and human systems, it is vital to represent the social dynamics, demand-related and policy, by reflecting the associated uncertainties. Based on the research of Sharmina et al. (2019), four attributes of socio-natural systems have been identified, i.e., '*stochastic events*', '*diversity of behaviour'*, '*policy interventions'* and '*co-evolution'*. The first three attributes are in fact the input variables for models, while '*co-evolution*' covers the interactions between the variables ensuring that those relationships are not simplified to the extent where the reality is compromised. In this respect, Table 1 provides an overview of the sources of uncertainty encapsulated in each of the four attributes, along with illustrative variables that may be useful in investigating water and energy demand in the context of *non-linearity*.

Table 1: The four attributes of socio-natural systems, based on Sharmina et al. (2019).

Attribute	*Sources of uncertainty captured*	*Examples of variables to be represented in models*
Stochastic process	Unpredictability, randomness, “black swan” events	Stochastic representation of hydrometeorological processes, technological breakthroughs, population growth, financial and geopolitical crises.
Diversity of behavior	Human behavior (from individual behavior to behavioral patterns and practices at a society level	Social networks exerting group/peer pressure; attitudes towards energy and water conservation, consumer classifications, diffusion of information, social and cultural norms.
Policy interventions	Planned or not ‘shocks’ with unpredictable, particularly unintended, consequences.	Standards for fuel and water efficiency, a feed-in tariff, a carbon tax, changes in levels of service provision.
Co-evolutions	Interactions and feedback loops, path dependency, emergence, temporal scales, non-linear developments	Key relationships and interactions between the variables specified within the other three attributes.

3.2.2 Treatment of uncertainty in common modelling approaches

The incorporation of the extremely complex and uncertain social factor within the technical (i.e., water- energy) system is inherently a highly challenging task, with numerous issues to address. In the literature, the human behavioural models originate from psychology (particularly social psychology) and sociology, but they are broadly used in other sciences (i.e., economic, political, statistics etc.). Pentland and Liu (1999) revealed the capacity of system dynamic models (SDM), in order to model and eventually, predict the aggregated human behaviour. Other popular modelling attempts to describe the human factor and its interactions with the water-energy systems are agent-based modelling approaches (ABM). Both approaches are the two most popular mathematical modelling methods for evaluating complex systems; while SDM are used to study macro-level system behaviour such as the movement of resources or quantities in a system over time, ABM capture micro-level system behaviour, such as human decision-making and heterogeneous interactions between humans. An alternative approach for identifying and interpreting stakeholder behaviours, in order to handle conflict resolutions within water management, is game theory (Madani, 2010). However, to overcome the limitations of system dynamics and game theory of representing the inter-connections between humans statistical models, by means of random graphs, are used (Newman et al., 2002). In this thesis, the emphasis is given to system dynamics and agent-based models, and thus the following paragraphs are dedicated to these two approaches.

3.2.2.1 Agent-based modelling

Currently, agent-based models are recognized as the state-of-the-art approach for representing the human behaviour in a wide range of applications, i.e., health systems, engineering, ecological etc. Their history begins from the early 70's, when Thomas Schelling discussed the basic concept of agent-based models as autonomous agents interacting in a shared environment with an observed aggregate, emergent outcome. In 90's this conceptualization is employed, while the current definitions of "agents" are based on the research of Holand and Miller (1991) that concerns the economic theory. In the terms of Farmer and Foley (2009), "*An agent-based model is a computerized simulation of a number of decision-makers (agents) and institutions, which interact through prescribed rules*". Decades later, the conceptualisation, architecture and implementation is still evergreen, while the applications are uncountable. Several major advantages credited to ABM have made it powerful in modelling of coupled human and natural systems. Specifically, ABM has the ability to model individual decision making, while accounting for heterogeneities, interactions, and feedbacks. In addition, ABM is able to merge institutional aspects, behavioural structure and norms with natural processes (Hare & Deadman, 2004). Finally, it offers a spatial ability, making it possible to "[put] people into place (local social and spatial context)" (Entwisle, 2007). However, the coupling of natural and human system requires the ability to merge two conceptually different approaches, i.e., bottom-up, ABM, and top-down.

In addition and besides the wide use of ABM there are still many open methodological issues to address and questions about their operational use (Berglund, 2015; Polhill et al., 2019). As pointed by Magliocca (2020), most of modelling approaches do not contain agent interactions or do not base agent decision-making on existing behavioural theories. Focusing on the water-energy nexus and the modelling of human factor, by means of demands and policy making, several efforts have been made to address and eliminate these issues. For instance, Zhu et al. (2023) explore and simulate the complex dynamic interactions in the supply and demand process of water-energy- food nexus sectors. In addition, Guo et al. (2022) model through agent-based models the agricultural water-saving compensation policy, responding to anthropogenic and environmental interventions.

From the consumption perspective, in order to simulate human consumers as agents, ABMs, which are in fact inspired by the game theory and build upon the aforementioned social network context, use relatively simple rules to represent behaviors, social connections, and reactions of a population (Kaiser et al., 2020; Yuan et al., 2014), as well as interactions among the end-users and the water or energy utility. In the field of water resources, their use is mainly restricted to explain water consumptions, urban (Blöschl et al., 2019; Darbandsari et al., 2017; Koutiva & Makropoulos, 2019) and agricultural (Huber et al., 2022; e.g., Marvuglia et al., 2022), which is an important, yet not the sole anthropogenic footprint across the water cycle. On the other hand, regarding the practical use of ABM's in energy systems, Yazdanie and Orehounig (2021) highlight the need for improving uncertainty analyses against human-induced factors, such as socio-economic and technological development, population changes, future costs and policies, and sudden large-scale changes, also referred to as "black-swan" events.

From the policy-making point of view, a rigorous policy analysis requires some means to define and identify the most important scenarios. For our good fortune, agent-based models are suitable for enabling decision-making in an uncertain world. Specifically, these simulation methods explicitly consider policy decisions as a dynamic response, adaptive over time to new information, rather than any fixed set of actions. In this respect, Carley's (2002) agent-based simulators relate the overall behavior of organizations to data on the knowledge, capabilities, tasks, procedures, and networks of communication for the agents of which they consist.

Recently, focusing on the water-energy-food nexus, Mirzaei et al. (2023) coupled two different groups of stakeholders, i.e., farmers and government to describe their cooperation and the social pressure, extracting the policies options that optimize the coupled (technical and social) system. Generally, ABM is the best-compromise approach for modelling heterogeneity in individual attributes and in the network of interactions among population elements. However, this has a cost; this means that requires more data at the level of individuals, which in turn lead to a slower modelling process, higher computational costs, and more difficult calibration in the AB modelling, compared to other approaches.

3.2.2.2 System dynamics

‘’*The human mind is not adapted to interpreting how social systems behave. Social systems belong to the class called multi-loop nonlinear feedback systems*”. In the mid-1950s, Jay W. Forrester inspired from the human nature and based on this declaration, created the concept of system dynamics. The main idea based on the fact that people would never send a space ship to the moon without first testing prototype models and making computer simulations of anticipated trajectories. Even if such models and tests do not guarantee the possibility of no failure, they do identify many weaknesses which can be corrected before they cause large-scale catastrophes. In this respect, system dynamics are built upon the idea and represent various of systems, including, the feedback loops of human and natural systems. The core concepts of the system thinking, such as interconnectedness, feedbacks, adaptive capacity/resilience, self-organization, and emergence (Williams et al., 2017) are addressed in that modelling approach, helping people making the best-compromise decisions.

From the modelling perspective, there are two types of diagrams that fulfil the “bathtub” of the system dynamics, namely causal loop and stock-flow. Causal-loop diagrams are, generally, employed for qualitative modelling, while stock-and-flow diagrams are applied in quantitative modelling, leading to the development of models that can be consequently simulated and analysed. In Figure 3.5**,** two simple examples of these two components are demonstrated, regarding the water demands.

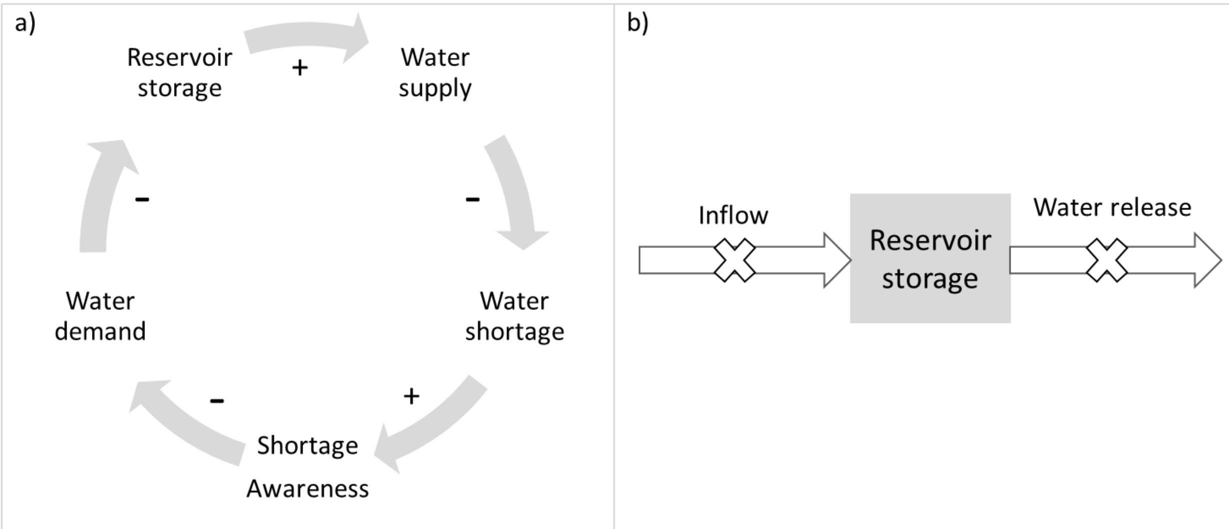


Figure 3.5: a) Causal-loop diagram for water demand. b) Stock-flow diagram for a simple operation of a water reservoir.

The system dynamics has been widely used to analyze the WEF nexus worldwide at different spatial scales, such as global (Sušnik, 2018), national (Linderhof et al., 2020) and basin scales (Ravar et al., 2020). Also, its application has been widely used for describing the social factor across the water-energy nexus (Guemouria et al., 2023; Keyhanpour et al., 2021; Phan et al., 2021). In addition, Zeng et al. (2022) researched the human sensitivity indicated by environmental awareness, that can adjust the co-evolution behaviours of the WEFS nexus through feedback loops. In this scene, Giuliani et al. (2016) developed a coupled human natural model, investigating the adaptation of agricultural users against the climate change scenarios and different policy options.

However, system dynamics are more suitable to closed than to open systems, originating from their conceptual architecture. In this respect, this modelling approach tailored for social components appears to have limitations, regarding the external influences, outside of the system. Another crucial disadvantage relies on its lack of ability to offer "*grey*" options. Specifically, since the "decisions" are described from pure mathematical expressions, these cannot be influenced from game theory, strategic rules and behavioural adaptation, thus leading to "white" or "black decisions", i.e., outputs.

3.2.3 Human factor model

3.2.3.1 Concept

The proposed human-oriented simulator is called to represent the human behaviour within sociotechnical systems, by accounting for decision, choice and action theories and by representing at least all major intra- and inter-sector interactions. Due to the explicitly stochastic nature of ABM, this simulator is built upon this approach. In particular, it allows for representing memory effects, spatial heterogeneity and mobility, and interactions among population elements.

As already mentioned, the agent-based approach follows by definition a bottom-up perspective, thus a fundamental challenge is ensuring a satisfactory equilibrium between accuracy and computational effectiveness. The first requirement presupposes a representative classification of the society's components (agents) and a realistic mathematical description of their behavioural rules, which in turn may result to an over-detailed model. On the other hand, this not impose formidable barriers to the overall computational procedure, which also includes a time-demanding simulation model of the technical system. Another crucial point is the derivation of a stable and self-adaptive society, after upscaling the individual social components, which are (and should be) biased.

All above requirements and specifications are addressed within the proposed model. This ABM is tailored for producing dynamic water and energy demands, by simulating the consumers behaviour. This simulation requires the exploration two key aspects in integrating individual water/energy users into management: (a) accurately foreseeing household demand behaviour, (b) assessing how this behaviour is impacted by water and energy management interventions and strategies such as awareness campaigns and price regulations and c) describing the social network of each user. To address them, we are taking advantage of theories from social psychology to simulate the consumption behaviour of urban households, drawing on concepts like the influence of social norms and the relationship between attitudes, intentions, and actual behaviours. By employing methodologies rooted in theories like Social Impact Theory (Latané, 1981), we aim to understand how attitudes towards water conservation can shift, particularly influenced by early adopters of conservation behaviours whose attitudes deviate from the social norm.

We argue that the incorporation of the complicated and unpredictable social factor within technical systems is inherently a demanding task, with numerous issues to address. In particular, in large cities the society of is highly disparate and extended, thus a parsimonious yet representative classification of its components is critical. As shown in Figure 3.6, this should allow for linking several user profiles with consumption habits, awareness of saving, adaption to changes, willingness to adopt green economy policies, and tendency to follow others.

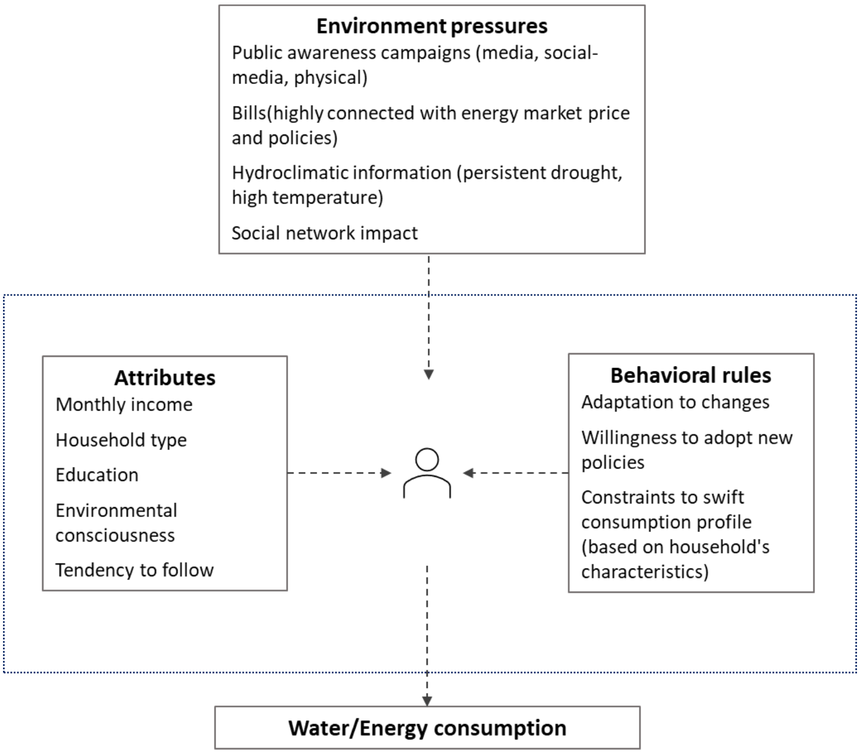


Figure 3.6: Outline of agent's behaviour with respect to external pressures and reactions against water and energy consumption.

3.2.3.2 Model architecture

To unwrap the complexity of this modelling approach, the ODD protocol (Grimm et al., 2020) is followed, to describe the ABM:

- Emergence: Herein, emergence refers to how the individual behaviors of household agents collectively shape the overall behavior of the community, which is then translated into water demand through a water-energy system simulation.
- Adaptation: Household agents adapt their behavior firstly by changing their attitude on water conservation due to the social impact exerted on them (e.g., tendency to follow others), by means of network and public awareness campaigns (agent-environment). Then, household agents review their decision regarding water demand behavior based on a) the structure of their behavior (e.g., willingness to adapt) and b) the water bills.
- Fitness: At an individual agent level, households measure the fitness of their decision by assessing their goal of reducing their water bills. Global "fitness" is measured after aggregating the decisions and result to the monthly domestic water demand.
- Prediction: Household agents anticipate the reduction of their water bill, and keep memory of previous mechanisms/decisions.

- Interaction: Household agents interact with each other forming social networks and influencing each other's water conservation attitude. In particular, the agents interact with their social network (agent-agent) and are affected by policy measures.
- Stochasticity: All households are spatially distributed in the urban boundary (which is configured as a grid), and they can move by following a random uniform distribution in order to interact with their immediate neighbors and influence each other''s water consumption attitude.

Entities and state variables

Each household agent consists of three essential parts, i.e., attributes, behavioral rules, and memory, which vary across households in the initial set up of the model, and they change during the simulation, due to both external and internal influences. In the model, we consider two entities, i.e., the *Households* and the *Water/Energy Saving Campaigns*, the interactions of which are assumed independent, while their further taxonomy is described below.

In particular, the Households are classified into categories according to their income (Hussien et al., 2016) and their environmental consciousness, in order to describe the range of their water and energy consumption. The consciousness is further distinguished into three sub-categories, namely low, moderate, high. Thus, their behavior/adaptation is depended on all these characteristics and their tendency to be influenced by their social network.

The *Water/Energy Saving Campaigns* are also distinguished in into a number of categories, according to their type, namely physical, media and social media based. The physical campaigns reflect the messages on newspaper, leaflets, workshops in schools, universities, jobs etc. On the other hand, media and social media campaigns represent the messages on TV and the Internet, and on the platforms of social media (Borawska, 2017). In general, a predefined distribution is made but in abnormal conditions (e.g., low water availability) the campaigns are potently activated.

Process overview

The modelling of urban consumers is based on the simultaneous interaction between the Households and their external influences. The latter originate from the household's environment and include the water/energy bills and water/energy saving campaigns. At each computational step (month), the moving agents (Households and Water/Energy Saving Campaigns) take a random step within the feasible model space, while the household agent receives the bills and compares the current bill with the previous one and decides to change its water and energy demand behavior state or not. On top of this, if the household meets a campaign, it decides to adopt saving water/energy policies or to stay stable even in extreme conditions (e.g., persistent droughts, highly electricity prices). This decision is based on the agent's characteristics, regarding its environmental consciousness and the intensity of the campaign.

At the end, the individual consumption values by all households are aggregated to represent the performance of water and energy usage at the macro level. The aggregated consumption is used as input to the water-energy system (now expressed in terms of demand) and the water-energy fluxes and associated costs are recalculated, by considering all inputs as dynamic variables. More details of model coupling, assumptions and results are given in section 6.5.3, in which the proposed ABM is adapted to represent water demands.

3.3 Energy market uncertainty

3.3.1 Europe’s Energy History: A Complicated Tale

Since 1973, when the first oil price shocks occurred, these have led to recession for many economies and hampered their growth. In this respect, policy makers have been incited to explore alternative energy sources, to address the increasing environmental consequences and to protect their economies from violent changes. Energy-related steps are taken by the Maastricht Treaty (1992) and the Single European Act (1986), which acknowledge the Community's relevant jurisdiction. In particular, the Single European Act (SEA) was signed with the goal of establishing a single market by tearing down the obstacles preventing the free flow of capital, people, products, and services. The energy sector started to liberalize with the introduction of market prices, division of energy production, transportation, and distribution activities, and rivalry among operators that eventually became Trans European. Nonetheless, each Member State continued to be in charge of choosing its own energy mix.

In 2008, an "energy-climate package" was adopted by European leaders. Specifically, they established a goal for 2020, and the committee chose to translate it into a formula—the 3 times 20, or 3x20 network—in honour of the collective agreement. The requirement for Member States to cut greenhouse gas emissions by 20%, enhance by 20% and raise the proportion of renewable energy sources to 20% of total energy used. Because of its varying degrees of accomplishment, the European Union modified the three 2030 objectives in 2014. Following to these measure, the European Union conducted the so-called “Green Deal”, which aims to eliminate net greenhouse gas emissions by 2050. According to this, by 2030, the states must have decreased by a minimum of 55% when compared to 1990 values, leading to "carbon neutrality" or "climate neutrality". The plan primarily centred on the phase-out of fossil fuels, electric vehicles, technology advancements, circular economy principles, building retrofitting, and sustainable agriculture. However, the European Union was compelled to reconsider its position on "energy sovereignty," or the necessity of not relying too much on foreign sources for its energy supplies, after Russia invaded Ukraine in February 2022. In this vein, the European Community launched the REPowerEU plan that is based on three blocks, i.e., saving energy, diversifying supplies and supporting our international partners, accelerating the rollout of renewables.

Therefore, this integrated European energy market is expected to offer a more economically efficient and competitive electricity system, that will increase the liquidity and social welfare, simultaneously enhancing the security of supply and cross-border trade. To the road of European energy integration and liberalization, a set of rules and policies are developed to the individual energy markets of all member states, thus introducing the Target Model. This comprises four markets, i.e., day-ahead, intraday, forward, and balancing. The member states participate in the Target Model in a single coupling mode, at day ahead market level, auctions are held, whereas at intra-day market level continuous trading takes place. All participant’s orders are collected and allocated at a pan European level, constrained by the inter-zonal capacity for different bidding areas. Currently, this model is adopted by twenty-six European countries (Austria, Belgium, Czech Republic, Croatia, Denmark, Estonia, Finland, France, Germany, Hungary, Italy, Ireland, Latvia, Lithuania, Luxembourg, the Netherlands, Norway, Poland, Portugal, Romania, Slovakia, Slovenia, Spain, Sweden, Greece, and Bulgaria).

3.3.2 Treatment of uncertainty in common modelling approaches

The energy market, which is a major driver of the water-energy systems, as it is operating, has a short history but the fluctuations of the last years, due to the energy crisis, have many effects. In this vein, Bohi (1991) studied the macroeconomic effects of the energy price shock in the 1970s and concluded that in a dataset of four countries there was no correlation between the price shock and the operation of industry. On the contrary, Van de Ven (2017) concluded that the impacts of the energy shocks are correlated with the economic development and the associated circumstances, considering that the economies are dependent on a single source. In the scene, the future of this energy crisis is unclear. Some economists predict that reshoring will slow the global energy transition as markets fragment (Goldthau & Tagliapietra, 2022), while some researchers disagree. Nevertheless, the initial goal of European Commission to increase the social welfare of this transition is stress-tested from the recent energy crisis that began in the aftermath of COVID-19 pandemic and escalated due to the Russian invasion in Ukraine (Ozili & Ozen, 2023; Shaikh, 2022). An important lesson of this situation was that the energy transition process rendered the whole energy market vulnerable to rising prices and uncertainty of the power supply. In this respect, the configuration and description of uncertainty in the energy market is crucial for decision-making in investing and policy design in regional and local scale (Fuss et al., 2008; Venetsanos et al., 2002). Besides the black-swan events and abnormal situations in a global scale, e.g., pandemics, the energy market's uncertainty with respect to electricity prices originates from swifts to policies, geopolitical changes, development of new infrastructures and governments' decisions. In this respect, Nikkinen and Rothovius (2019) decomposed the uncertainties in the energy sector, concluded that the two main drivers are the crude oil and the stock market uncertainty. In addition, Haugen et al. (2023) focused on the European energy transition, that regards to a renewable-based system and the associated effects in the operation and the forecast of electricity prices.

From a modelling perspective, different approaches have been adopted to represent the various sources of uncertainty across the energy market and its components. For instance, the fundamental models that are physical-based and consider the technical characteristics of the electricity sector, i.e., capacities and constraints in the transmission systems are popular (Bello et al., 2016; Kallabis et al., 2016). On the other hand, more theoretical models that originate from statistics and stochastics are applied to simulate and forecast the electricity prices (Borovkova & Schmeck, 2017; Higgs & Worthington, 2008; Hou et al., 2017; Möst & Keles, 2010; Shenoy & Gorinevsky, 2016). In addition, the agent-based simulation models (ABMs) have experienced an increasing popularity amongst electricity market modelers, since the key characteristics of a market-based sector, i.e., learning properties, asymmetric information and imperfect competition can be represented (Weidlich & Veit, 2008). For instance, Fraunholz et al. (2021) took advantage of ABMs to forecast electricity prices, while Kell et al. (2020) simulated in the long-run the transition from coal to gas that was observed in the UK between 2013 and 2018. Furthermore, financial tools and econometric models to model the price paths correlated with explanatory variables (e.g., temperature, time, contracts etc.) are used (Kremer et al., 2021; Narajewski & Ziel, 2020). Another kind of tools originates from game theory and are used to model the equilibrium of market in competitive electricity markets (Abapour et al., 2020; Hobbs & Kelly, 1992; Khalid et al., 2019).

Apart from individual models, recent efforts in this field have provided combined approaches to simulate the variability of electricity prices across scales. In this respect, Torralba-Díaz et al. (2020) coupled a fundamental electricity market model with agent-based simulation to highlight the resulting inefficiency and increasing prices, due to renewable sharing and poor information. In addition, he fundamentals models have been hybridized with economic and business models in order to forecast the electricity prices at the short-term scale (Lu et al., 2020; de Marcos et al., 2019).

We argue that all these approaches and techniques underlie the need of decision support tools, in the field of newly introduced liberalized energy markets, that account for the uncertain aspects that shape electricity prices. Undoubtedly, an uncertainty-aware representation of the electricity price as a random process is subject to several challenges, including its double periodicity, induced by seasonality (monthly scale) and the intraday cycle (hourly scale), as well as the detection of spikes, as an after effect of the already mentioned pandemic and the energy crisis. In addition, the problem is further complicated, due to the limited statistical information of historical data under the current energy market structure.

3.3.3 Electricity price generator

The proposed electricity price generator is built upon the idea of the hydrometeorological process generator, as described in 3.1.3. In contrast to the climate-oriented generator, the electricity price one follows a two-level simulation scheme to preserve the probabilistic properties at the daily and hourly timescales. The electricity price process is also characterized by a) long-range dependence in the daily scale, b) double seasonality (month to month, hour to hour), and c) existence of negative values (occasionally). In this respect, the proposed generator is adjusted to describe different states of the energy market system, to capture the usual fluctuations across days and seasons, as well as long-term spikes, by means of shifts, trends and persistent periods of high and low electricity prices (Gudkov & Ignatieva, 2021).

3.3.3.1 Modelling procedure

As before, the proposed generator is built upon the Symmetric Moving Average To Anything (SMARTA) scheme by Tsoukalas et al. (2018) that couples three major modelling elements: (a) the theoretical autocorrelation function (ACF), introduced by Koutsoyiannis (2000a), to reproduce a given autocorrelation structure, (b) the Symmetric Moving Average (SMA) generation procedure, as formalized by Koutsoyiannis (2000a) in order to be aligned with the ACF, and (c) the Nataf's joint distribution model (Nataf, 1962).

Let $\underline{x}_t$ be a discrete-time stochastic process to simulate (in our case, daily electricity prices), for which we aim to provide a synthetic time series of a large (theoretically infinite) length. The process is considered to be stationary and follows a specific cumulative distribution function (CDF), $F_{\underline{x}}$. The overall idea behind SMARTA lies in introducing an auxiliary Gaussian process z_t, simulated through the SMA model, with such parameters that after applying the inverse of their distribution function, results in the target process $\underline{x}_t$ with the desirable correlation structure and marginal distribution.

Key requirement of the generation procedure is the reproduction of long-term changes within synthetic electricity price data, in order to represent abnormal spikes and volatilities of the energy market, as the ones observed during the running energy crisis. This feature is demonstrated, by embedding the Cauchy-type autocovariance structure within the SMA generation scheme, following the eq. 3.12. In that case, the ACF remains high for many lags. An example of this fitting is demonstrated in Figure 3.7, that represents the empirical autocorrelation for the daily electricity price dataset of France. Next, according to the SMA rationale, the auxiliary stochastic process $\underline{z}_i$ is expressed as a weighted sum of a finite number of backward and forward random variables, as expressed in eq. 3.16.

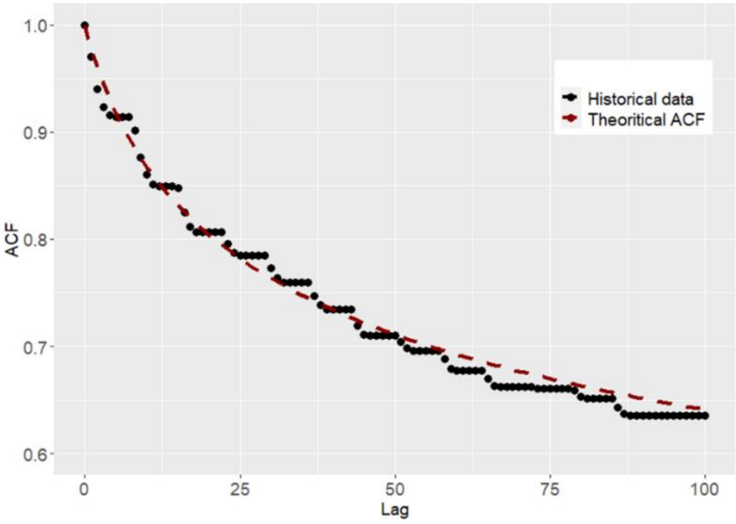


Figure 3.7: Fitting of theoretical autocovariance function to empirical autocovariances, estimated on the basis of daily electricity prices of France.

As already mentioned, the above procedure is applicable to stationary processes that follow given CDFs. Actually, electricity prices are significantly affected by seasonality effects, which is in contrast to the stationarity hypothesis. To remedy this inconsistency, we apply a standardization approach to the original data, in order to remove the monthly seasonality. In this vein, the daily data are grouped by month and they are transformed as follows:

$$x_t^* = \frac{x_t - \mu_m}{\sigma_m} \tag{3.18}$$

where μ_m and σ_m are the mean value and standard deviation of month m. After running SMARTA, we apply the inverse procedure to the simulated price data, in order to obtain the final synthetic time series.

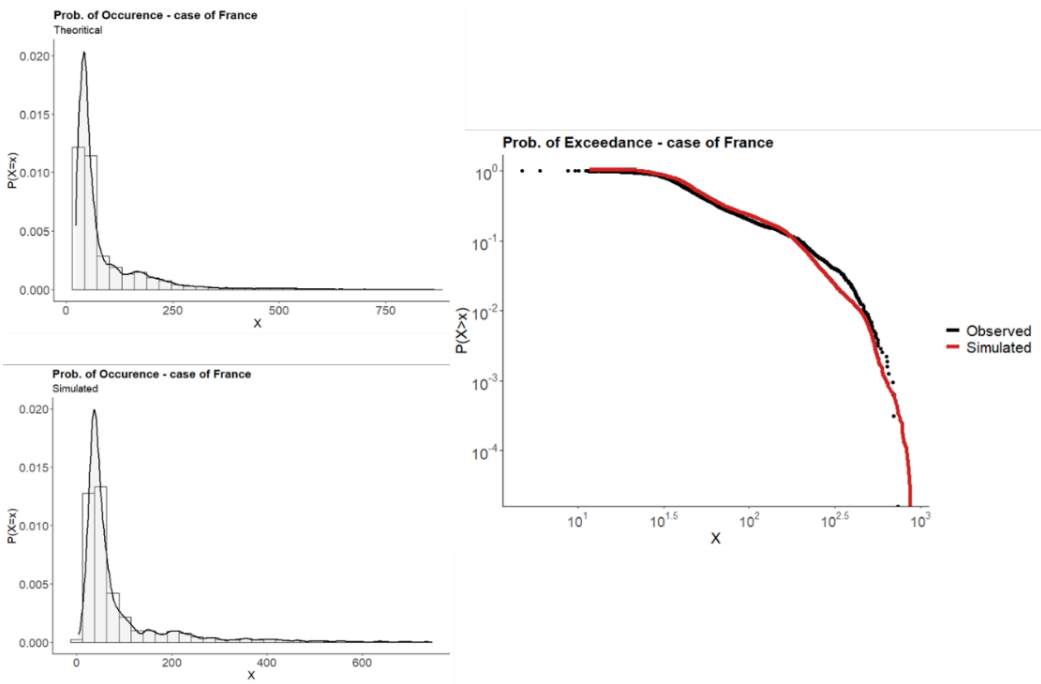


Figure 3.8: Fitting of three-parameter Gamma distribution function to the historical and simulated electricity price data of France.

To summarize, from the modeler's perspective, the essential tasks include the standardization of historical data and the assignment of the target autocovariance function, as well as the target CDF. An example of CDF fitting is given in Figure 3.8.

Next, the synthetic daily data is disaggregated by preserving the seasonally varying marginal distributions and the lag-1 hour-to-hour autocorrelation structures. To simulate a cyclostationary process, we are taking advantage of Stochastic Periodic AutoRegressive To Anything (SPARTA) (Tsoukalas et al., 2018a). This scheme is able to simulate such processes, by defining the marginal distribution of each hour and establishing the dependence patterns across seasons (hours). In this research, daily electricity price timeseries will be used for the water-energy systems, since finer scales cannot be applicable in the long-term management and assessment. An application of this framework is presented in **Chapter 4.**

3.4 Epistemic (endogenous) uncertainty

3.4.1 Definitions and modelling approaches

Besides the inherent uncertainty of the natural systems, further complexity is established by using models to describe their mechanisms. The models transfer their errors and assumptions, thus introducing the epistemic uncertainty that spans from the field observations to the conceptualization of processes and the parameter estimation strategy. This may be done on the basis of expert judgement, while in the case of observed response data the common approach relies on model fitting techniques, also referred to as calibration (or training, for data-driven models).

Epistemic uncertainty has been researched in numerous scientific disciplines (Sankararaman & Mahadevan, 2011), i.e., hydrology (Efstratiadis et al., 2015; Merz & Thieken, 2005), medicine (Tonelli & Upshur, 2019), energy (Clavreul et al., 2013; Sakki et al., 2022), etc. In water resources modelling (including hydropower systems), this has been mainly described in terms of parameter uncertainty and less often in model structure (Benke et al., 2008; Jiang et al., 2018; Moges et al., 2020).

As summarized by Efstratiadis and Koutsoyiannis (2010), when the model parameters are inferred through calibration, the epistemic uncertainty is related to the following factors: (a) measurement errors; (b) use of over-parameterized model structures, whose complexity is inconsistent with the available information about the system behaviour; (c) inappropriate representation of the temporal and spatial variability of model inputs; (d) poor identification of initial and boundary conditions; (e) non-informativeness of calibration data with regard to the entire system regime; (f) use of statistically inconsistent fitting criteria within calibration (e.g. error metrics not accounting for heteroscedasticity); (g) weaknesses of nonlinear optimization algorithms on rough and high-dimensional response surfaces; and (h) inconsistent assumption of parameters constant in time whilst the environment is changing, e.g. due to urbanization, deforestation, stream lining and other human interventions. We have to come in terms that model uncertainty will always exist since, by definition, models are imprecise representations of the real world, even though some of the aforementioned components may reduce it.

Let consider a model of the following form:

$$\underline{y} = f\left(\underline{x}, \vec{\theta}\right) \tag{3.19}$$

where $\underline{x} \coloneqq \left[\underline{x}_1, \underline{x}_2, \dots, \underline{x}_m\right]$ is a set of external drivers and $\vec{\theta} \coloneqq [\theta_1, \theta_2, \dots, \theta_n]$ refers to a set of parameter of the model, and $\underline{y} \coloneqq \left[\underline{y_1}, \mathrm{y}, \dots, \underline{y_m}\right]$ corresponds to the model outputs that are approximations of the real system's responses. For instance, for a rainfall-runoff model $\underline{x}$ regards to rainfall and potential evapotranspiration processes, and $\underline{y}$ is the resulting runoff, while $\vec{\theta}$ comprises a set of parameter that depend on the modeler choice. Herein, we will focus on two kinds of epistemic uncertainty, i.e., the parameter estimation uncertainty and the model structural uncertainty. In particular, the first one refers to the inability to uniquely locate a 'true' parameter set based on the available information. On the other hand, the model structural uncertainty originates due to simplifications and/or inadequacies and/or ambiguity in the processes they describe. It is clear that the choice of parameter as well as the structure of the model is crucial to describe the associated uncertainty. If we consider that the structure of the model is chosen, the estimation of the parameters is made by a model fitting on observed data. This is made by employing optimization techniques based on performance criteria. Undoubtedly, the building models should be consistent, both in terms of structure and parameters, with the behaviour of the real system. However, the global optimal set of parameters does not often exist (Wagener & Gupta, 2005). The issue of multiple set of parameters was discussed by Beven & Binley (1992), introducing the term "equifinality" to underscore the existence of multiple "behavioural" parameter sets, which are all acceptable albeit not equivalent, on the basis of different conceptualizations, data and fitting criteria. Since now, many efforts have been made to explore the map of equifinal sets of parameter, even when assuming a specific structure and a single performance measure (Beven, 2019; Ford et al., 2017; Khatami et al., 2019).

It is clearly admitted that the poor parameter identifiability may result in considerable uncertainty in the model outcomes. In this vein, a variety of computational techniques is offered to deal with these limitations and eventually quantify the model predictive uncertainty, by seeking for promising pathways of its outputs on the basis of different parameter sets. A common uncertainty assessment procedure across the hydrological sciences has been proposed by the instigators of equifinality, Beven and Binley (1992), namely Generalized Likelihood Uncertainty Estimation (GLUE). This methodology estimates the overall predictive uncertainty of the model, ignoring the individual effects of the input, parameter and model structure components. To fill this limitation, other approaches attempt to handle them individually, by employing different techniques, e.g., simple uniform random sampling (Charron et al., 2010), Markov Chain Monte Carlo methods (Luengo et al., 2020), meta-Gaussian techniques (Montanari & Brath, 2004), sequential data assimilation (RUIZ et al., 2013), multi-model averaging methods (Arsenault et al., 2015) and joint schemes (Zhang et al., 2012).

The following sections provide three different approaches to incorporate the concept of epistemic uncertainty, with respect to available information. The first approach, as presented in section 3.4.1, deals with a priori quantification of parameter uncertainty, while the other two sections refer to a posteriori analyses of total model uncertainty under observed response data. In particular, section 3.4.2 discusses the use of a stochastic approach to generate synthetic model errors (where the errors originate from conventional calibration approaches). Lastly, the third approach regards to the calibration uncertainty *per se*, providing a two-step procedure to account for the associated data and the objective function.

3.4.1 Modelling parameter uncertainty

Let consider a model following the eq. 3.19, where the governing laws and thus the model structure are a priori known, but the real response of the system is undetermined. In this respect, this uncertainty can merely be translated by means of randomly varying model parameters. In order to represent the system's response under uncertainty, we can assign suitable distribution functions to the parameters, to preserve specific statistical characteristics (e.g., asymmetry) based on expert judgment. In this respect, we next run the model in a Monte-Carlo context, by sampling the parameter values from the corresponding distributions.

In our case studies, we mainly employ this approach to "fuel"-energy conversions, which are further developed in section 5.2.2.

3.4.2 Modelling parameter and structural uncertainty

In contrast with the previous approach, the existence of observed response data significantly assist the parameter estimation procedure by allowing to infer the parameters through calibration. However, the *utopian* fitting of the model to the real system's response does not exist, thus a deterministic approach may lead to misperception of the complex mechanisms. In this respect, a methodology to effectively use the residuals of the model is provided.

Let consider a calibrated conversion model following the eq. 3.19, and the error timeseries, e_t, is the differences between the observed and simulated quantities. The error is desirable to follow three specifications (Sorooshian & Dracup, 1980): (1) the error is uncorrelated with the simulated quantity; (2) the error is uncorrelated with itself (zero autocorrelation); and (3) the error is an independent and identically distributed random variable, i.e., without periodicity or other kind of time variation in its statistical properties. To respect of these we first transform the runoff by applying:

$$y' = \varepsilon \, ln(1 + y/\varepsilon) \tag{3.20}$$

where ε is a scale parameter introduced to avoid zero flow values, which was set the 1% of the mean daily observed runoff (ε = 0.01 mm). The rationale of this transformation is explained by Koutsoyiannis (2014). Following to this, the error process w_t is expressed by:

$$w_t = ln\left(1 + \frac{y_{sim,t}}{\varepsilon}\right) - ln(1 + y_{obs,t}/\varepsilon) \tag{3.21}$$

where $y_{sim,t}$ and $y_{obs,t}$ are the simulated and observed quantity at time t, respectively.

If the system of interest is subject to periodicity, the error process w_t is next grouped by season (e.g., month) and is "unlocated", in order to avoid the negative parameters, by using the location parameter:

$$w'_{t,s} = w_{t,s} - \left[min(w_{t,s}) - \sqrt{var[w_{t,s}(t)]}\right] \tag{3.22}$$

where s refer to each month. Next, we generate a stochastic timeseries of errors, taking advantage of the Symmetric Moving Average (neaRly) To Anything (SMARTA) scheme by Tsoukalas et al. (2018). In this respect, the target auto-correlation structure is estimated by using the eq. 3.12. In addition, the marginal distribution for each month is assigned.

Next, the generated $w'_{t,s}$, are transformed by using the inverse transformation of eq. 3.22, while the final error, $e_{gen,s}$, is expressed by:

$$e_{gen,s} = (y_{sim,s} + \varepsilon)[e^{-w_s} - 1] \tag{3.23}$$

In this respect, the final simulated quantity, accounting for the model error is given by:

$$y_{gen,s} = (y_{sim,s} + \varepsilon)e^{-w_s} - \varepsilon \tag{3.24}$$

By employing the above methodology of residuals, we are able to account for the predictive uncertainty of our model and its effects to the downstream models.

This approach is suitable for rainfall-runoff transformations (see application in chapter 5). We argue that the introduction of hydrological models within the representation of water-energy nexus augments the total uncertainty, but it is crucial. Specifically, in many cases, the rainfall data samples are quite longer than the runoff ones, thus such models are essential to increase the available hydrological information. Furthermore, the parent processes of the changing climate are the atmospheric ones, not the streamflow, thus a rainfall-runoff model should be established to investigate the impacts of changing input processes.

3.4.3 Modelling calibration uncertainty

Another aspect of model uncertainty is the calibration itself. Specifically, different time-periods or performance metrics result to different set of “optimal” parameters (the well-known issue of equifinality). In this respect, we propose a stochastic calibration approach, following the ideas by Gharari et al. (2013) and Efstratiadis & Koutsoyiannis (2010). In particular, Gharari et al. (2013) proposed the “sub-period calibration”, which aims at identifying a time consistent parameterization for a certain model structure and data set. This approach involves two steps. First, the available input and output data sets are split into (ideally equal length) k sub-periods. The second step regards to the calibration metric, by employing n different objective functions. Then, each sub-period is calibrated individually by sampling the parameter space and identifying the n-dimensional Pareto front for each sub-period, leading to k parameter set. On the other hand, Efstratiadis & Koutsoyiannis (2010) discussed the multi-objective calibration challenge, emphasizing to the use of multiple fitting criteria. Specifically, they provided a calibration methodology, in which the individual uncertainties of the calibration procedure are directly related through the model structure. In this respect, instead of minimizing the errors, they consider a proper multi-objective configuration of the calibration problem, assuming a limited number of fitting criteria that account for different aspects of the model performance.

By merging the two aforementioned approaches, i.e., the “sub-period calibration” and the different performance measures, we employ a two-step procedure in order to calibrate, in an uncertainty-wise manner, a rainfall-runoff model. First, we split the historical data into k different windows of length N. Next, we create k calibration scenarios, in which we apply randomly varying weights to a multi-objective performance measure comprising different goodness-of-fitting metrics. Eventually, k parameter sets are extracted, which are considered as equifinal, since they correspond to optimal solution for each calibration scenario. This methodology will be employed in chapter 7.

3.5 Quantifying uncertainty through copulas

3.5.1 Definitions and specifications

Copula theory (Sklar, 1973) enables the construction of multivariate joint distributions with arbitrary marginals. Specifically, copulas are used to describe and model the dependence (inter-correlation) between random variables. Due to this flexibility and the need of describing the correlations between variables, the use of these tools have been spread in a variety of scientific fields ,including economics (Patton, 2012), renewables (Otero et al., 2022) and their interface (Mejdoub & Ghorbel, 2018). In this vein, Klein et al. (2016), by taking advantage of the copula estimates the predictive uncertainty of hydrological multi-model predictions, while Fan et al. (2022) used copulas schemes to filter the model errors, and eventually limit the uncertainty. Besides, the predictive uncertainty copulas are widely used for forecasting weather conditions, wind speed and economic fluctuations (Möller et al., 2013; A. Patton, 2013; Wang et al., 2018). In our research, copulas will be used as a key tool for quantifying uncertainty in forecast terms and in the post-processing of dependent variables across the water-energy nexus, by means of predictive uncertainty, in order to offer insights to the policy-makers. In terms of forecasting, copulas allow for estimating the level of uncertainty in the medium-term scheduling, while in terms of post-processing these are able to quantify the uncertainty after employing an uncertainty-aware framework that supports stakeholders. Regardless of the application, copula-based tools will be able to offer the level on uncertainty, by means of a more nuanced understanding of uncertainty, that will be further translated in terms of associated risk. A brief mathematical description of constructing copulas follows.

3.5.2 Brief mathematical framework

For sake of brevity, we give only a short overview about copulas here. For a more detailed description of the theory, the reader is referred to (Joe, 1997; Nelsen, 2006). Copula function has a material effect on the shape of the joint distribution, so the selection of copula function should be reasonable. There are many type of copula functions that allows for describing the patterns of tail dependence, ranging from tail independence to tail dependence, and different kinds of asymmetry. Among all copula types, frequently-used ones include Gaussian and t copulas, from the elliptical copula family, and Gumbel, Clayton, Frank and Joe copulas, from the Archimedean copula family (Skoglund, 2010). Their shapes are presented in Figure 3.9**.**

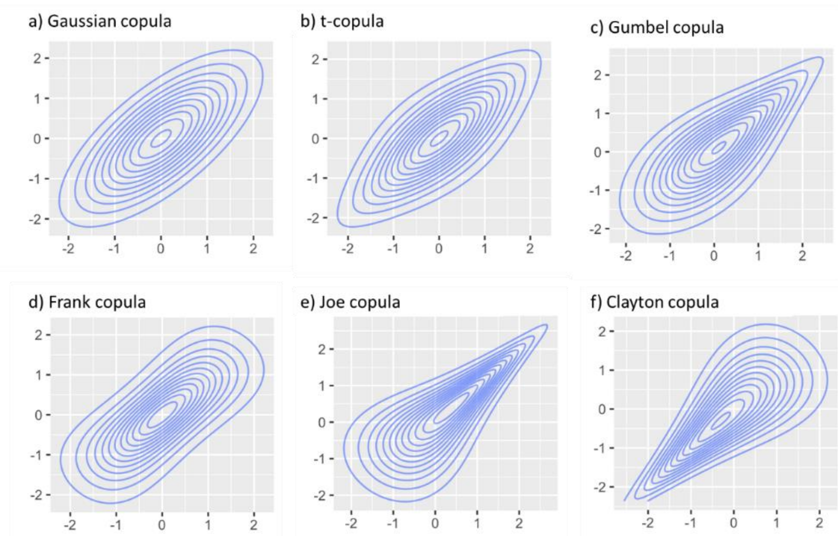


Figure 3.9: Contour plots of PDF for Caussian, t, Gumbel, Frank, Joe and Clayton copulas.

For convenience, we will focus on the case of the Gaussian copula, which is the simplest approach. We remind that these copulas are also used for the construction of non-Gaussian conditional distributions, based on the method by Tsoukalas (2018).

Let consider X and Y two random variables, while $F_X(x)$ and $F_Y(y)$ are their cumulative distribution functions (CDFs) and $u_X = F_X(x)$ and $u_Y = F_Y(y)$ are uniformly distributed in the range [0, 1].

According to copula theory, their joint CDF can be expressed by:

$$F(x, y) = P\{X \leq x, Y \leq y\} = C\big(F_X(x), F_Y(y)\big) = C(u_X, u_Y) \tag{3.25}$$

where $C(,)$ denotes the selected copula CDF.

For a given correlation matrix $R \in [-1, 1\,]^{dxd}$ (where d is the dimension- in our case $d = 2$, the Gaussian copula with a parametric R is expressed by:

$$C(u_X, u_Y) = \Phi_R(\Phi^{-1}(u_X), \Phi^{-1}(u_Y); R) \tag{3.26}$$

where Φ_R and Φ stand for the joint cumulative distribution function and univariate Gaussian CDF respectively.

The conditional CDF of the $X|Y = y$, that is $F_{X|Y=y}(x) = P\{X \leq x|Y = y\}$ can be obtained through the following relationship:

$$F_{X|Y=y}(x) = \frac{\partial C(u_X, u_Y)}{\partial u_Y} \coloneqq C_{X|Y}(u_X|u_Y) \tag{3.27}$$

where $C_{X|Y}$ stands for the so-called conditional copula. For the case of the Gaussian copula, the latter relationship reads as follows:

$$a \coloneqq F_{X|Y=y}(x) = C_{X|Y}(u_X|\, u_Y) = \Phi\left(\frac{\Phi^{-1}(u_X) - \mathrm{R}\Phi^{-1}(u_Y)}{\sqrt{(1 - R^2)}}\right) \tag{3.28}$$

which can be inverted to:

$$u_X^{a|u_Y} \coloneqq C_{X|Y}^{-1}(a|\, u_Y) = \Phi\left(R\Phi^{-1}(u_Y) + \sqrt{(1 - R^2)}\Phi^{-1}(a)\right) \tag{3.29}$$

in order to find the value of u_X that corresponds to a desired probability of non-exceedance $a \coloneqq C_{X|Y}$ given the (known) value of u_Y (compactly written as $u_X^{a|u_Y}$). Finally, one can also obtain the quantile that corresponds to that conditional probability level by employing the inverse cdf of X, i.e., $F_X^{-1}(\cdot)$. The latter reads:

$$x^{a|F_Y(y)} = x^{a|u_Y} = F_X^{-1}\left(u_X^{a|u_Y}\right) \tag{3.30}$$

while for the Gaussian copula case it only entails a substitution of eqs. 3.29 and 3.30.

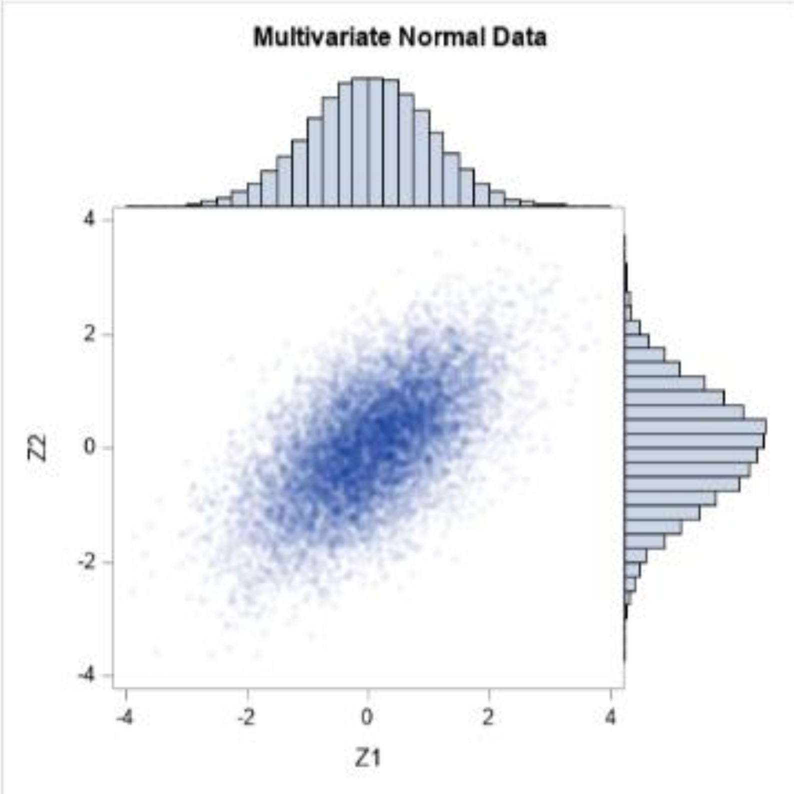


Figure 3.10: A scatter plot of the bivariate normal data with histograms for each marginal distribution.

3.6 Conclusions

In conclusion, this chapter has made significant strides in advancing our understanding and management of the intricate interplay between water resources, energy systems, and societal dynamics within the water-energy nexus. Through the development of comprehensive models, we have effectively accounted for hydroclimatic variability, social complexities, and uncertainties inherent in energy markets. Regarding the representation of climatic and energy-market uncertainty, we consider their processes as random variables, and use stochastic models for the generation of synthetic rainfall and electricity price data. Next, for the description of the human-induced procedures, an agent-based model, which is the sole approach that explicitly accounts for internal interactions across the social network, is developed tailored for the water-energy nexus. Specifically, this enables the swift from the steady-state hypothesis to a dynamic social subsystem, simulating the household’s behavior with respect to water and energy consumption.

Besides the climatic, social and energy market uncertainty, three pathways of representing the internal uncertainty are offered. In particular, all approaches focus on the parameter and structural uncertainty, but its one is discuss different aspects. The first approach is tailored for the statistical representation of “fuel”-energy conversion models, while the second one presents a methodology of generating synthetic residuals, accounting for the uncertain calibration parameters. The last method is dedicated to the calibration itself, merging two different uncertainty-aware approaches.

Finally, a framework for quantifying the uncertainty is presented, based on the copula theory. This tools will be employed in forecasting and in the post-processing of dependent variables across the water-energy nexus, in order to offer insights to the policy-makers.

By integrating these multidimensional factors, varying from climate to the socioeconomic environment and the modelling approaches, our research provides a robust modelling framework capable of accounting for the multifaceted uncertainties within the water-energy nexus. The methodologies developed in this thesis will be further employed in chapters 4, 5, 6 and 7 in order to offer valuable tools for policymakers, planners, and stakeholders to make informed decisions and formulate robust strategies for managing water and energy resources in an uncertain future. Specifically, chapter 4 is dedicated to the energy market and its major component ,i.e., electricity prices, offering two different analyses, namely the long-run simulation of electricity prices and forecasting across different scales of interest. In addition, chapter 5 discusses the combined uncertainty of climatic, economic and technological, in the design and assessment of renewable-related works. Following to this, chapter 6 step from the single work to a water-centric system, strongly driven by climatic, social and electricity price fluctuations. Finally, chapter 7 focuses on the key element of water-energy nexus, multipurpose hydropower plants, and its long-term management under the joint uncertainties.

4 From long-run simulation to forecasting of EU electricity market

Preamble

The applications of the *uncertainty-aware simulation-optimization framework* revealed that a key driver of the water-energy nexus originates from the socioeconomic environment. In this respect, this chapter focus on the energy market and its footprint, namely electricity prices. Specifically, this comprises two different analyses of the electricity prices, i.e., simulation of electricity prices and forecasting across different scales of interest. The first approach is applied to six European Energy Market by following the framework of 3.3.3, while the second one is stress-test to the Greek Energy Market by introducing a copula-based tool, following the mathematical framework of section 3.5. This chapter is based on these publications:

Efstratiadis, A. and **Sakki**, G.-K.: Driving energy systems with synthetic electricity prices, EGU General Assembly 2024, Vienna, Austria, 14–19 Apr 2024, EGU24-3165, https://doi.org/10.5194/egusphere-egu24-3165, 2024.

4.1 Simulation of the European Energy market

Before employing the proposed *electricity price generator* to the water-energy systems under study, this is stress-test to six European countries, i.e., Switzerland, France, Greece, Italy, Portugal, Netherlands. These are chosen due to several reasons. Specifically, most of them are interconnected, as depicted in Figure 4.1, while their energy mix is radically different, as demonstrated in Table 2. For instance, the Switzerland's electricity mix is based on hydropower (more than 50%), while France's is dependent on nuclear power. Other criteria are originated by their economic and climate conditions, fiscal compliance, and financial sector development. In this vein, two groups can be discriminated, i.e., the southern and northern. Particularly, the southern European countries favours the renewables investments, and their economic development was static for several years, due to the financial crisis of 2007-2008.

All data are extracted from the official database of the European Network of Transmission System Operators for Electricity (ENTSOE-E) and refer to the daily scale for years 2016-2022, as demonstrated in Figure 4.2. In case of the Italian energy market, the corresponding data begin from 2006. We remark that this period includes two periods of interest, namely the low prices during 2016-2020 and the spikes of 2021-2022. As already mentioned, the methodological framework and eventually the simulation of both periods is a key challenge of this research.

Table 2: Electricity mix of European countries (%). The raw data are provided by Eurostat.

Country	RES	Bio	Solar	Wind	Hydro	Nuclear	Gas	Coal	Oil
Switz.	0.0	0.2	4.3	0.1	54.8	37.0	0.0	0.0	3.6
France	0.1	2.1	4.3	8.2	9.8	63.3	9.2	0.9	2.1
Greece	0.0	1.0	12.6	20.7	9.0	0.0	37.3	10.4	9.0
Italy	2.0	6.6	9.9	7.1	10.7	0.0	50.7	7.6	5.3
Port.	0.4	8.5	6.5	28.3	16.2	0.0	37.0	0.1	3.1
Neth.	0.0	8.0	13.9	17.9	0.0	3.4	39.6	12.1	5.0

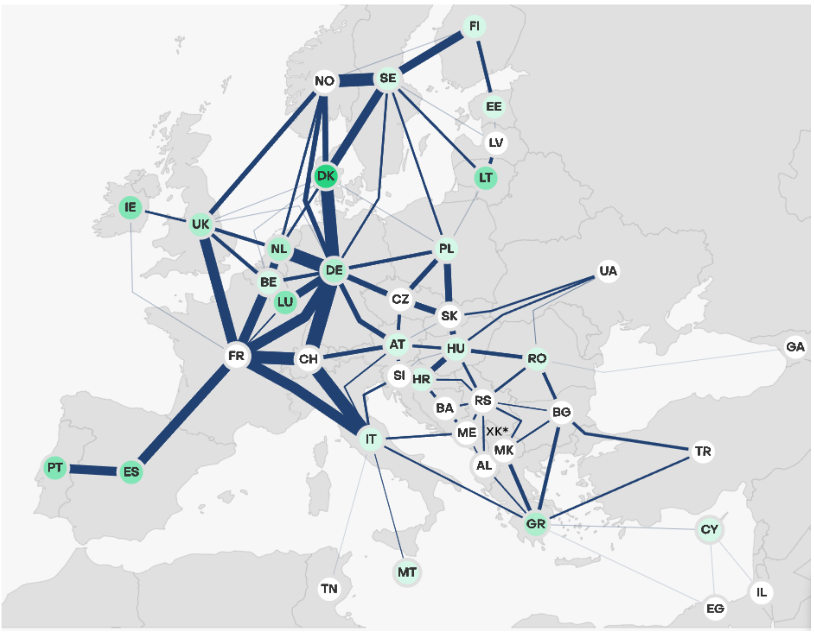


Figure 4.1: Interconnections of European electricity markets. (source: Ember)

4.2 Results

The proposed generator, as described in 3.3.3, is employed to simulate a 1000-year dataset of daily electricity prices for the six countries, i.e., Switzerland, France, Greece, Italy, Portugal, Netherlands. For all countries the 3-parameter Gamma distribution function (Pearson3) is fitted and the ACF of eq. (3.12) is applied with the scale and shape parameters as demonstrated in Table 3. The demonstration of fitting the theoretical autocorrelation is given in Appendix, Figure 10.1, while from Figure 10.2 to Figure 10.7 the estimation of the marginal distribution for each country are given.

For all countries, we compare the observed and simulated daily mean, standard deviation, skewness coefficient and lag-1 autocorrelation, which are given at Table 4. As already mentioned, the electricity price's process is characterized by seasonality at the monthly scale. In this respect, a generator should account for this characteristic and reproduce the process' regime at both scales, daily and monthly. In Figure 4.3 and Figure 4.4, the monthly-based mean and standard deviation values of electricity prices compared with the simulated timeseries are demonstrated. In addition, Figure 4.5 presents the five-number summary, through boxplots, i.e., the minimum, first quartile, median, third quartile, and maximum of the historical and the simulated electricity prices for the six energy markets under study. As expected, the simulated time series take advantage of the available statistical information to expand the data, since it covers a period of 1000 years against the small sample of the observed (6 years).

Table 3: Shape parameters of target autocorrelation functions for Switzerland, Netherlands, France, Greece, Portugal, and Italy.

Country	κ	β
Switzerland	0.013	5.12
France	0.021	6.02
Greece	0.010	5.75
Netherlands	0.019	5.46
Portugal	0.073	22.82
Italy	0.012	6.15

Further to this statistical analysis, for each country a selected time-window of the simulated timeseries is contrasted against the historical data (Figure 4.6). The key question of representing accurately not only the statistical characteristics of the observed data *per se*, but also the persistence of low and high electricity prices is addressed herein. Specifically, as demonstrated in Figure 4.3 and Figure 4.4 and Table 4, the proposed generator is able to reproduce the statistical regime of the observed data at the daily and the monthly scales. In addition, it is capable to move beyond the statistical characteristics, by representing precisely the season-to-season volatilities, the daily spikes and the low-frequency events in the long run (Figure 4.6). Finally, this analysis indicated that this generator is generic and easily adjustable to different energy markets, by adopting appropriate assumptions in the model setup, i.e., selection of marginal distribution and selection of shape parameters for the theoretical autocorrelation function, κ and β.

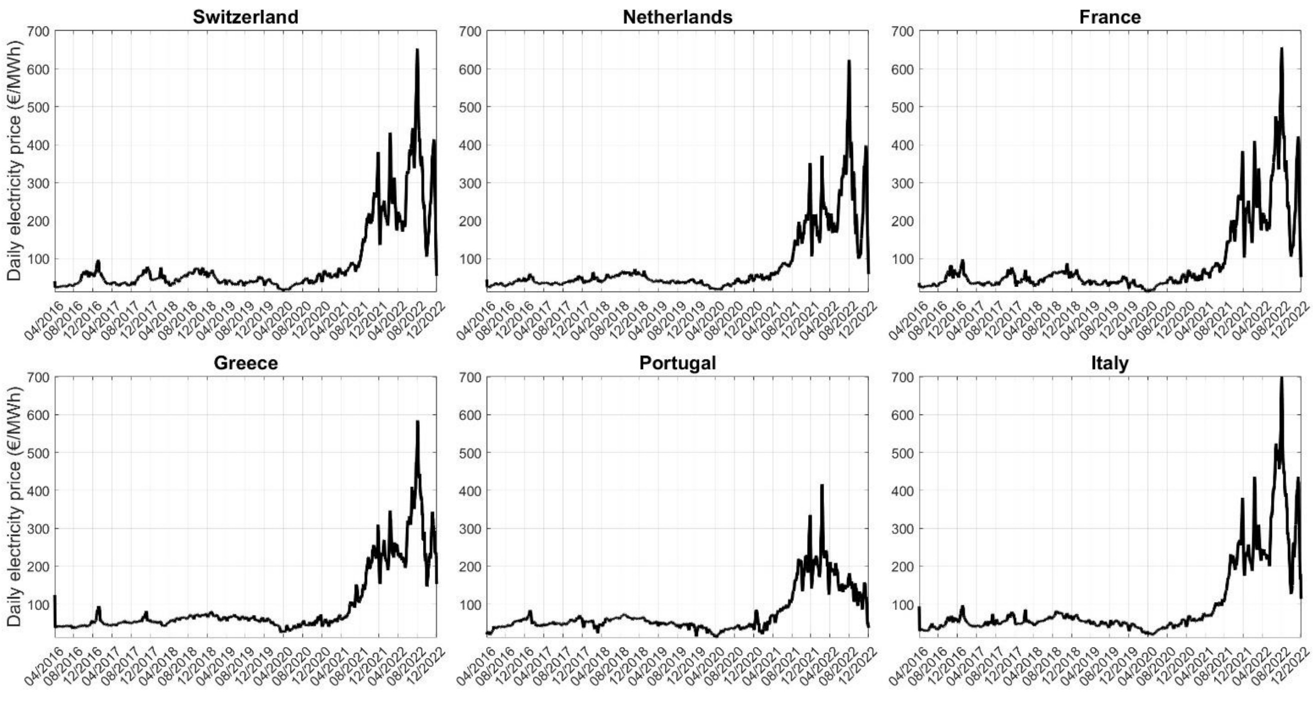


Figure 4.2: Historical daily electricity prices for Switzerland, Netherlands, France, Greece, Portugal, Italy.

Table 4: Comparison of daily statistical characteristics for all modelled variables.

Country		Mean (€/MWh)	St. deviation (€/MWh)	Skewness	Lag-1 Autocorrelation
Switzerland	Historical	84.9	92.1	2.75	0.984
	Simulated	85.0	83.6	2.3	0.984
France	Historical	81.9	92.5	2.93	0.971
	Simulated	92.9	101.4	3.00	0.979
Greece	Historical	89.4	86.1	2.61	0.976
	Simulated	90.1	81.4	2.54	0.988
Netherlands	Historical	75.9	79.9	2.97	0.969
	Simulated	79.3	74.5	2.64	0.981
Portugal	Historical	70.2	55.6	2.44	0.969
	Simulated	73.9	61.3	2.35	0.951
Italy	Historical	78.7	71.8	4.30	0.977
	Simulated	82.1	75.5	3.56	0.988

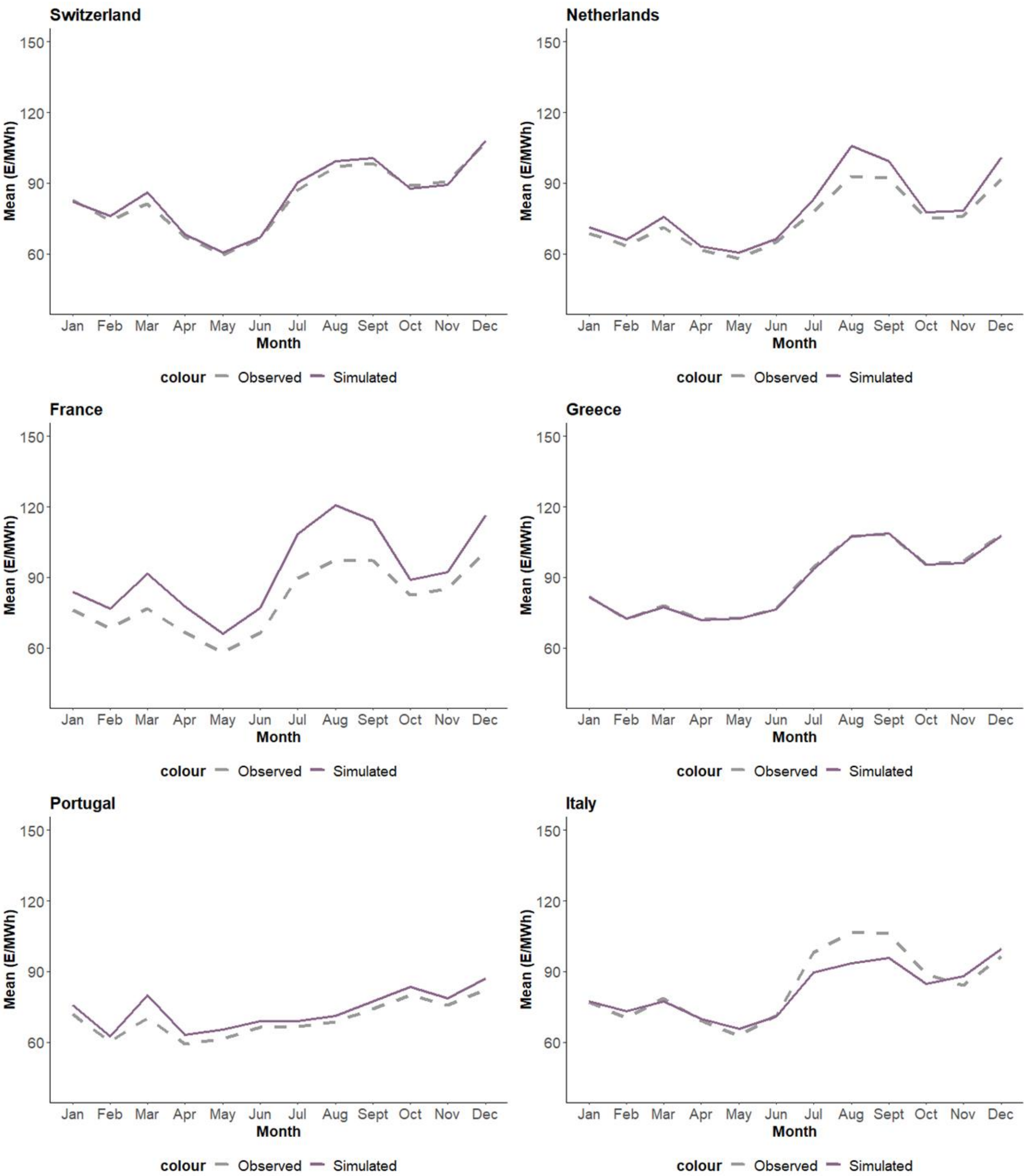


Figure 4.3: Monthly-based comparison of historical monthly mean values with the simulated ones for Switzerland, Netherlands, France, Greece, Portugal, Italy.

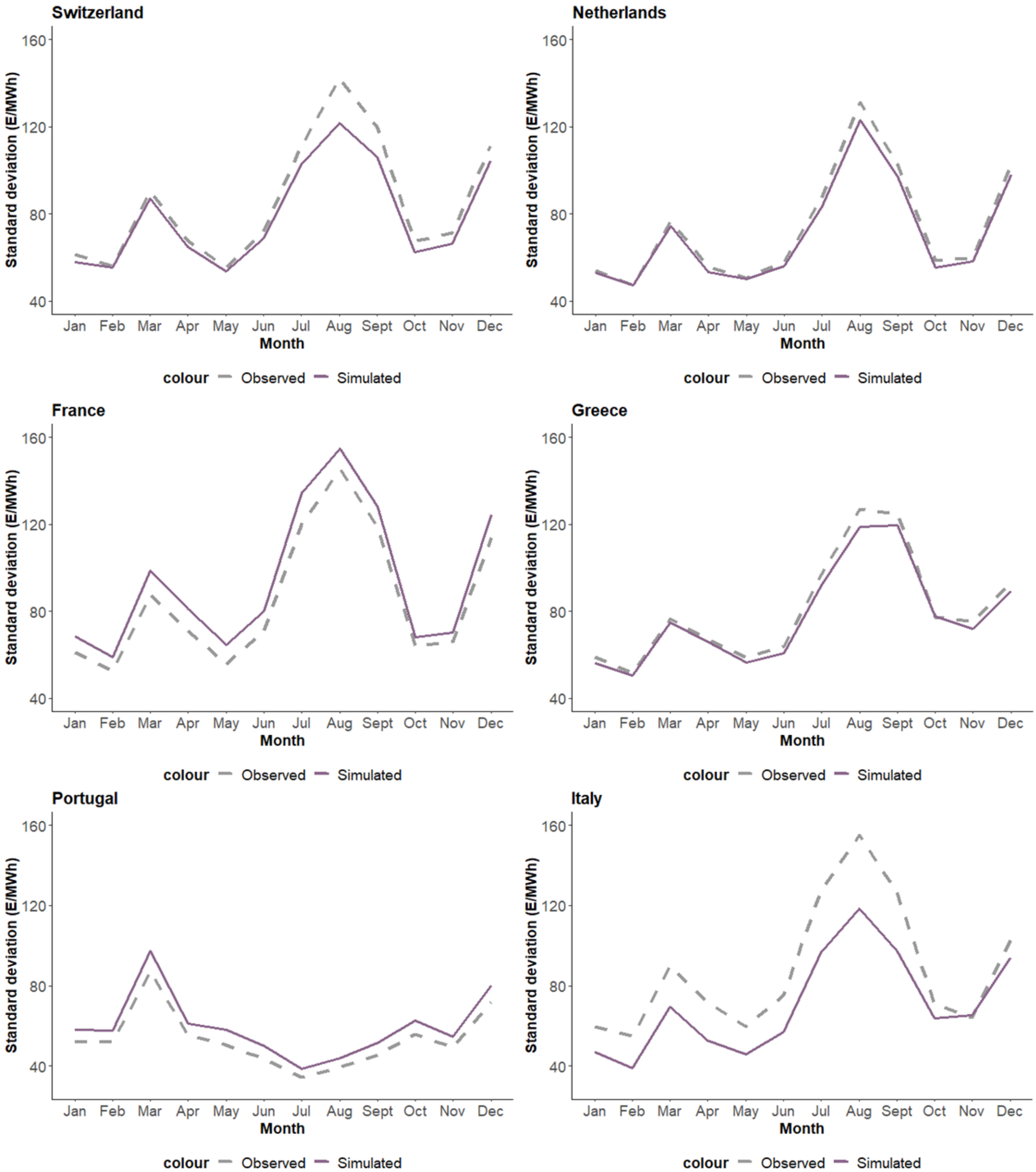


Figure 4.4: Monthly-based comparison of historical standard deviation values with the simulated ones for Switzerland, Netherlands, France, Greece, Portugal, Italy.

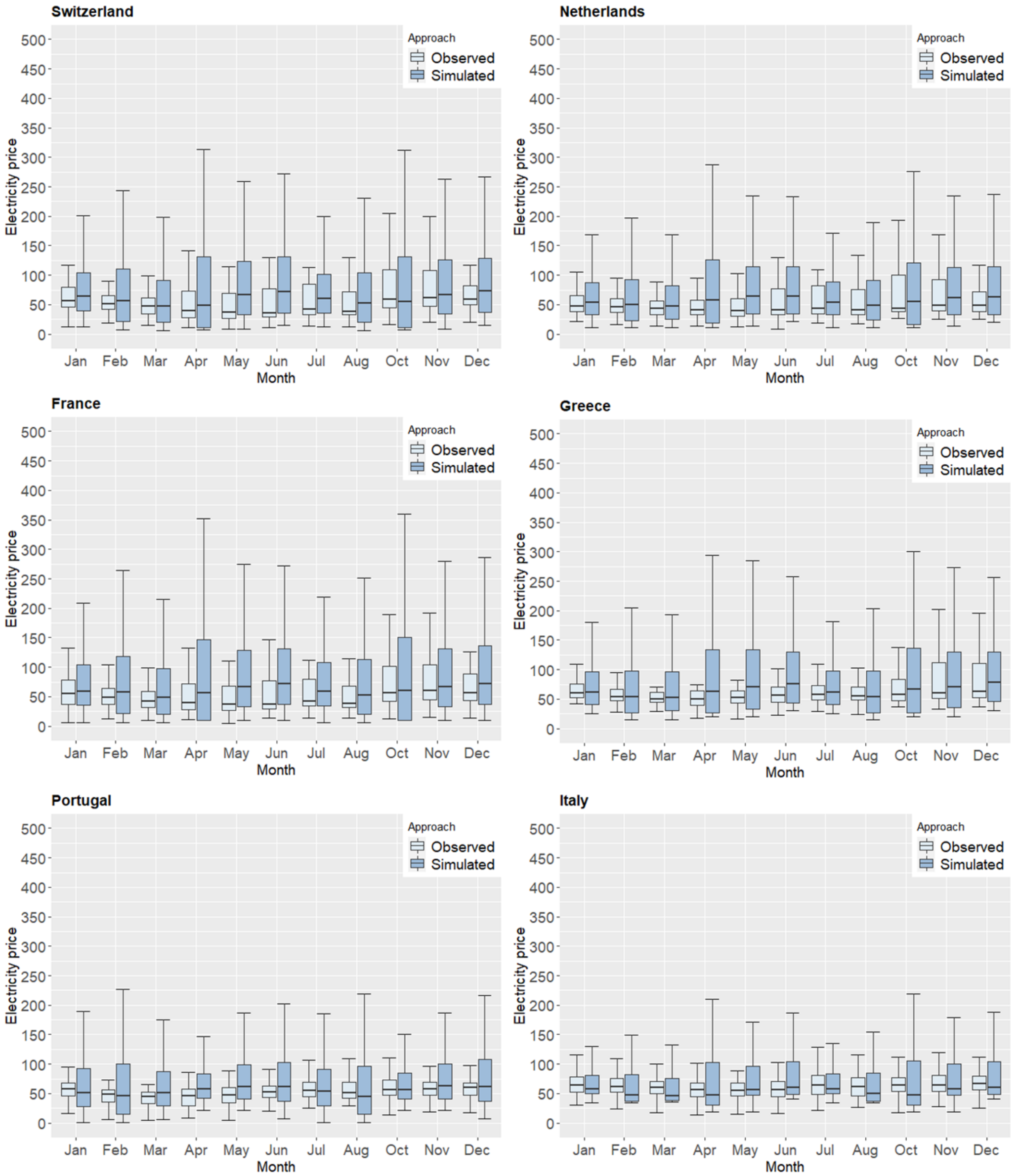


Figure 4.5: Monthly-based boxplots that compare the historical with the simulated electricity price for Switzerland, Netherlands, France, Greece, Portugal, Italy.

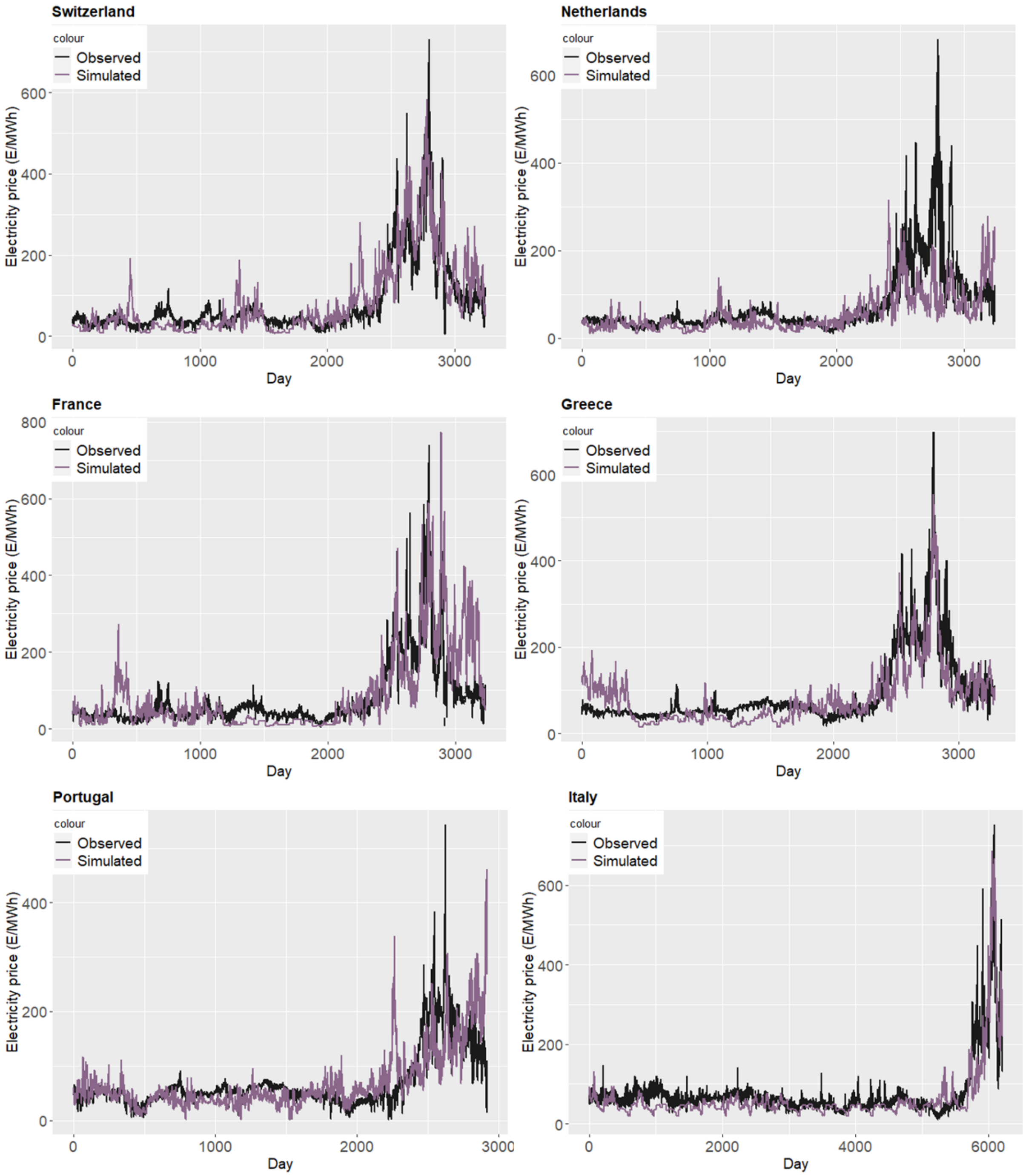


Figure 4.6: Window of historical and simulated timeseries of electricity price for Switzerland, Netherlands, France, Greece, Portugal, Italy.

4.3 Forecasting of electricity prices across scales via copulas

The second application across electricity markets refers to the forecasting of electricity prices across multiple scales of interest, i.e., daily, weekly, monthly, quarterly. As already mentioned in section 3.3.1, the energy market comprises different structures, one of them being the day-ahead scheduling. In this respect, the day-to-day variations are crucial for the operation of all energy-related projects (e.g., wind and photovoltaic parks, small and large hydropower plants). On the other hand, the coarser timescales serve median and long-term management policies, mainly regarding the human-controlling projects, e.g., large hydropower plants. In general, considering multiple time scales for forecasting electricity prices allows for a more comprehensive understanding of the market dynamics and helps stakeholders make better-informed decisions. In particular, numerous target groups of stakeholders in the electricity sector, such as power generators, distributors, and consumers, have different planning horizons and decision-making processes. By providing forecasts at various time scales, analysts can cater to the needs of these stakeholders, enabling them to make informed decisions about production, procurement, pricing, and consumption. In addition, energy trading and investment decisions involve managing various types of risks, including price risk. By forecasting electricity prices at different time scales, market participants can better assess and manage their exposure to short-term volatility as well as longer-term trends.

In this respect, we are taking advantage of the Greek Energy Market data to forecast the electricity prices for the aforementioned timescales. The data are separated into training and testing, that correspond to 80% and 20% of the sample, respectively. For the construction of copulas, we follow the mathematical framework, as described in section 3.5.2. In brief, we first assign to each random variable, e.g., electricity price of the day and the day-ahead, the marginal distributions. Next, we select a well-suitable joint distribution for these variables, thus for each quantile an estimation of electricity price results, given the "current" (daily, weekly, monthly) price. We remark that these only incorporate the information of the past energy market dynamics, ignoring weather and demands forecasting. In this respect, these tools are able to provide macroscopic insights of how the market is moving, regardless of other forecasts. This happens because copula methods are only based on the relationships and dependence structures between the variables of interest. This allows them to provide insight into market analysis and dynamics, regardless of the accuracy or instability of other forecasts. Thus, even if this approach is not entirely accurate, it provides significant understanding of the structure and dynamics of the electricity market.

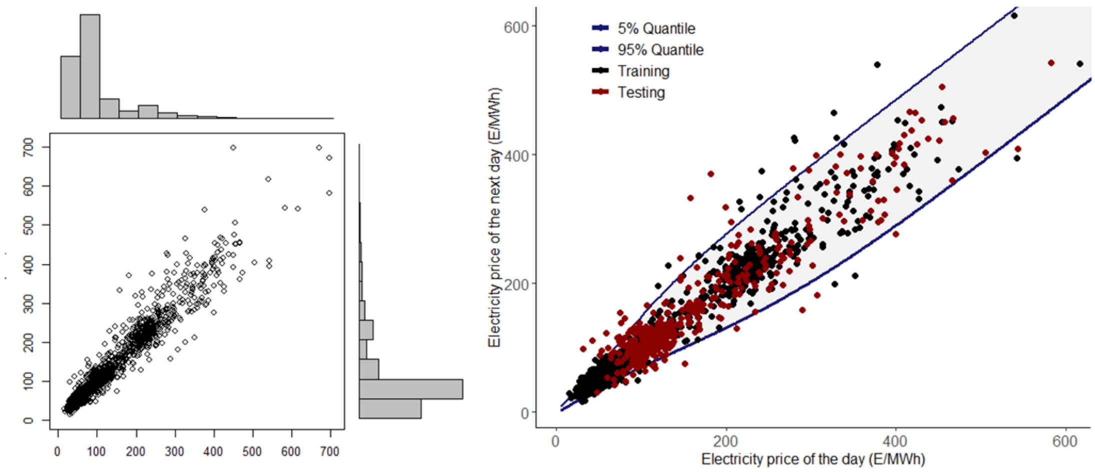


Figure 4.7: Histogram and copula-based tool for prediction of electricity price at the daily scale.

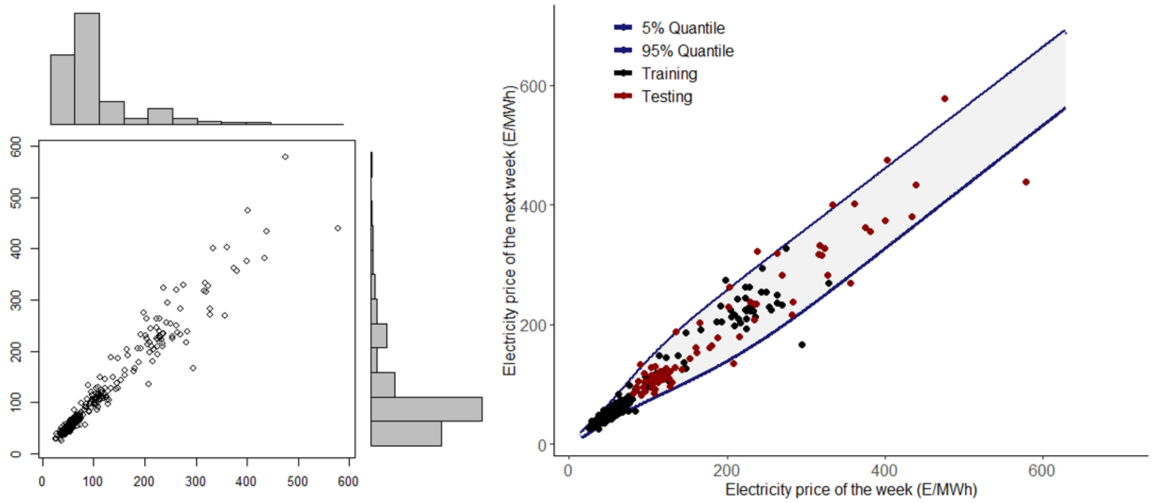


Figure 4.8: Histogram and copula-based tools for prediction of electricity price at the weekly scale.

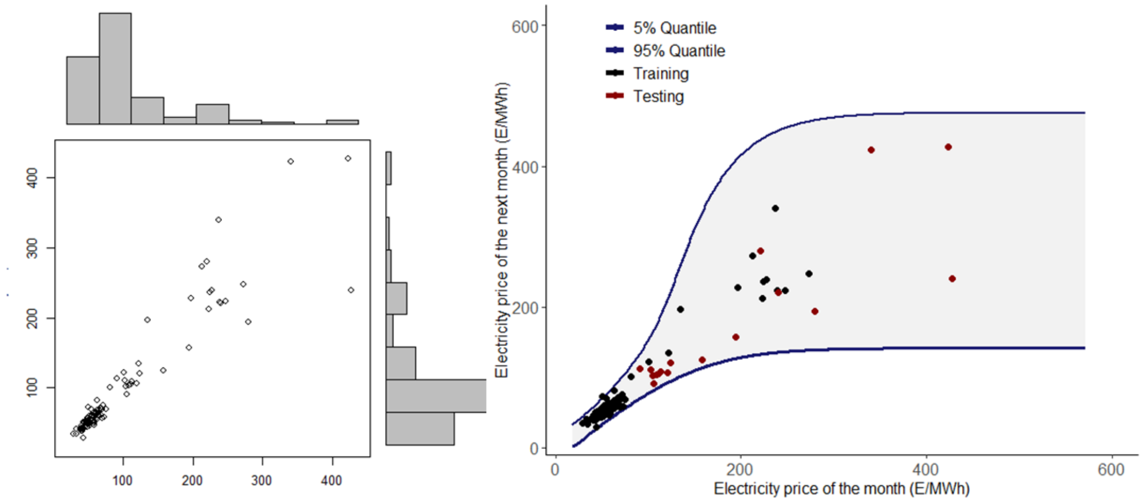


Figure 4.9: Histogram and copula-based tools for prediction of electricity prices at the monthly scale.

These simple, yet accurate, copula-based tools for predicting the electricity prices are demonstrated in Figure 4.7 (refers to the daily scale-BB1 copula is fitted), Figure 4.8 (refers to the weekly scale-BB1 copula is fitted), and Figure 4.9 (refers to the monthly scale-Frank copula is fitted). It is clear that we can group two areas of interest, i.e., low ($<$ 200€/MWh) and high ($\geq$ 200 €/MWh) electricity prices. Specifically, for the first group the level of prediction is quite narrow, while for the second one the predictive uncertainty is wider. This is more obvious in the forecasting tool at the monthly scale, whereas the uncertainty is high due to inherent and non-inherent reasons. For instance, given an average monthly electricity price of 300 €/MWh, the prediction ranges from 190 to 500 €/MWh. The inherent reasons refer to the scale of interest *per se*, the day- to day prediction is less uncertain. Oppositely, the non-inherent ones regard to the uncertain policymaking of all participants, government regulations and interventions for the next month.

4.4 Combination

An interesting approach arises from the combination of the two aforementioned tools. Specifically, the generation of long synthetic data, allows for capturing a wide "window" of data. In addition, the copula-based tool for forecasting offers the range of the predictive uncertainty given the value of the current electricity price. In this respect, the coupling of these tools allow the stakeholders to simulate their system with various scenarios of forecasting to policy-making in the mid-term scale.

Let consider a forecasting horizon of N days for which we aim to provide m equally probable scenarios to drive the short-term scheduling of an energy-related system. The first step regards to the generation of $m \times N$ ensembles of daily electricity prices by employing the methodology as described in section 3.3.3. The second step includes the estimation of the copula-based tool for prediction as presented in section 4.3. Then, we extract only a part of the $m \times N$ ensembles, as indicated by the uncertainty bounds of copulas.

Herein, we are taking advantage of the Greek Energy Market to employ this procedure. In this respect, 200 scenarios of 5 years (1825 days) are generated, while the copula tool refers to a mid-scale forecasting. In particular for the forecasting through copulas, the known variable is the average electricity price for the period January-March and the predictive variable refers to the rest of the year, i.e., April to December (Figure 4.11). We remark that the sample of historical data is too small, only 7 years, thus the copula is constructed, by using synthetic data. In this respect, we are taking advantage of the stochastic regime of the historical data in order to generate long synthetic data and eventually estimate the appropriate copula scheme. Figure 4.11 presents the copula scheme that was selected, i.e., BB7, compared with the historical data (red color). In addition, Figure 4.10 presents the mean electricity price for the period April to December for each scenario, which varies from 20 to 400 €/MWh.

In this respect, stakeholders are able to simulate and optimize their mid-term system's operation, for an horizon of nine months by selecting the most suitable scenarios. For instance, if the mean electricity price of the first three months is 200 €/MWh, the prediction of the mean electricity price for the next nine months corresponds to 97 to 310 €/MWh. Thus, the suitable scenarios for this state of the system are selected, accounting for the mean electricity price of the period April to December. Eventually, these scenarios are only 65, compared to the initial sample of 200. These scenarios are the most appropriate of the energy market's conditions, thus allowing the energy system's operator to decision-making conditioning their external environment.

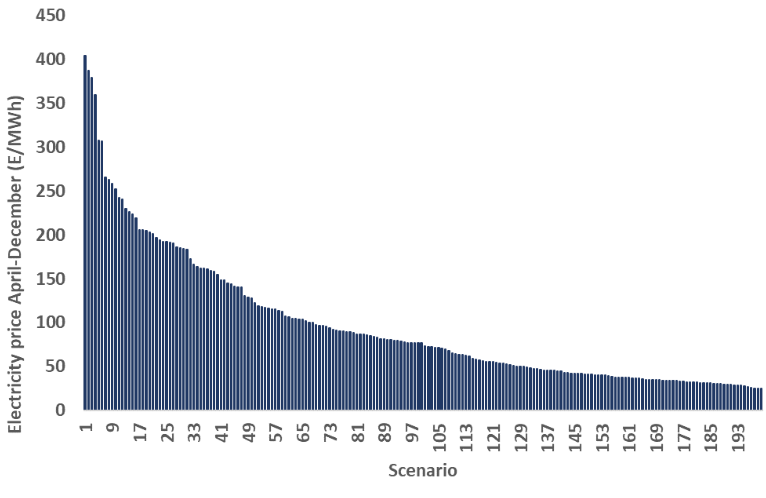


Figure 4.10: Copula-based tool for prediction of electricity price at a mid-term scale.

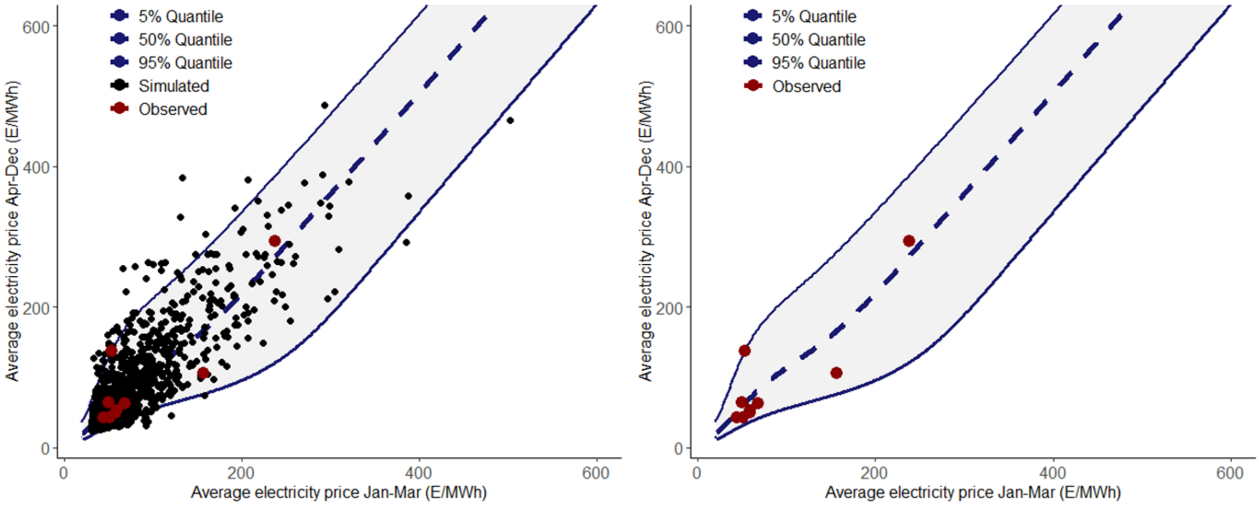


Figure 4.11: Copula-based tool for prediction of electricity price at a mid-term scale.

4.5 Conclusions

To end with, this chapter encloses the energy-market uncertainty within two operational approaches. The first one includes the simulation of daily electricity prices in the long-run, by using the proposed electricity price generator, as described in section 3.3.3. The second approach refers to the forecasting of electricity prices across several timescales , i.e., daily, weekly, monthly, taking advantage of the copula theory as formalized in section 3.5. The first approach is implemented for six European Energy Markets, with varying energy mix, while the second is established to the Greek Energy Market.

Both case studies have a significant footprints for the scheduling, operation and long-term management of water-energy systems and energy-related projects. The simulation of electricity prices offers the ability to stakeholders and investors to design or assess existing projects, accounting for the energy market uncertainty of the host state. On the other hand, the proposed simple forecasting scheme has a scheduling and mid-operation character. Specifically, these copula-based tools offer a macroscopic prediction, under the expected uncertainty levels, of the energy market dynamics, considering the past information and describing the dependencies. This has a major advantage arises due to is independent of other forecasted variables, e.g., weather conditions and demands. In addition, the combination of both tools offers the significant advantage to the stakeholders to make informative decisions, by quantifying a priori the evolution of their system under uncertainty, depending on the forecasting of the electricity prices.

5 Uncertainty-wise design and assessment of renewable projects

Preamble

This chapter is dedicated to the renewables under uncertainty; from the description of each source, the general simulation scheme to a valuable toolbox for stakeholders. Specifically, key objective is to formalize the endogenous and exogenous uncertainties across the input processes and model hypotheses, and eventually represent them under a novel uncertainty quantification framework, by coupling the methodological triptych of statistics, stochastics and copulas. Besides this, we set the methodology of representing the operation of renewables by means of random processes, thus allows to incorporate their uncertainties in stochastic terms. Following to this, we offer simple, yet generic toolboxes for policymakers, to facilitate the design and assessment procedure for renewable-based investments. As a proof of concept for the effectiveness and generality of the proposed framework, we analyze two different cases. The first involves the design of a run-of-river small hydropower plant, while the second one refers to the to the long-term economic assessment of a wind power plant. Most of the material here was prepared originally for the thesis, albeit a small part of it is also covered on our publications:

G.-K. Sakki, I. Tsoukalas, P. Kossieris, C. Makropoulos, and A. Efstratiadis, Stochastic simulation-optimisation framework for the design and assessment of renewable energy systems under uncertainty, Renewable and Sustainable Energy Reviews, 168, 112886, doi:10.1016/j.rser.2022.112886, 2022.

G.-K. Sakki, I. Tsoukalas, and A. Efstratiadis, A reverse engineering approach across small hydropower plants: a hidden treasure of hydrological data?, Hydrological Sciences Journal, 67 (1), 94–106, doi:10.1080/02626667.2021.2000992, 2022.

K.-K. Drakaki, **G.-K. Sakki**, I. Tsoukalas, P. Kossieris, and A. Efstratiadis, Day-ahead energy production in small hydropower plants: uncertainty-aware forecasts through effective coupling of knowledge and data, Advances in Geosciences, 56, 155–162, doi:10.5194/adgeo-56-155-2022, 2022.

5.1 Setting the scene

All European strategies (e.g., Green Deal, REpowerEU etc.) focused on the increasing share of renewables in the energy mix, promoting innovation and technological advancements in renewable energy technologies, enhancing energy efficiency, and fostering the transition towards a more sustainable and resilient energy system. As mentioned, the EU has set a target of at least a 45% share of renewable energy in the final energy consumption by 2030. Yet today, energy production and consumption based on fossil fuels still represent more than 75% of the EU’s greenhouse gas emissions, thus boosting EU members towards clean energy solutions. However, the systematically increasing penetration of renewable energy introduces further complexities to the global energy scene, due to multiple and interacting uncertainties (Alqurashi et al., 2016; Oree et al., 2017). This issue affects the entire life-cycle of renewable energy systems (RES), i.e., planning, design, policy management and operation (Rauner & Budzinski, 2017; Saxe et al., 2020).

As shown in Figure 2.1, multiple sources of uncertainty exist, from the input “fuel” to its conversion to electricity production, and eventually the energy market. Following the rationale of section 2.4, their disentangling requires to separate them into exogenous (external) and endogenous (internal). The former category mainly refers to the inherent uncertainty of the system's drivers, i.e. hydrometeorological processes, also involving highly-complex and unpredictable socioeconomic and environmental factors, as well as conflicts within the broader energy-society nexus, e.g., land development (Sargentis et al., 2021). On the other hand, internal uncertainties refer to conversion processes and underlying modelling assumptions.

The fact that renewable energy production is highly varying, intermittent and unpredictable across all scales, induces significant challenges to researchers and practitioners, in terms of successfully planning, scheduling, utilizing and controlling RES (Koutsoyiannis et al., 2009; Nakata et al., 2005). Nevertheless, it is recognized that the associated tasks, generally configured as optimization problems, can be effectively handled if uncertainties, probabilities, and fluctuating behaviors of renewable energy systems are properly represented (Zakaria et al., 2020).

This research highlights the importance of addressing the major facets of uncertainty, external and internal in combination, for two crucial life-cycle phases of RES, namely the technical design and the economic assessment. This problem is introduced in a generic simulation-optimization context, and then specified across the most popular types of RES, namely wind, photovoltaic and hydroelectric. The key objective is to formalize the endogenous and exogenous uncertainties across the input processes and model hypotheses, and eventually represent them under a novel uncertainty quantification framework, by coupling the methodological triptych of statistics, stochastics and copulas.

As a proof of concept for the effectiveness and generality of the proposed framework, we analyze two different cases. The first involves the design of a run-of-river small hydropower plant (SHPPs) in Pamisos River basin, Western Greece, and particularly the estimation of the optimal mixing of its turbines. The underlying optimization problem aims to maximize the anticipated revenues from the long-term operation of the power plant, contrasted to the investment costs of the electromechanical equipment and the overall technical efficiency of the project, expressed in terms of capacity factor. The second case study refers to the long-term economic assessment of a planned wind power plant in the island of Ikaria (Greece). Both cases are handled through a modular scenario-based scheme, starting from the benchmark scenario, i.e., the conventional deterministic practice, and redounding to an integrated stochastic-probabilistic approach. This allows for capturing the key exogenous and endogenous uncertainties, and simultaneously providing decision support tools for the design, strategic management, and evaluation of RES.

5.2 Generic simulation-optimization framework for RES

5.2.1 Simulation procedure

In contrast to power systems using fossil fuels, where energy production is predictable and controllable, in the case of RES the production follows the variability of the inflow source (wind, solar radiation, water). This variability can be mathematically described on the basis of statistical or stochastic terms, assuming a simulation context to link the power production, $\underline{p}$, with the hydrometeorological input, $\underline{x}$, which are both handled as random (better referred to as stochastic) processes.

The transformation of the randomly varying input process, $\underline{x}$, to the output power, $\underline{p}$, is a nonlinear function which is generally expressed as:

$$\underline{p} = \begin{cases} 0 & x < x_{min} \\ \eta(\underline{x})\, p_0(\underline{x}) & x_{min} \le x < x_{max} \\ I & x_{max} \le x < x_s \\ 0 & x \ge x_s \end{cases} \tag{5.31}$$

where $p_0(\underline{x})$ is the theoretical power, I is the power capacity (also referred to as nominal power), and $\eta(\underline{x})$ is the total efficiency, which are both driven by the stochastic process $\underline{x}$. The limits x_{min} and x_{max} are characteristics of the specific RES, while x_s represents a cut-out value, above which the machine stops for safety reasons.

The theoretical power depends on the location, layout and particular technical characteristics of the RES. In this respect, the theoretical wind power is given by:

$$p_0(\underline{v}) = \frac{1}{8}\, \rho_\alpha\, \pi\, D^2 \underline{v}^3 \tag{5.32}$$

where ρ_α is the air density, D is the diameter of the wind turbine and $\underline{v}$ is the wind velocity. Typical values of v_{min}, v_{max} and v_s are 3.0, 12.0 and 25.0 m/s, respectively.

For the common type of solar energy systems, namely the photovoltaic (PV) ones, the theoretical power is given by:

$$p_0(\underline{r}) = S\, \underline{r} \tag{5.33}$$

where S is the net area of photovoltaic panels and $\underline{r}$ is the incoming solar radiation. The operation of PVs is simpler than other RES, since their nominal power is by definition achieved at $r_{max} = 1000$ W/m2.

Finally, the theoretical output power by a hydroelectric system is expressed in terms of hydrodynamic power:

$$p_0\left(\underline{h}, \underline{q_T}\right) = \rho\, g\, \underline{h}\, \underline{q_T} \tag{5.34}$$

where ρ is the water density, g is the gravity acceleration, $\underline{h}$ is the gross head, i.e., the elevation difference between the upstream water level and the outlet of the power station, and $\underline{q_T}$ is the flow passing through the turbines. Regarding the limits $q_{T,min}$, $q_{T,max}$ and $q_{T,s}$, these depend on the turbine characteristics, as further discussed in the first proof-of-concept study (section 4).

We underline that, in contrast to wind velocity and solar radiation, the turbine flow is not a purely natural process, but a spatiotemporal transformation (regulation) of the runoff produced over a catchment through a system of hydraulic works, employing diversion, storage, water transfer, etc. In this respect, the representation of the regulated process, $\underline{q_T}$, implies the use of an operation model of the associated water resource system, e.g., hydroelectric reservoir (Efstratiadis et al., 2021a). This model, symbolized, $\underline{q_T} = \Phi(\underline{q})$, gets as input the "primary" stochastic process, by means of streamflow $\underline{q}$, and accounts for the constraints and decisions induced by the system's characteristics (e.g., reservoir and penstock capacity, storage-elevation relationship) and assigned management practices, respectively. Similarly, the gross head $\underline{h}$ derives from the operation model, since its variability is mainly dictated by the variability of the upstream reservoir level.

On the other hand, the total efficiency, $\eta(\underline{x})$, is the product of individual efficiency values that refer to different components of the power transformation system, to express the associated energy losses. This involves the mechanical and mass losses in turbines, as well as the power losses in the generator and the transformer. In general, these are subject to complex physical laws that make hard to establish accurate analytical expressions (Gottschall & Peinke, 2008). In this respect, each power machine has its own efficiency function, expressed by nomographs that are provided by the manufacturer, on the basis of laboratory results. Particularly for the case of hydropower, the hydraulic losses across the water conveyance system (penstock) augment the uncertainty, since they are calculated based on quite uncertain technical components (e.g., roughness, Reynolds number etc.). Specifically, the hydraulic losses are the sum of friction and minor losses across the conveyance system. The friction losses across a pipe of length and diameter L and D, respectively (both expressed in m), are estimated through the Darcy-Weisbach formula:

$$h_f = f\,\frac{L}{D}\frac{V^2}{2g} = f\,\frac{8\,L\,Q^2}{g\,\pi^2 D^5} \tag{5.35}$$

where V is the velocity (m/s) and f is a dimensionless friction factor. For turbulent flow conditions, the friction factor is estimated through the Colebrook-White formula:

$$\frac{1}{\sqrt{f}} = -2.0\ log\left(\frac{k_s/D}{3.71} + \frac{2.51}{Re\sqrt{f}}\right) \tag{5.36}$$

where k_s is the equivalent roughness (typical design values 0.5-2.0 mm), and Re the Reynolds number:

$$Re = \frac{V\,L}{\nu} \tag{5.37}$$

where ν is the kinematic viscosity of the fluid (m^2/s); for water under typical temperature and pressure conditions (i.e., $T = 16$ oC, $P = 1.0$ atm), we get $\nu = 1.1 \times 10^{-6}$m^2/s.

In addition, the losses are generally expressed as a fraction of kinetic energy:

$$h_L = k\,\frac{V^2}{2g} \tag{5.38}$$

where V is the larger velocity value across the transition and k is a dimensionless factor, depending on the geometrical and hydraulic characteristics of the transition. The value of k is strongly affected by the shape of the transition. Well-rounded transitions ensure minimal local losses (which is an issue of good design and good construction, as well).

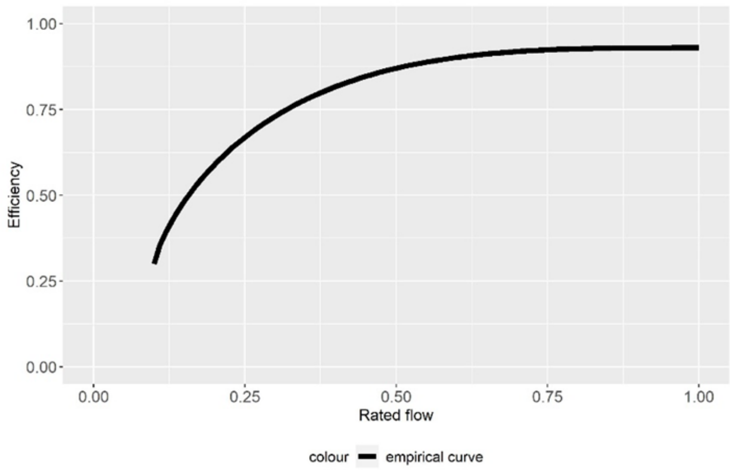
5.2.2 Insight to efficiency

As already mentioned, the ability of the "fuel" to become energy depends on the efficiency of the system, $\eta(\underline{x})$. This element is associated with the internal operation of the system, but it strongly depends on the external driver, i.e., "fuel". For renewable energy projects, the driver is the streamflow, the wind and the solar radiation. The efficiency of each convertor (i.e., hydroturbines, wind turbines, and solar panels) is typically estimated by employing experiments. However, the real-world operation differs from the experimental tests.

Characteristic examples of efficiency curves for wind and hydro-turbines, as function of the associated input process, $\underline{x}$, are demonstrated in Figure 5.1. It is interesting to remark that in all cases, the function $\eta(\underline{x})$ is not monotonic. Nevertheless, the estimation of efficiency is subject to three key sources of uncertainty. The first is due to deviations between the actual performance of the power machine in the field and its prototype (Yan et al., 2019). A characteristic example is the control of the pitch angle of wind turbines, which may significantly affect their real performance (Astolfi, 2019). The second source of uncertainty originates from the drop of efficiency due to deterioration, damage and ageing of equipment over time (Hamilton et al., 2020; Rahman et al., 2023). The last feature, which introduces further complexity and thus uncertainty, is the dependence of efficiency not only on the input, $\underline{x}$, but also on additional stochastic processes, such as the sediment transport causing erosion to hydro-turbines (Felix et al., 2016) or the temperature and other meteorological processes that affect the actual efficiency of PV panels (Elbreki et al., 2016). For instance, in eq. 5.39 denotes that the rate of PV efficiency decrease for every unit increase of temperature above 25°C, i.e.:

$$n_{actual} = n_{nom} - a_T \cdot max(T - 25,0) \tag{5.39}$$

where a_T is a power temperature coefficient (%/°C).



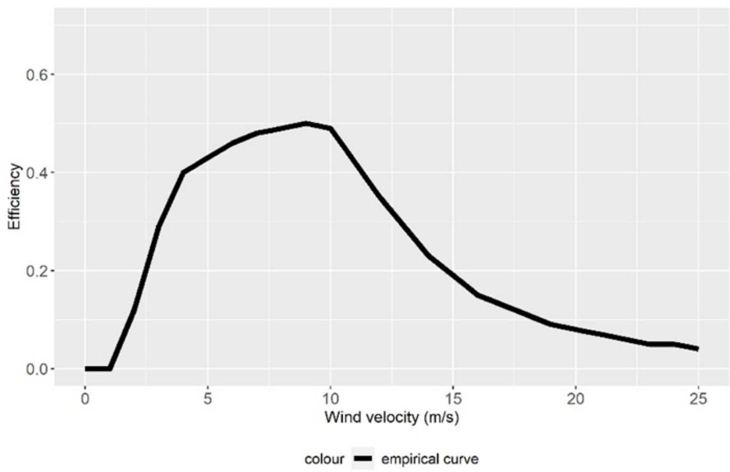


Figure 5.1: Examples of efficiency functions for a Pelton-type turbine (up) and a wind turbine (down).

To describe the efficiency as function of the input process, $\underline{x}$, we introduce an analytical formula, symbolized $\eta(\underline{x}, \theta)$, for the associated machine, where θ is a set of parameters that describe the shape of the curve. Since the efficiency is lower and upper bounded, we can presented by assigning a distribution with these characteristics. Herein, we are taking advantage of Kumaraswamy's double bounded distribution, which the cumulative distribution function is:

$$\mathrm{F}(x; a; b) = 1 - (1 - x^a)^b \tag{5.40}$$

where a and b are shape parameters. In this vein, this analytical formula is fitted to the commercial curve, and a set of parameters, i.e., a and b are extracted.

To account for all possible fluctuations of the real world operation against the standard commercial curve, we represent the set of parameters as random variables, thus this is written as $\underline{\theta}$. By assigning an appropriate distribution functions to $\underline{\theta}$, i.e., $\underline{a}$ and $\underline{b}$ and then employing random sampling of these, we able to describe different possible curves around the commercial one.

5.2.3 The design optimization context

Herein we formalize the design optimization problem in multicriteria terms, involving the estimation of a key characteristic of the RES, namely the determination of the total power capacity and its sharing to its individual components. In this respect, we consider a given layout of the system, such as a wind park, a solar park or a hydroelectric station, where the siting of all supporting infrastructures, by means of civil works (e.g., power station house, road network), are already specified. We remark that the design of most of civil-related infrastructures is strongly related the power capacity of the overall system and its individual components. In this vein, the design variables to optimize are expressed as a vector $\boldsymbol{I} = [I_1, I_2, \dots, I_{NS}]$, where NS is the number of the system's components.

The standard technoeconomic optimization problem is formalized as the maximization of financial quantities, such as the net present value (NPV). According to this concept, the discounted value of future net cash flows should exceed the investment cost, so as to ensure a sustainable investment (Yildiz & Vrugt, 2019). In our case, the cash flows derive from the production of electrical energy during the entire life-cycle of the system, while the investment cost, involving the electromechanical (E/M) equipment and the civil works, is directly or indirectly associated with the power capacity.

Following this, by considering a financial period of n years with a specific interest rate $\underline{i}$, the equivalent annual cost of the investment is given by:

$$A = C \, \frac{i \, (1 + \underline{i})^n}{(1 + \underline{i})^n - 1} \tag{5.41}$$

where C is the total investment cost, which is the sum of individual costs, C_i. We remark that the interest rate is also considered as a random variable, since it depends on various socioeconomic criteria, namely inflation, risk aversion of the investor etc. All these costs are subject to the key principle of economy of scale, thus expressed as:

$$C_i = f(I_i^{\lambda}) \tag{5.42}$$

where $\lambda < 1$ is a shape parameter, expressing the reduction of unit cost with respect to power capacity.

In order to implement the aforementioned cash-flow method in a risk-aware context, the expression of future revenues should be determined in terms of mean annual energy production, $E_a = \mathrm{E}\left[\underline{p}\right] T_a$ (where T_a denotes the annual duration), multiplied by a unit price, $\underline{u}$. The estimation of power production requires running a simulation model, thus E_a is actually a stochastic variable. In addition, the unit price $\underline{u}$ can also generally be considered as a stochastic process (Borovkova & Schmeck, 2017), since it varies in the context of free electricity market trade and supply. Under this premise, the objective function of the design optimization problem is expressed in annual profit terms as:

$$F\left(\boldsymbol{I}, \underline{p}\right) = \underline{u} \, E_a(\boldsymbol{I}, \underline{p}) - A(\boldsymbol{I}) \tag{5.43}$$

This function is strongly nonlinear and contains two conflicting components, namely the mean annual energy production, $E_a(\boldsymbol{I}, \underline{p})$, to maximize, and the equivalent annual cost, $A(\boldsymbol{I})$, to minimize.

To ensure robust solutions, in the multicriteria optimization problem we also embed a third component, which is the resulting capacity factor, CF, of the system under study. According to its common definition, CF is expressed as the ratio of the mean annual electrical energy output to the maximum possible one (Mamassis et al., 2021), i.e.:

$$CF\left(\boldsymbol{I}, \underline{p}\right) = \frac{E_a\left(\boldsymbol{I}, \underline{p}\right)}{T_a \sum_{i=1}^{N} I_i} \tag{5.44}$$

where T_a is the annual duration.

Although CF seems being a rather technical quantity, it is actually a fundamental performance metric of power systems, thus its interpretation plays key role in the evaluation of the viability of a RES. In particular, a low CF is not necessarily associated with poor performance in terms of energy production, but may also be due to the application of a too large installed capacity that is activated a small portion of time.

Since the other two criteria are given in monetary terms, the incorporation of CF within the generic optimization problem is made by assigning a penalty term, to achieve CF values over or close to a desirable threshold, CF^*. The latter is site-specific and varies across different RES types (Miller & Keith, 2018). Under this premise, the proposed multi-objective function to maximize is written as:

$$F'\left(\boldsymbol{I}, \underline{p}\right) = F\left(\boldsymbol{I}, \underline{p}\right) - \max\left[0, CF\left(\boldsymbol{I}, \underline{p}\right) - CF^*\right] w \tag{5.45}$$

where w is a suitable weighting coefficient.

5.2.4 The triptych of statistics, stochastics and copulas in practice

As shown in Figure 5.2**,** the proposed modelling framework under uncertainty follows the Monte Carlo paradigm, which makes use of three tools from the broader probability theory, i.e., stochastics, statistics, and copulas. The first two aim at capturing the major aspects of uncertainty that originate from the inherently random input processes and the model hypotheses, while copulas are used for expressing the socioeconomic uncertainty and in the post analysis phase, as well.

The Monte Carlo approach is applied to the simulation model, which involves most of practical issues of renewable energy (planning, design, long-term assessment, short-term control, etc.). This is configured by means of equally probable simulation scenarios that correspond to m different system's states and input processes. Each hypothetical state runs for N years, which equals the economic life of the project of interest. The state is expressed through three key characteristic properties, namely the efficiency function $\eta\left(\underline{x}, \underline{\psi}\right)$ the unit price, $\underline{u}$, and the interest rate, $\underline{i}$. The first is associated with the internal operation of the RES per se, while the other two derive from the uncertain socioeconomic environment. As mentioned in section 5.2.2, the formulation of efficiency under uncertainty presupposes to introduce an analytical formula, symbolized $\eta\left(\underline{x}, \underline{\boldsymbol{\psi}}\right)$, for the associated machine, where $\underline{\boldsymbol{\psi}}$ is a set of parameters that describe the shape of the curve. These are also represented as random variables, in order to capture all possible fluctuations from the standard commercial curve. This issue is further discussed in the two case studies, providing probabilistic parametric formulas for the power conversion curves of hydro and wind turbines, respectively.

Under this premise, the Monte Carlo scenarios are configured by assigning appropriate distribution functions to $\underline{\boldsymbol{\psi}}$, $\underline{u}$ and $\underline{i}$ and then employing random sampling to define the m potential states of the system. Furthermore, in order to express the external uncertainties induced by the local hydrometeorological regime, each scenario is driven with long synthetic data of length N for the corresponding input processes $\underline{x}$. In this respect, a stochastic model is applied to generate $m \times N$ years of synthetic data, and this sample is then split into m sub-sets, also referred to as ensembles. The temporal resolution of the data depends on the specific process (e.g., hourly for wind velocity and solar radiation, daily for streamflow).

Consequently, outcomes of the simulation scenarios are m ensembles of output processes (e.g., power production) and associated design components (e.g., optimized power capacity) and performance assessment metrics (e.g., mean annual revenues, capacity factor). In this vein, all outputs are represented in stochastic terms, which also allows for quantifying their uncertainty through statistical analyses of the corresponding simulated data. For instance, we can fit suitable probability density functions (pdfs) to individual design and performance assessment metrics. Further insight can be provided by accounting for the joint uncertainty induced by cross-dependencies between the derived design variables and performance metrics. The underlying methodology is based on the work of Tsoukalas (2018), and relies on the use of (Gaussian) copulas to establish the conditional distribution of two (non-Gaussian) random variables. A summary of the employed method is provided in the Appendix A.

The generic algorithmic procedure for the design case, which also contains the assessment problem, is depicted in Figure 5.3. The application of the aforementioned framework is demonstrated by means of two case studies, where a modular approach is adopted, thus adding progressively more sources of uncertainty within simulation and optimization.

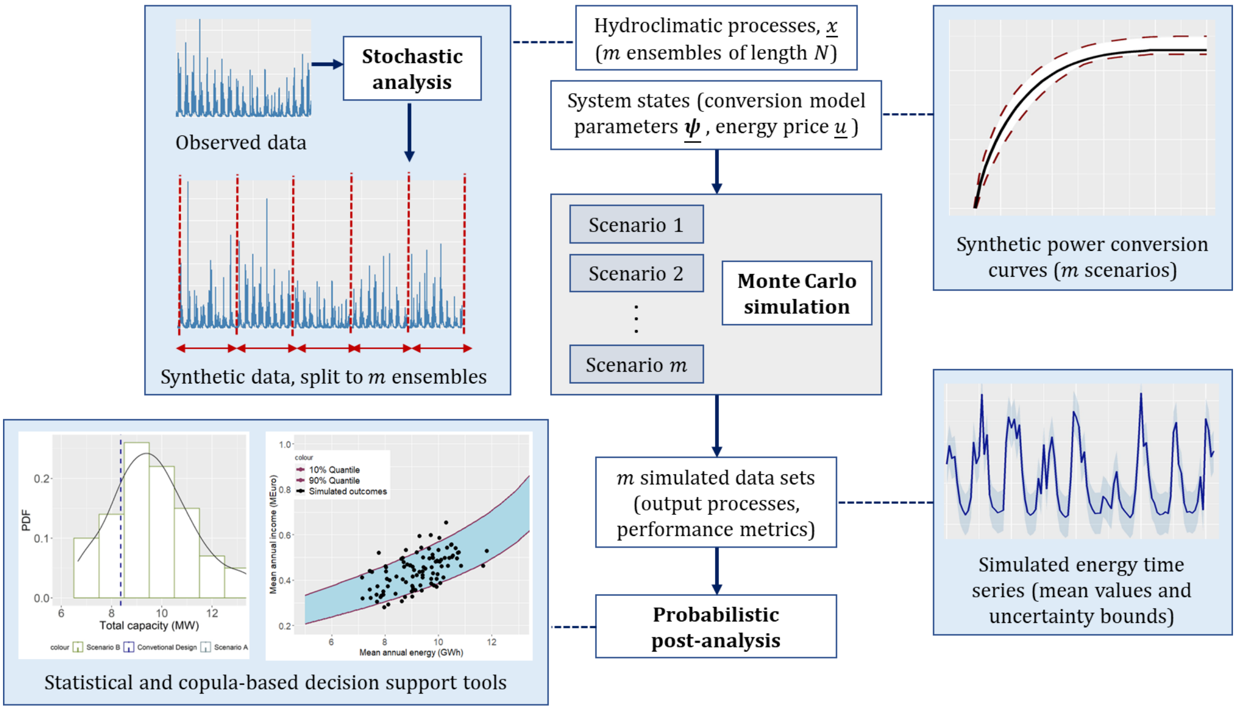


Figure 5.2: Schematic layout of the proposed framework.

Summary of algorithmic procedure for the design of RES under uncertainty

Step 1: Generation of $m \times N$ years of synthetic driving data (e.g., streamflow, wind velocity, solar radiation) at the appropriate temporal resolution (N: project lifetime).

Step 2: Generation of m equally probable system states (e.g., power curves, energy price)

Step 3: Formulation of m Monte Carlo simulation scenarios by splitting synthetic drivers into m ensembles of N-year length and by sampling random system states from the corresponding set

Step 4: Set up of the optimization procedure (*design variables*: power capacity values of system's components, *objective function* as formalized in eq. 5.36)

Step 5: Extraction of m optimized design variables and associated performance metrics

Step 6: Statistical processing of simulation-optimization outcomes:

- Marginal analysis by fitting probability density functions
- Dependence analysis through copulas

Step 7: Selection of final design quantities accounting for their uncertainty

Figure 5.3: Logical flow of the proposed framework regarding the design optimization problem.

5.3 Optimal Design of run-off-river hydroelectric plant under uncertainty

5.3.1 Key principles of hydropower system operation

The uncertainty-aware framework, in the design context, is stressed for a run-off-river (RoR) small hydropower plant, which is a quite complex and promising renewable source. This type of hydroelectric system diverts part of the streamflow arriving to an intake structure, located in the riverbed, to a forebay tanks and then to the power station, which is generally located far from the intake, to create a significant elevation difference. In Figure 5.4, a part of the holistic representation of the water-energy nexus (Figure 1.1) is presented.

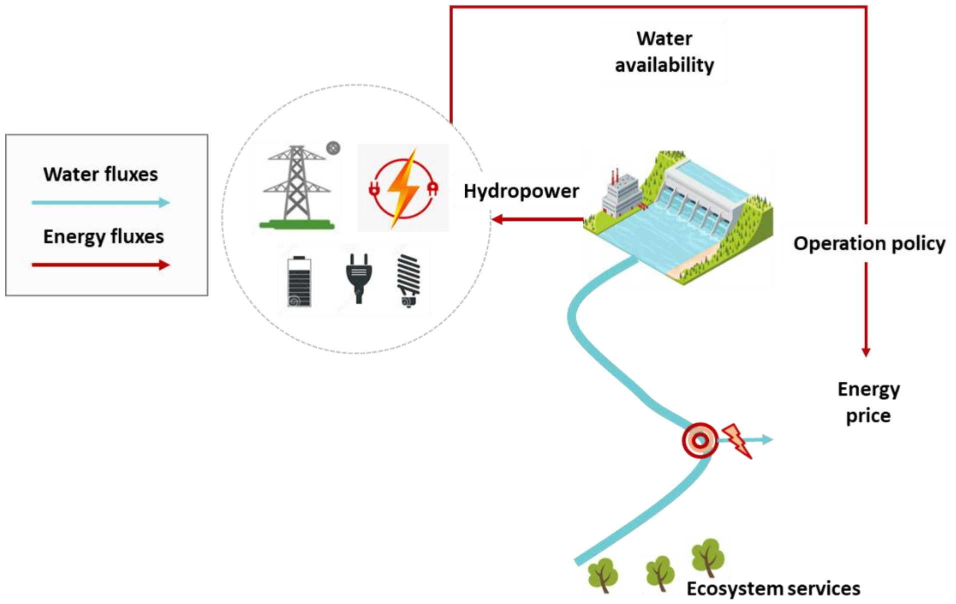


Figure 5.4: Schematic layout of an in-stream hydropower plant. This is a part of **Figure 1.1** (the holistic water-energy nexus) that will be discussed herein.

For a given layout, the design problem lies in the selection of an optimal mixing of turbines, in order to capture as much as possible of the streamflow variability. Let consider a RoR plant comprising two turbines of power capacity, I_1 and I_2, operating within flow ranges ($q_{1,min}$, $q_{1,max}$) and ($q_{2,min}$, $q_{2,max}$), respectively. The range of operation of each turbine is determined by its power capacity. In particular, the maximum discharge is given by:

$$q_{i,max} = \frac{I_i}{\rho\, g\, \eta_{i,max}\, h_n} \tag{5.46}$$

where $\eta_{i,max}$ is the total efficiency of the electromechanical equipment, and h_n is the net head, i.e., the difference between the gross head and the hydraulic losses across the water conveyance system. These losses can be analytically estimated, on the basis of discharge, diameter and other properties. On the other hand, the minimum operational discharge is simply expressed as portion of the maximum one, i.e., $q_{i,min} = \theta\, q_{i,max}$, where θ depends on the turbine type.

The mixed scheme operates from the minimum flow between $q_{1,min}$ and $q_{2,min}$, and the sum $q_{1,max} + q_{2,max}$. A typical operation policy implies the use of the large turbine in priority, while the small one receives the surplus flow, up to its capacity (Anagnostopoulos & Papantonis, 2007). In some cases, a safety limit, q_s, is also imposed, to interrupt the operation of turbines during significant flood events (Hänggi & Weingartner, 2012). Finally, the turbine efficiency can be expressed through the following parametric formula, by adapting eq. 5.40:

$$n = n_{min} + \left(1 - \left(1 - \left(\frac{q^* - \theta}{1 - \theta}\right)^a\right)^b\right)(n_{max} - n_{min}) \tag{5.47}$$

where $q^* = q_T / q_{max}$ is the rated flow, n_{min} and n_{max} are the upper and lower efficiency values, and a and b are shape parameters depending on the turbine type. The total E/M efficiency is obtained by multiplying with an adjusting factor, with typical value 0.95.

5.3.1 Rainfall-runoff model

The estimation of the generated runoff over the upstream catchment is an essential part of this framework, instead of using the historical inflows. Even if the employment of a rainfall-runoff model increases uncertainty, it is “necessary evil” since the historical inflow data are significantly smaller than rainfall’s one. In addition, by employing a rainfall-runoff model, we can incorporate the initial source of uncertainty, i.e., climate.

4.3.1.1 Simulation procedure

To estimate the runoff generated over the upstream catchment, a flexible, parsimonious, and easily adjustable model should be selected. This must combine the ability to run long-term simulations in daily time intervals with minimal computational burden. In our case, we are taking advantage of the lumped scheme proposed by Efstratiadis et al. (2015), which is applicable for long-term simulations accepting stationarity of input processes and both steady-state and changing basin properties. To calibrate the model and extract the optimal set of parameters (totally eight), the use of the multi-objective performance measure is necessary, since it aggregates three typical goodness-of-fitting metrics (NSE, KGE, bias). The outcome of this model, i.e., the daily runoff, will next feed the simulation model of the run-off-river hydroelectric. The conceptual scheme of the hydrological model is depicted in Figure 5.5.

Input data to the simulation procedure are the time series of precipitation, P, and potential evapotranspiration, PET. The storage terms are expressed in units of equivalent water depth (mm), while flows are given in units of water depth per unit time, Δt. In the description of the equations, the time step index (in this case, day) is omitted, for simplicity.

At the beginning of each time step, the storage of the three reservoirs is known, from the solution of the previous step, i.e. the temporary water retention at the soil surface, I_0 (upper reservoir), the moisture storage in the unsaturated zone, S_0 (intermediate soil moisture reservoir) and the groundwater storage, W (lower reservoir storage).

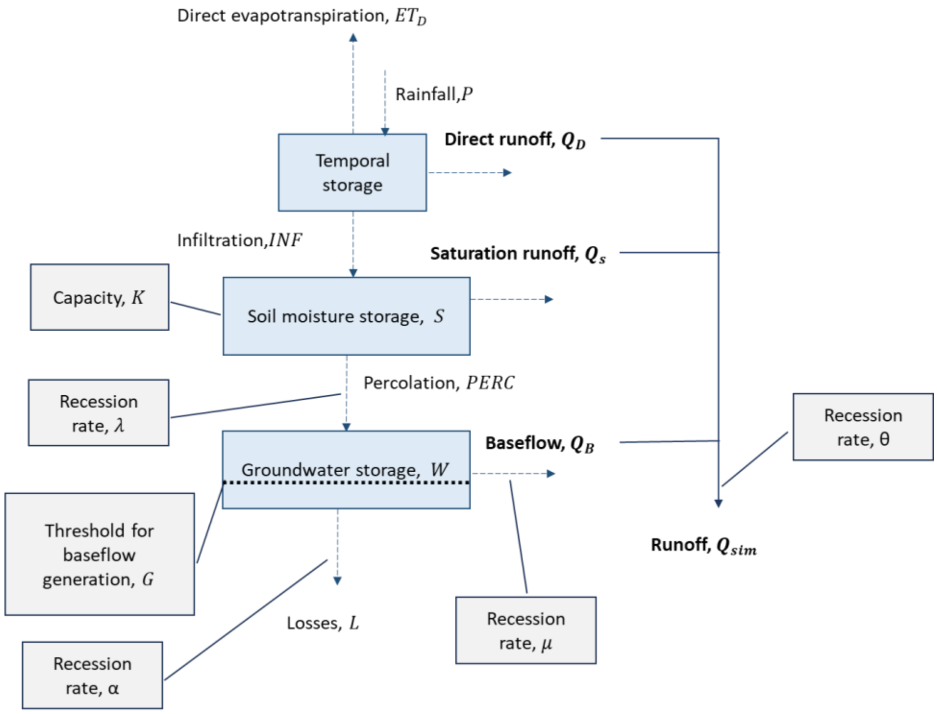


Figure 5.5: Conceptual illustration of hydrological model processes and parameters.

The precipitation is temporarily retained in the upper tank, with a capacity of I_{max}. According to the approach of the Soil Conservation Service (USDA, 2004), this capacity is estimated as a percentage, β, of the maximum potential retention, i.e., the amount of water that the unsaturated zone can hold. This quantity is generally equal to $K - S$, while at the beginning of the time step $S = S_0$ applies. Therefore, the surface retention capacity is given by :

$$I_0 = \beta(K - S_0) \tag{5.48}$$

If the precipitation value exceeds the available storage of the surface retention tank (temporal storage) i.e. if $P > I_{max} - I_0$ then direct (surface) runoff is produced, through the relationship:

$$Q_D = v\,(P - I_{max} + I_0) \tag{5.49}$$

The amount (percentage) v is not constant but also depends on the current soil moisture conditions, and is estimated based on the relationship of the Soil Conservation Service (USDA, 2004), namely:

$$v = \frac{P - I_{max} + I_0}{P - I_{max} + I_0 + K - S_0} \tag{5.50}$$

This zone is represented by the intermediate reservoir, whose capacity is equal to K, while its storage is equal to S (in this case it is set equal to the known storage, S_0, at the end of the previous time step). It is pointed out that the capacity K is a parameter of the model, while the quantity S is a state variable of the model. In the calculations, S is taken to be the moisture storage at the end of the previous time step. Conversely, if $P \leq I_{max} - I_0$, then no surface runoff is produced.

In any case, the available amount of water retained on the ground and by the vegetation is available for the production of direct evapotranspiration, through the relationship:

$$ET_D = \min(PET, I_0 + P - Q_D) \tag{5.51}$$

The amount of water that cannot be retained on the surface is filtered, through the soil, into the intermediate reservoir (soil moisture reservoir), through the relationship:

$$INF = \max(0, I_0 + P - Q_D - ET_D - I_{max}) \tag{5.52}$$

Therefore, at the end of the step, the soil moisture retention is:

$$I = I_0 + P - Q_D - ET_D - INF \tag{5.53}$$

Also, the moisture available at the beginning of the time step is:

$$S = S_0 + INF \tag{5.54}$$

Subsequently, three types of outflows from the intermediate reservoir take place, namely soil evapotranspiration, infiltration to the lower reservoir, and overflow due to soil saturation. In particular, the losses due to soil evapotranspiration depend on the filling rate of the tank and are estimated by:

$$ET_S = \frac{S\left(2 - \frac{S}{K}\right)\tanh\left(\frac{PET - ET_D}{K}\right)}{1 + \left(1 - \frac{S}{K}\right)\tanh\left(\frac{PET - ET_D}{K}\right)} \tag{5.55}$$

where S/K is the tank filling ratio, and $ET - ET_D$ refers to the remaining demand for evapotranspiration production. Obviously, if the “demand” from precipitation on the ground has been met, then no further evapotranspiration is required to be produced through the unsaturated zone. The above relationship is semi-empirical, and is based on Turc-Budyko's theoretical nomograms, which link actual evapotranspiration to water and energy availability, as defined by precipitation and potential evapotranspiration, respectively (Andréassian & Perrin, 2012).

Finally, the total losses due to evapotranspiration are:

$$ET = ET_D + ET_S \tag{5.56}$$

The amount of water infiltrating to the lower tank is estimated as a percentage of the stored moisture:

$$PERC = \lambda S \tag{5.57}$$

where λ refers to the recession rate, which is a parameter of the model.

The excess quantity that overflows, namely:

$$Q_S = \max(0, S - K) \tag{5.58}$$

referred to as runoff due to saturation, and together with direct runoff constitute the surface runoff, which passes through the hydrographic network of the basin, and finally reaches its outlet with a time lag and smoothing. The particularly complex process of surface runoff routing, the modeling of which will be further described, is symbolized through the transformation function:

$$Q_R = f(Q_D + Q_S) \tag{5.59}$$

The final balance of the soil moisture reservoir is written:

$$\Delta S = INF - ET_S - PERC - Q_{\mathrm{S}} \tag{5.60}$$

The infiltration from the upper reservoir feeds the lower reservoir is increased its initial reservoir to:

$$W = W_0 + PERC \tag{5.61}$$

In this tank, which has no capacity limit, the processes of the aquifer are realized (saturated zone). In particular, two outflows take place, one horizontal and one vertical. The first represents the source (base) runoff, in the form of outflow from a horizontal hole, through the relationship:

$$Q_{\mathrm{B}} = \max[0, \mu\,(W - G)] \tag{5.62}$$

where G is the water height (threshold) for the production of underground runoff and μ is the recession rate, which is a parameter of the model. The above expression allows or not the production of base flow, thus the possibility of representing intermittent flow basins, depending on the range of variation of the groundwater reservoir. For this purpose, a special control parameter is introduced in the model.

The second (vertical) outflow represents deep infiltration, which is not discharged into the basin but is routed into downstream aquifers, constituting, in essence, losses from the system. These losses are estimated by the relation:

$$L = \alpha\, W \tag{5.63}$$

where α refers to the recession rate, which is a parameter of the model.

The final balance of the groundwater reservoir is written:

$$\Delta W = PERC - Q_{\mathrm{B}} - L \tag{5.64}$$

Making the above assumptions, the runoff that ends up at the outlet of the basin is the sum of the diverted surface runoff and the base flow, that is:

$$Q = Q_R + Q_B \tag{5.65}$$

It should be pointed out that if the hydrological simulation is done on a longer time scale (e.g. monthly), then it can be considered that the surface runoff component, i.e. the quantity $Q_R + Q_S$ reaches the outlet of the basin as it is, i.e. without requiring its transformation due to routing processes. However, on the daily scale, the concept of tolling is particularly important, and for this purpose an additional computational procedure was developed, as explained below.

The routing processes are described through a two-stage combinatorial scheme, which allows for the smoothing and time-shifting of the produced surface runoff. Specifically, in a first stage a smoothing transformation is applied through a linear reservoir, and then a linear smoothing-displacement filter based on unit hydrograph theory is applied.

The operation of the linear reservoir is based on the consideration of a reservoir of unlimited capacity, fed by a varying input $i(t)$, while the output $y(t)$ is a linear function of the storage $x(t)$, ie:

$$y(t) = \frac{dx}{dt} = \frac{1}{k}\, x(t) \tag{5.66}$$

where k parameter, with dimensions of time, controls the outflow rate. In this case, the surface runoff is considered as input, i.e. the sum, $Q_R + Q_S$, and the routed runoff as output, given by the equivalent relationship (in discretized form):

$$Q_{R1} = \theta\, X \tag{5.67}$$

and θ is the recession rate (dimensionless, since both outflow and storage are expressed in units of water equivalent height), which is a parameter of the model. The smaller the value of θ, the more smoothing is achieved. If X_0 is the storage at the beginning of the time step, then to it is added the surface runoff produced by the model, through the corresponding relations so the routed runoff is:

$$Q_{R1} = \theta\, (X_0 + Q_D + Q_S) \tag{5.68}$$

at the end of each time step, the storage is replenished to:

$$X = X_0 + Q_D + Q_S - Q_{R1} \tag{5.69}$$

In the second routing stage, a linear filter is applied given by the relation:

$$Q_{R2,t} = \sum_{j=0}^{N} \alpha_j\, Q_{R1,t-j} \tag{5.70}$$

where $Q_{R1,t-j}$ are the values of the surface runoff routed through the linear reservoir, for lag from 0 to N time steps (days), and α_j refer to the weight factors, which satisfy the relationship:

$$\sum_{j=0}^{N} \alpha_j = 1 \tag{5.71}$$

With the above procedure, the finally produced surface runoff, Q_{R2}, is expressed as a linear combination of the routed runoff of the current and N previous time steps.

For the estimation of the weight coefficients α_j we assume that the above transformation follows the form of the unit hydrograph (UH) of the basin. In this case, the standard synthetic hydrograph developed by NRCS (2007), called Standard PRF 484 (PRF stands for peak rate factor), and which has been widely applied in flood studies (among others, was applied generally in the hydrological analyzes of Directive 2007/60/EC). The components are given in non-dimensionalized form (time t to rise time t_p, and flow q to peak flow q_p), based on the following table (Table 5).

Table 5: Components of the Standard PRF 484.

t/t_p	q/q_p	t/t_p	q/q_p	t/t_p	q/q_p
0.0	0.000	0.9	0.970	2.0	0.320
0.1	0.015	1.0	1.000	2.2	0.240
0.2	0.075	1.1	0.980	2.4	0.180
0.3	0.160	1.2	0.920	2.6	0.130
0.4	0.280	1.3	0.840	2.8	0.098
0.5	0.430	1.4	0.750	3.5	0.036
0.6	0.600	1.5	0.650	4.0	0.018
0.7	0.770	1.6	0.570	4.5	0.009

0.8	0.890	1.8	0.430	5.0	0.004

4.3.1.2 Routing procedure

A key element of the UH is the lag time, t_L, defined as the distance of the center of gravity of the UH, duration D (practically identical to the peak time, t_p) from the center of gravity of the precipitation, which corresponds to the time instant $t = D/2$. According to common hydrological practice, the lag time can be estimated as a constant percentage of the concentration time t_c, ie:

$$t_L = 0.6\, t_c \tag{5.72}$$

On the assumption that the center of gravity of the UH coincides in time with the peak, the rise time t_p is estimated as a function of the rain duration D and the concentration time t_c, through the relation:

$$t_p = t_L + \frac{D}{2} = 0.6\, t_c + \frac{D}{2} \tag{5.73}$$

By its conceptualization, the Standard PRF 484 has a base time $t_b = 5\, t_p$, while in the estimation of the rise time two quantities are introduced, namely the rain duration, D, and the concentration time, t_c. In the present modelling, 12 hours (i.e. half of the time step) is conventionally considered as the rainfall duration, while the concentration time is estimated by the well-known Giandotti relation, namely:

$$t_c = \frac{4\sqrt{A} + 1.5L}{0.8\sqrt{\Delta z}} \tag{5.74}$$

where $t_c$is the concentration time (h), A the area of the basin (km^2), L the length of the longest water path in the basin (km) and Δz the altitudinal difference of the average elevation of the basin from the elevation of its outlet node (m). Given the time quantities t_p and t_b, the UH of the basin is obtained, in which its ordinates (provisions) are given in undistributed form. Then, the UH is reformulated in a discretized form, i.e. in a daily time step, so correspondingly the non-statistical benefits are reported on a daily scale. These values, divided by the total non-dimensional zed runoff, correspond to the weighting factors, α_j, applied by the linear pass filter.

4.3.1.2 Calibration of the model

Eventually for the calibration of this model, we need to define the eight parameters, i.e.,

(a) The recession rate β, referred to in the literature as the initial loss percentage
(b) the capacity of the soil moisture tank, K, expressing the storage capacity of the unsaturated zone of the soil
(c) the recession rate for infiltration production, λ, expressing the percentage of water moving from the soil moisture tank to the groundwater tank, i.e., the water flowing from the unsaturated to the saturated zone of the soil (infiltration)·
(d) the recession rate for baseflow production, μ, expressing the percentage of stored groundwater above the threshold G, which is discharged through point or distributed sources into the river
(e) the baseflow production threshold, G, expressing the quantity of groundwater that must be stored in order to produce baseflow
(f) the recession rate, ξ, determining the minimum groundwater level during the dry period, and consequently controlling whether the flow can become intermittent or not

(g) the recession rate, for deep infiltration and/or underground escapes, α, expressing the percentage of groundwater diverted to deeper layers and ultimately discharged outside the basin
(h) the recession rate, θ, of the routing shape through the linear reservoir, controlling the smoothing of surface runoff during its transfer through the soil surface to the basin outlet.

A critical aspect of the modelling procedure of evaluating the predictive ability of the model is the formulation of a performance measure, which evaluates the fitting of the simulated discharges to the observed, and the generally good hydrological behavior of the model. This measure, which is also used as an objective function during the calibration process, includes three terms.

The first term is the efficiency measure, known in hydrological literature as the Nash-Sutcliffe efficiency index, given by the equation:

$$NSE = 1 - \frac{\sum_{t=1}^{N}(Q_{obs,t} - Q_{sim,t})^2}{\sum_{t=1}^{N}(Q_{obs,t} - \mu_{obs})^2} \quad (5.75)$$

where $Q_{obs,t}$ is the observed value at time step (day) t, $Q_{sim,t}$ the corresponding value estimated by the simulation model, μ_{obs} is the mean value of observations, and N is the length of the control horizon. The value of NSE ranges from -∞ to 1, where 1 indicates perfect fit. A characteristic value of $NSE = 0$ indicates a model with predictive ability equal to the mean value of observations, μ_{obs}, while negative values indicate models with even more limited predictive ability. For representing basin outflow, efficiency values in the range of 0.80-0.90 are considered very satisfactory, while values around 0.30 are considered marginal for characterizing a model as representative of the physical system (Efstratiadis & Koutsoyiannis, 2010).

The second term is the Kling-Gupta efficiency index, KGE, given by the equation (Gupta et al., 2009):

$$KGE = 1 - \sqrt{(\rho - 1)^2 + \left(\frac{\mu_{sim}}{\mu_{obs}} - 1\right)^2 + \left(\frac{\sigma_{sim}}{\sigma_{obs}} - 1\right)^2} \quad (5.76)$$

where ρ is the correlation coefficient between observed and simulated runoff values, μ_{sim} and μ_{obs} are the mean values of simulated and observed runoff, respectively, and σ_{sim} and σ_{obs} are the standard deviations of simulated and observed runoff, respectively. In recent years, this measure, which has become popular in hydrology, gradually replacing the more classical NSE index, is used to ensure that the statistical characteristics of the simulated runoff are maintained compared to the observed runoff.

The third term is a transformation of the NSE index, given by the equation:

$$logNSE = 1 - \frac{\sum_{t=1}^{N}(\ln(Q_{obs,t}) - \ln(Q_{sim,t}))^2}{\sum_{t=1}^{N}(\ln(Q_{obs,t}) - \ln\,(Q_{mean}))^2} \quad (5.77)$$

This index, which implements a logarithmic transformation of flows, is introduced to ensure a better fit of the model to low flows, the accurate reproduction of which is particularly critical in the design of small hydropower plants. Similar to NSE, the theoretically maximum values of the KGE and $logNSE$ indices are unity, indicating a perfect fit, while there is no lower limit regarding the minimum value.

In this research, as a performance measure and thus as the objective function for the calibration problem, the average of the three aforementioned indices is taken, considering them equally essential and focusing on different aspects of model fitting:

$$F = (NSE + KGE + logNSE)/3 \tag{5.78}$$

5.3.2 Study area, data and design assumptions

The hydropower plant under design is established in a sub-catchment of Pamisos River in Thessaly, Greece, taking advantage of a gross head of 45 m. The penstock length and diameter are 500 m and 1.5 m, respectively. The available historical data comprises daily rainfall and runoff records for 39 years, with mean annual values of 950 mm and 630 mm, respectively. Following the Greek legislation, we apply an environmental flow to be released downstream of the intake, which equals to 0.20 m^3/s.

Regarding the calibration of the rainfall-runoff model, the parameters are given in Table 6, while the performance metrics are $NSE = 0.486$, $KGE = 0.658$, and $logNSE = 0.714$.

Table 6: Parameters of rainfall-runoff model.

Parameter	Value	Parameter	Value
β	0.10	G	100.0
K	293.6	ξ	0.951
λ	0.399	α	0
μ	0.0363	θ	0.50

The key design objective involves the setting of two Francis-type turbines. Their efficiency is approximated by eq. (11), where $n_{min} = 0.30$, $n_{max} = 0.93$, $a = 0.80$ and $b = 3.75$. For the estimation of hydraulic losses across the penstock, we consider a roughness coefficient up to 1.0 mm.

5.3.3 Deterministic optimization context

Since the configuration of the major system components (intake and power station sites, layout of diversion, penstock diameter) are already specified, their investment costs are fixed. In this respect, the annual profit component (eq. 5) includes the cost of E/M equipment, which implies a high percentage (30-40%) of the total budget of a typical small hydropower plant (Ogayar & Vidal, 2009). In the literature, this cost is linked with the power capacity, I, and the gross head, h, through empirical relationships. In the present study we apply the following formula, proposed by Aggidis et al. (Aggidis et al., 2010):

$$C = C_0\, I^{\alpha}\, h^{\beta} \tag{5.79}$$

where $C_0 = 14\,400$ €, $a = 0.56$ and $\beta = -0.112$.

The rest assumptions for the configuration of the objective function (eq. 9) involve the assignment of selling price of electrical energy and the capacity factor threshold, which are set equal to u = 0.087 €/kWh and $CF^* = 0.25$, respectively. We remark that, although this price should, in general, be handled as a random variable, here we employ a fixed value, according to the Greek legislation for small hydroelectric plants that are not yet entered the energy market model. On the other hand, the selection of CF^* is based on engineering evidence, and prohibits the derivation of oversized turbines, in order to exploit large yet low-frequency streamflows.

To insight to the optimization problem, we repeat the design procedure for a large number of turbine capacity combinations, driven by the historical streamflow data. We highlight that since the formulation of the problem is deterministic, it leads to a unique solution, i.e., the global optimum of the profit function. Interestingly, as shown in Figure 5.6, the response surface comprises two regions of attraction, and thus two optimal mixings, with quite close performance. These reveal two alternative operation policies, one by setting in high priority the large turbine (global optimum) and the other the small one (local optimum).

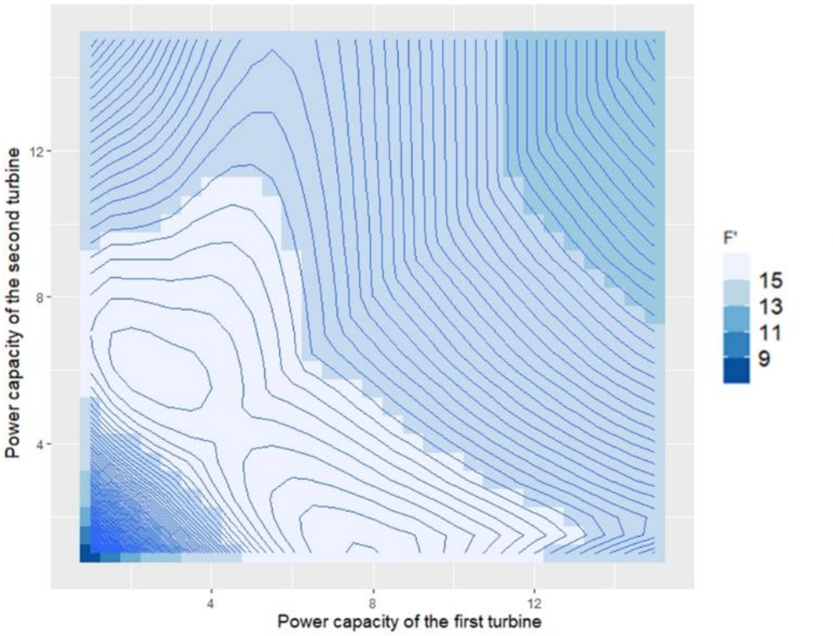


Figure 5.6:: Response surface of the profit function, highlighting the two optima points that indicate alternative turbine mixings.

5.3.4 Building the design procedure under uncertainty

In order to better reveal the potentials of the stochastic design framework over the conventional, deterministic one, we demonstrate a modular scheme to disentangle the key sources of uncertainty, aleatory and epistemic, exogenous and endogenous. In particular, we establish five settings of the optimization problem, herein symbolized A, B, C, D and E, with respect to the each source of uncertainty.

4.4.4.1 First setting: Generation of synthetic rainfall timeseries

The *first setting* aim to represent the aleatory uncertainty (exogenous) originating from the natural variability of rainfall. In this respect, we provide of m ensembles of synthetic precipitation time series (the primary climatic drivers of all hydropower systems) through the hydrometeorological process generator, as proposed in section 3.1.3. A window of generated rainfall timeseries compared with the observed is demonstrated in Figure 5.7. Next, these rainfall timeseries are used as inputs to the rainfall-runoff model, as described in section 5.3.1, by considering the set of optimized model parameters, thus providing m ensembles of simulated inflows.

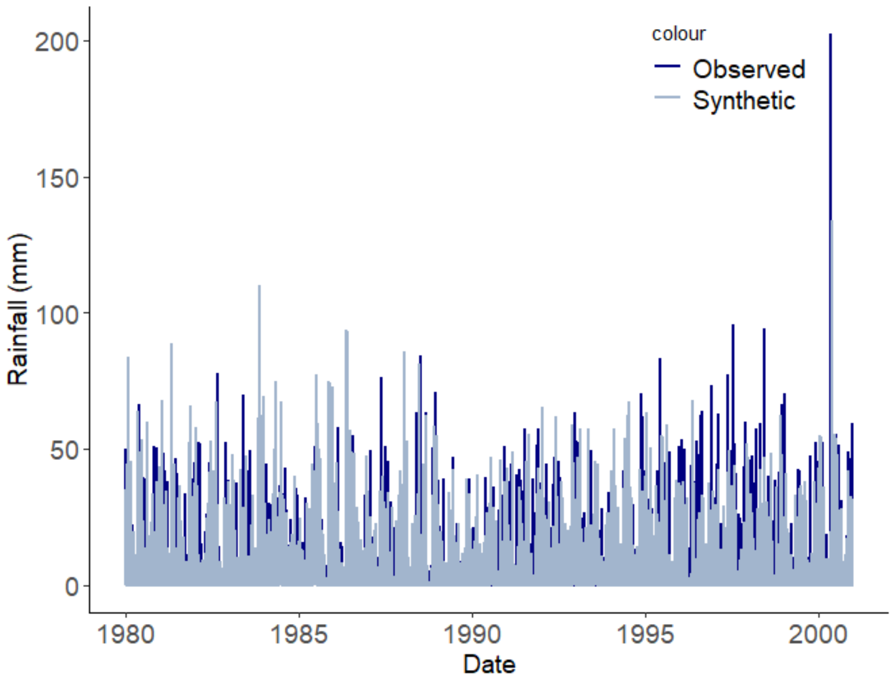


Figure 5.7: A window of generated rainfall timeseries compared with the observed ones.

4.4.4.2 Second setting: Generation of synthetic inflow timeseries

The second setting aim to represent the epistemic uncertainty (endogenous) originating from the lack of knowledge of the modelling of rainfall-runoff models. In this respect, we employ the methodology as described in section 3.4.2 In our case, all monthly-resolved error processes follow the Generalized Gamma distribution. An example of this fitting is given in Figure 5.8, while the rest of them are presented in the Appendix (section 10.2). In this addition, Table 7 presents the target autocorrelation structure for the errors. The comparison of the statistical properties (mean, standard deviation and skewness) between observed and simulated errors are given in Table 8. As before, an ensemble of $m \times N$ years of synthetic runoff timeseries are generated. In Figure 5.9, a window of the generated runoff timeseries, by means of quantiles, is compared to the observed runoff. As expected, the error is decreased for the low flow part of the data, while it exhibits large fluctuations for the peak flows.

Table 7: Shape parameters of the target autocorrelation structure for the errors $w'_{t,s}$.

Month	κ	β
January	0.60	4.40
February	0.21	0.01
March	0.21	0.01
April	0.12	0.01
May	0.17	0.09
June	0.18	0.01
July	0.15	0.01
August	0.11	0.01
September	0.10	5.00

October	0.10	2.20
November	0.24	1.05
December	0.19	0.01

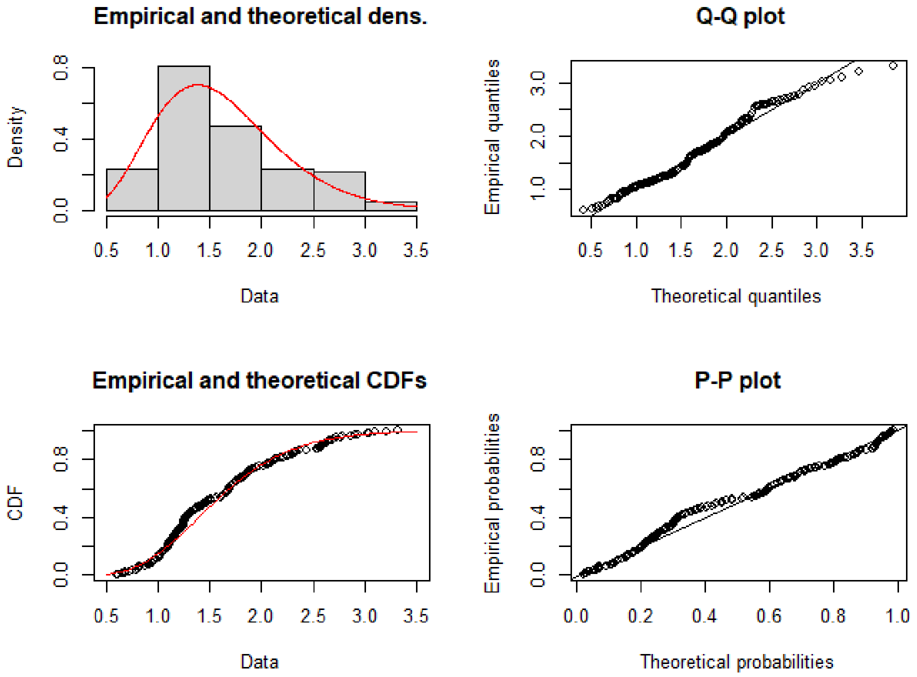


Figure 5.8: Fitting of marginal distribution of the monthly-based error processes, w'_s, regarding the April data.

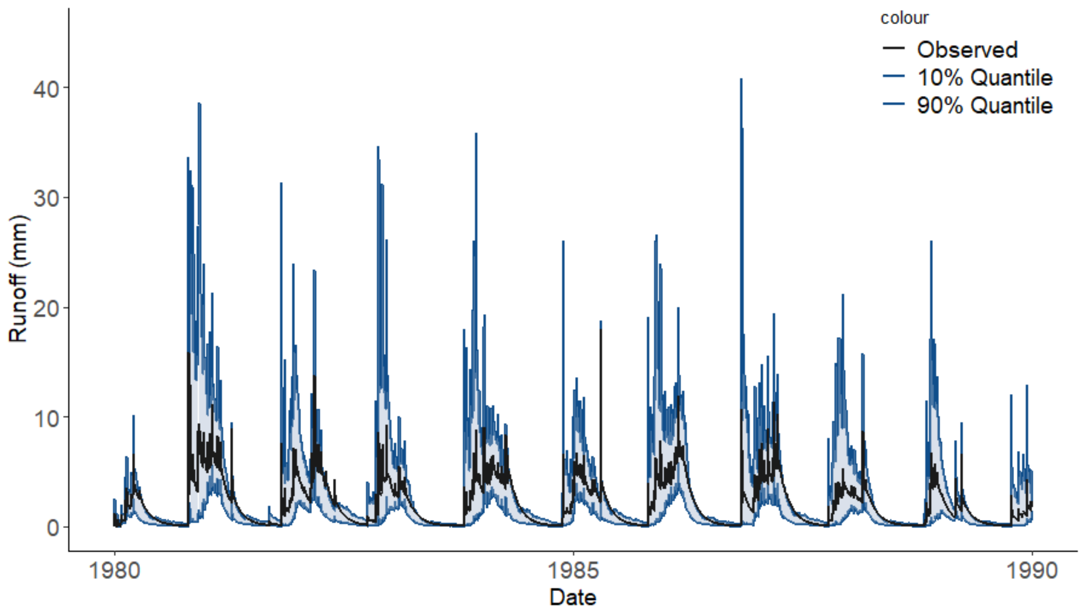


Figure 5.9: 80% uncertainty intervals of generated runoff timeseries compared with the observed ones.

Table 8: Statistical properties of errors (observed and simulated).

Month	error	Mean	Standard deviation	Skewness
January	Observed	-0.033	0.466	0.062
	Simulated	-0.033	0.461	0.065
February	Observed	0.022	0.462	-0.923
	Simulated	0.018	0.463	-0.932
March	Observed	0.449	0.506	-0.215
	Simulated	0.454	0.504	-0.198
April	Observed	0.851	0.609	0.697
	Simulated	0.846	0.604	0.719
May	Observed	0.919	0.485	-0.155
	Simulated	0.904	0.483	-0.149
June	Observed	0.294	0.656	1.208
	Simulated	0.296	0.670	1.223
July	Observed	-0.100	0.591	0.339
	Simulated	-0.103	0.592	0.321
August	Observed	-0.200	0.873	-0.193
	Simulated	-0.218	0.855	-0.190
September	Observed	-0.058	1.249	0.197
	Simulated	0.030	1.260	0.202
October	Observed	0.389	1.562	0.080
	Simulated	0.405	1.581	0.081
November	Observed	0.310	1.393	1.275
	Simulated	0.312	1.410	1.257
December	Observed	-0.009	0.618	0.395
	Simulated	-0.024	0.608	0.414

4.4.4.3 Third setting: Generation of synthetic efficiency curves

The *third setting* also aim to represent the epistemic uncertainty (endogenous) originating from the lack of knowledge of the modelling of turbine efficiency. In this vein, we repeat the m optimization scenarios, driven with equally probable efficiency formulas (Figure 5.10). Following the rationale of section 3.4.1 and 5.3.1, we consider the four parameters of eq. 5.47 as random variables, thus we sample the efficiency bounds $\eta_{\min}$ and η_{max} from a Beta distribution, and the shape parameters a and b from a Normal one. This ensures that the derived curves are asymmetrically spread around the standard one, to account for the effects of systematic drop of efficiency due to ageing.

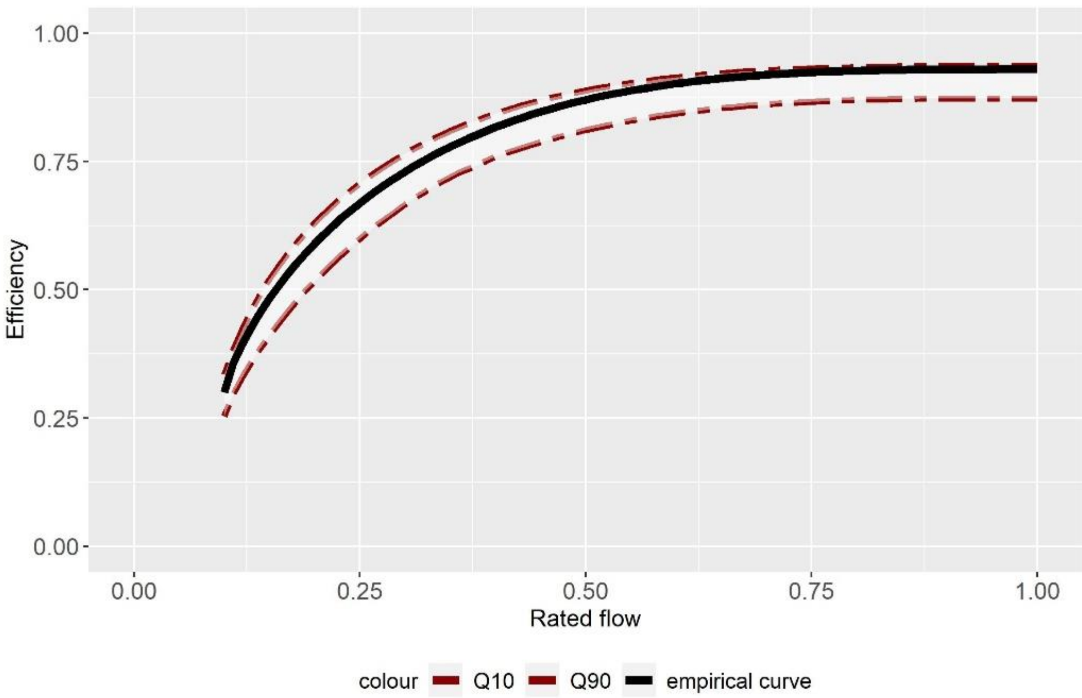


Figure 5.10: Equally probable efficiency curves asymmetrically spread around the standard (empirical) one to emphasize ageing effects.

4.4.4.4 Fourth setting: Generation of synthetic interest rates

The *fourth setting* aim to represent the economic uncertainty, originating from the broader socioeconomic environment. In particular, this aspect of uncertainty is expressed by means of the interest rate or the internal rate of return of the investment, $\underline{i}$. This component is a highly connected to the inflation (Figure 5.11), since when the inflation rate is high, interest rates tend to rise too – so although it costs you more to borrow and spend, you could also earn more on the money you save. When the inflation rate is low, interest rates usually go down. In this respect, to comply with this facet of uncertainty we generate m ensembles of interest rate to run the optimization procedure. Taking advantage of the copula-based theory, we estimate this element by employing the joint distribution of the inflation and the interest rate. The theoretical background to build copulas is given in section 3.5. In brief, we first select the appropriate marginal distribution for each variable, i.e., inflation and interest rate and the "best-fitted" copula from a range of family. In our case, the Generalized Gamma distribution is selected, while the Gaussian copula is the most appropriate.

Next, we generate m inflation values from its marginal distribution and make a random sampling of m quantiles. Eventually, for each set of inflation value and random quantile, the interest rate is extracted, thus providing m equally probable interest rates (Figure 5.12).

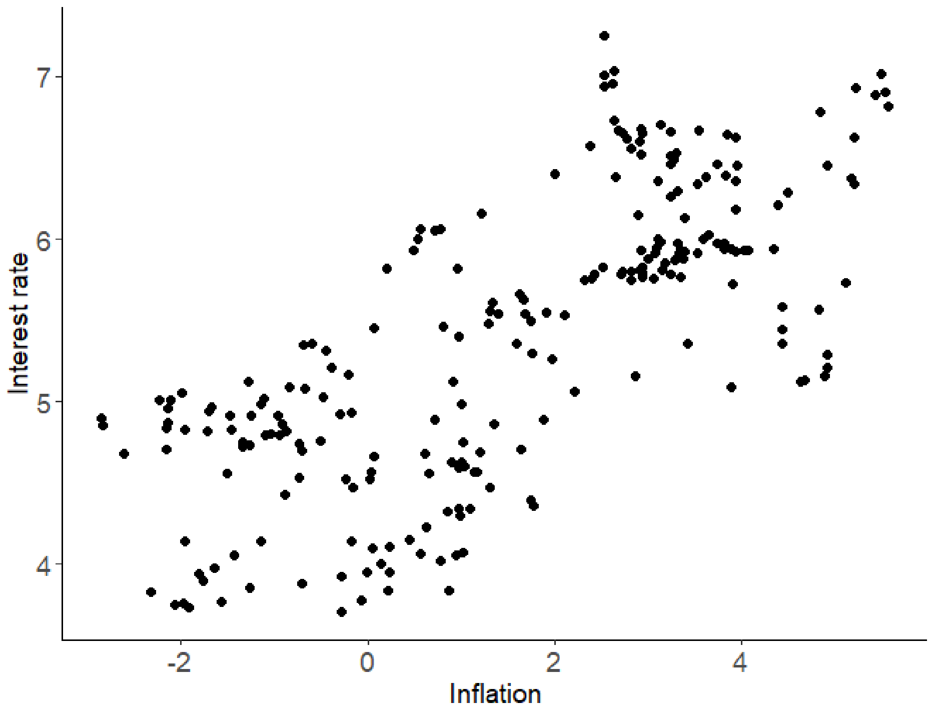


Figure 5.11: Scatterplot of the observed inflation (%) with interest rate (%) for renewable projects (source: Federal Reserve Bank of Cleveland).

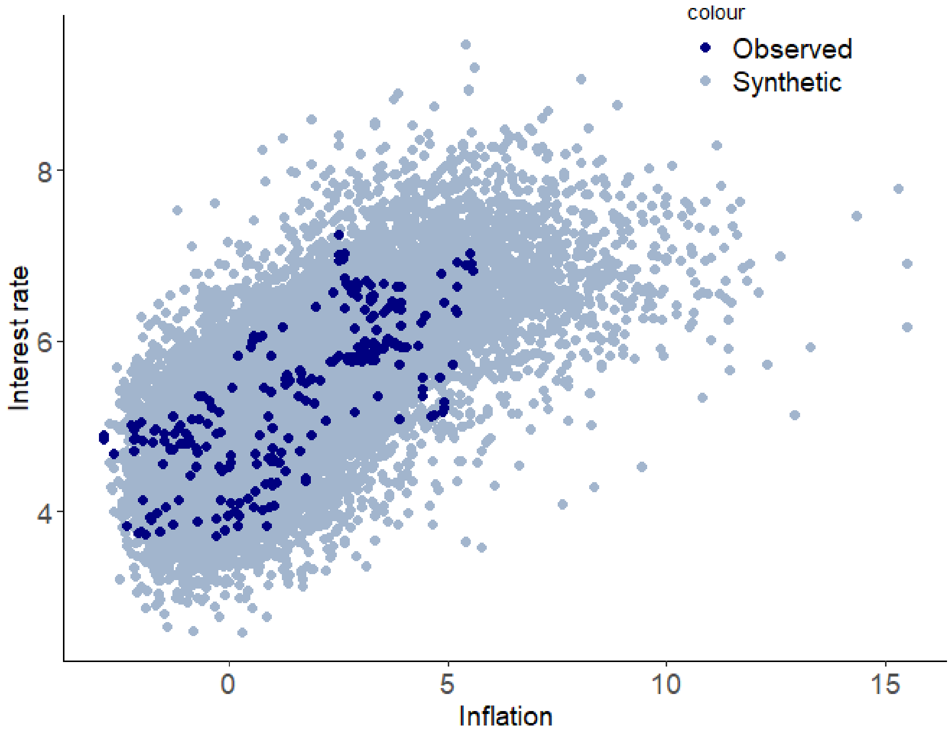


Figure 5.12: Comparison of generated and observed inflation and interest rates for renewable projects.

4.4.4.5 Fifth setting: Combination of the first fourth settings

The *fifth* and final *setting* refers to the combination of above settings, providing a holistic optimization context, since all aforementioned uncertainties are incorporated. In particular, $m \times N$ years of synthetic rainfall timeseries are generated. Then the rainfall-runoff model runs and an ensemble of generated inflows are provided. Next, $m \times N$ errors are assigned to the runoff ensemble, thus incorporating the first aspect of epistemic uncertainty. Finally, the simulation-optimization scheme runs by taking as inputs the above inflows, the uncertain efficiency curves of the turbines (refer to 4.4.4.3) and the m interest rates.

5.3.1 Results

Each optimization setting results to scenarios of 200 equally probable optimized sets of power capacity values and associated performance metrics. As shown in Figure 5.13**,** the uncertainty-aware design procedure leads to two characteristic patterns across the two regions of attraction, already revealed from the deterministic optimization approach. The lower right pattern, which implies the use of the larger turbine as primary, is well-approximated by a linear relationship, while the upper left one formulates an oval scheme. We highlight that as the description of uncertainty becomes more detailed, the spread of these patterns increases, and, furthermore, their distribution is the objective space changes significantly. As shown in Table 9, the incorporation of uncertainty leads to a wide range of optimal values across all key quantities of the design procedure (total capacity, energy production, etc.). As expected, these differ across the alternative settings.

In Figure 5.14, we demonstrate the histogram of the optimized total capacity values (for setting E, accounting for both external and internal uncertainties) and contrast it with the single value provided by the deterministic approach. Furthermore, in Figure 5.15, we apply the copula theory, in order to quantify the predictive uncertainty of the anticipated profits against the total power capacity. In a real-world practice, the user can first refer to Figure 5.14 for turbine sizing, by selecting an appropriate quantile (which represents the risk of the design policy), and next take advantage of Figure 5.15, in order to quantify the predictive uncertainty of the investment.

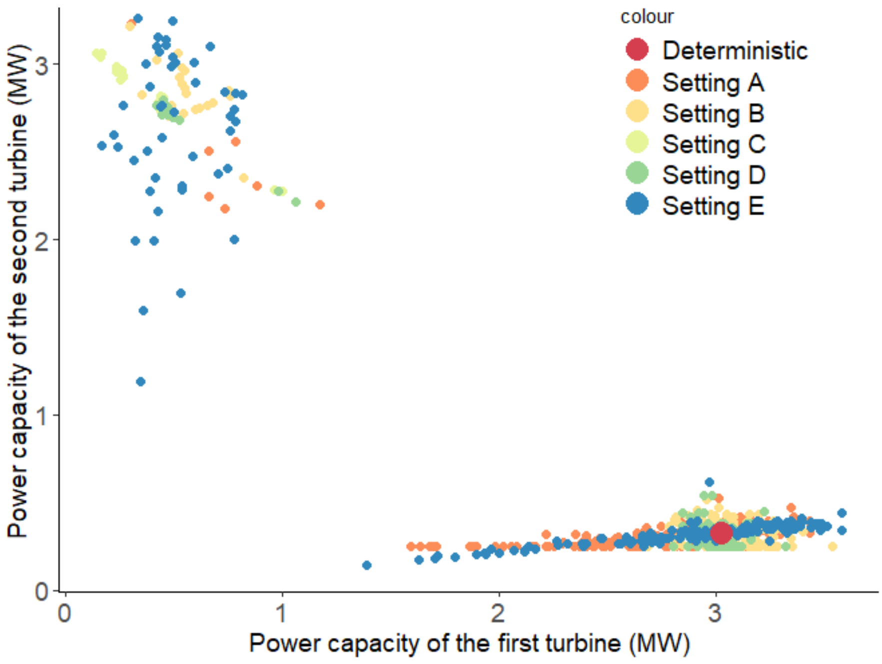


Figure 5.13: Optimized sets of turbine mixing for the three problem settings.

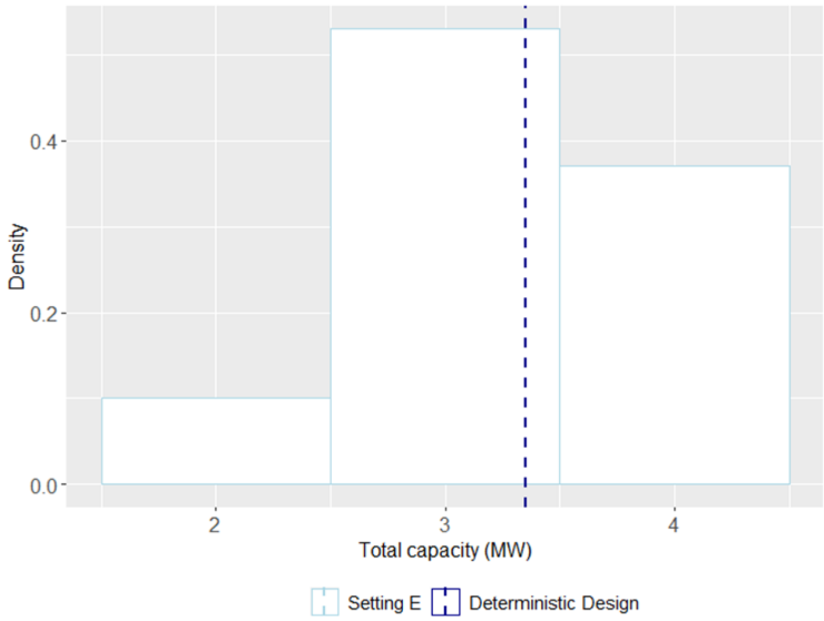


Figure 5.14: Histogram of the set of optimized total capacity values (setting E).

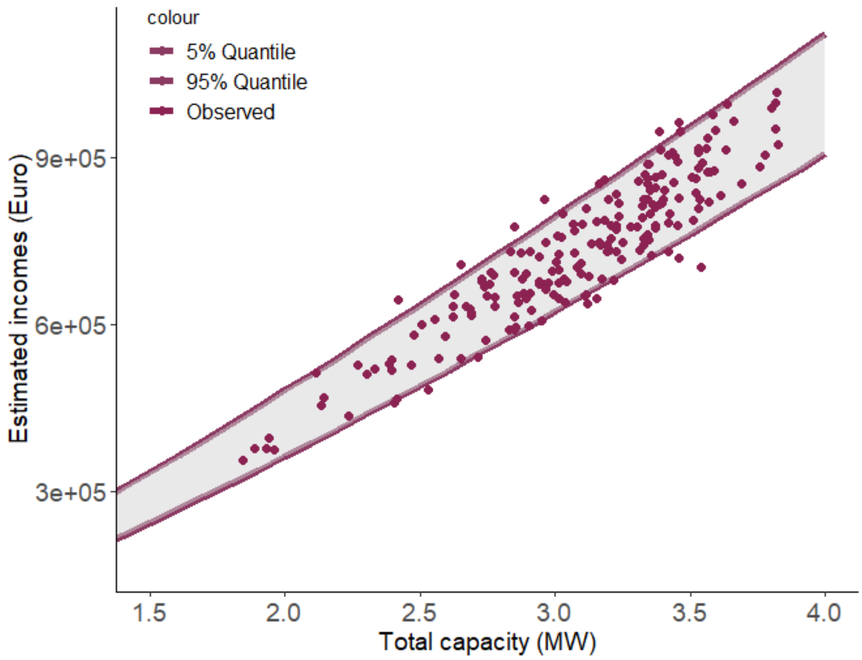


Figure 5.15: Fitting of Gaussian copula to total power capacity and mean annual profit (setting E).

Table 9: Summary of results from the alternative design approaches (the ranges refer to the minimum and maximum values of 200 scenarios).

Design approach	Deterministic	Setting A	Setting B	Setting C	Setting D	Setting E
Total capacity (MW)	3.35	1.84-3.83	2.93-3.79	3.16-3.38	3.05-3.81	1.53-4.02
Mean annual energy (GWh)	9.05	4.1-11.7	8.22-10.0	8.9-9.3	9.02-9.22	4.02-12.4
Capacity factor	0.31	0.25-0.37	0.24-0.27	0.30-0.33	0.28-0.34	0.25-0.30

5.4 From uncertainty assessment to an effective guide for preliminary design of SHHPs

Further to the optimization context, an effort is made to provide simple and generic tools for the estimation of the key components is the investment of small-hydropower plants. We remark that by taking advantage of 200 Monte Carlo scenarios as guide for the design of SHPPs, we employ a hypothetical design with perturbated characteristics (inflows, efficiency, curves, costs). In order to further augment this information we employ the above optimization procedure in two additional positions for small hydropower plants, in Achelous and Evinos basins. To conclude to a generic formula, for the estimation of optimal total capacity, we account for the hydrometeorological regime and the head, H, of the potential position. Specifically, for the first component, we apply two characteristic values, i.e., the inflows that correspond to 10% and 90% quantiles. Thus, the formula is:

$$P = a\, H^b\, Q_{10}^c\, Q_{90}^d \tag{5.80}$$

To estimate the parameters $a, b, c\ and\ d$, we employ a fitting by optimizing the NSE metric to the Achelous case. Then to stress-test this formula, we use the other two cases (Pamisos and Evinos) as validation. The fitting of the above formula is given in Figure 5.16, while the values of parameters are given in Table 10. In addition, the NSE for calibration and validation are 0.985 and 0.976, respectively.

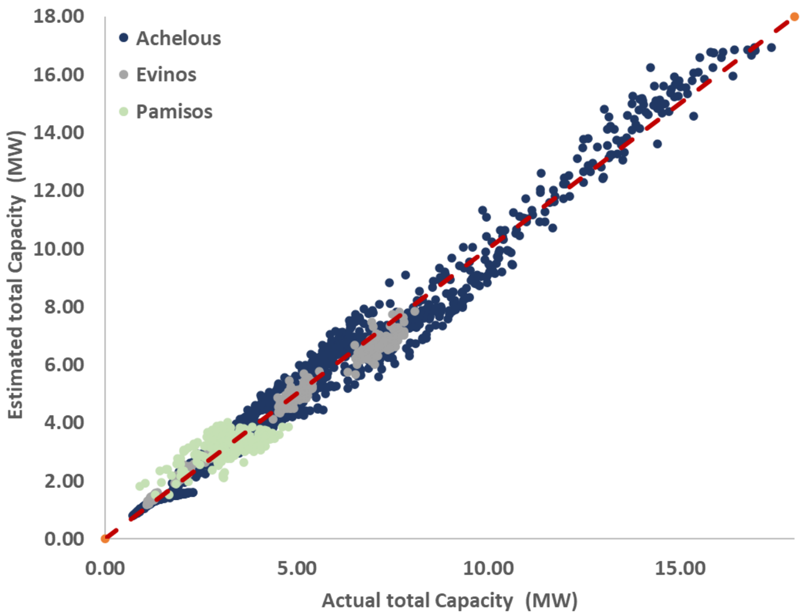


Figure 5.16: Fitting of a generic equation for the estimation of the optimal power capacity.

Further to this simple formula for the estimation of the optimal capacity, we offer two generic yet effective tools for the estimation of the total power capacity and the optimal mix of turbines, by means of nomographs. The first nomograph is presented in Figure 5.17, while the second one in Figure 5.18. The data presented in nomographs, extracted by employing the uncertainty-aware design context of setting E, for various potential positions in Greece and for various heads.

Table 10: Parameter values for the estimation of optimal power capacity.

Parameter	a	b	c	d
Value	0.05	1.28	0.772	0.087

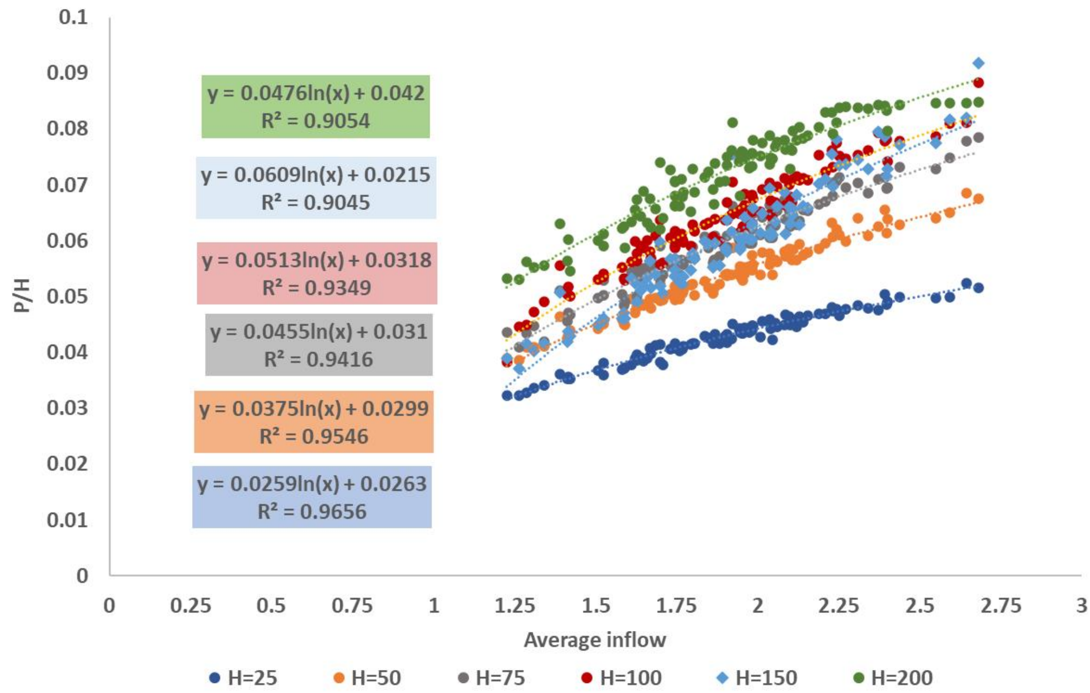


Figure 5.17: Nomograph for estimating the optimal installed capacity.

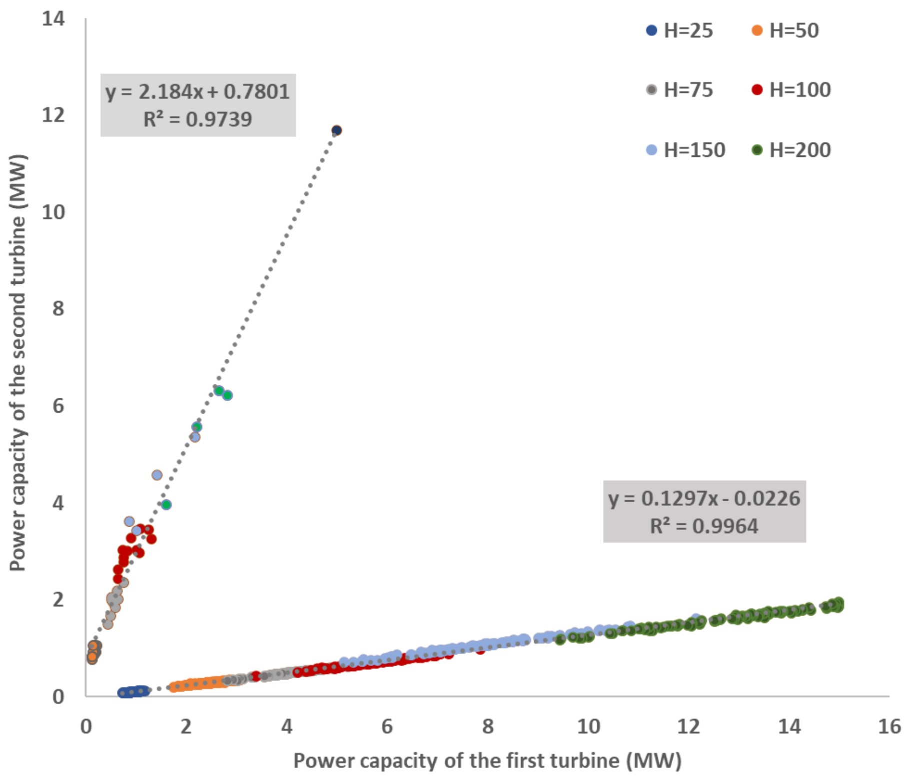


Figure 5.18: Nomograph for estimating the optimal mix of two turbines.

These are designed to be implemented in a sequel procedure. Firstly, the stakeholder needs to know the average inflow in the potential position of the intake, as well as the estimated head. By using the appropriate group (by head), the estimation of the $P/_H$ is made via the nomograph of Figure 5.17. As the total capacity is known, the key question is the optimal mix of the turbines. The answer is given through the nomograph of Figure 5.18, whereas depending on the estimated head the and the total capacity, the stakeholder is able to choose an optimal mix. For convenience a numerical example follows. Let consider an average inflow of 2 m^3/s and an estimated head of 200 m. Regarding the nomograph of Figure 5.17, the ratio $P/_H$ is about 0.06, thus leading to a total capacity of 12 MW. Step into the second nomograph of Figure 5.18, the optimal mix of the two turbines is 13 and 2 MW.

5.5 Proof of concept B: Long-term assessment of a wind turbine system performance

The second case study seeks for the long-term assessment of a wind power park, by accounting for its main internal and external uncertainties. This is established in a small Aegean island (Ikaria, Greece), and consists of two turbines with different power capacities, i.e., 1.0 MW and 2.3 MW, different hub heights, i.e., 59 and 85 m, respectively, and thus different power curves. These curves are also expressed by the parametric formula of the eq. (11), where the streamflow is replaced by wind velocity and thus $v^* = v_T/v_{max}$ is the rated wind velocity, n_{min} and n_{max} are the upper and lower efficiency values, and a and b are the shape parameters. The two curves are demonstrated in Figure 5.19.

The turbines are established in-line and aligned with the prevailing wind direction. Since the large turbine is upstream, for the energy production we account for the interaction (e.g., due to turbulence effects) between them, by decreasing the wind velocity to the second turbine as follows (Vasel-Be-Hagh & Archer, 2017):

$$v = v_o\left(1 - \frac{2a}{(1 + 2\,k\,L/D_L)^2}\right) \tag{13}$$

where v_o is the freestream wind velocity at the hub height level, k is the decay coefficient, and a is the induction factor. Here, for the decay coefficient and the induction factor we are applying the values proposed by Vasel-Be-Hagh and Archer (2017), i.e., $k = 0.038$ and $a = 0.10$. Following this, L is the distance between the two wind turbines and D_L is the diameter of the large turbine, which are equal to 400 m and 71 m, respectively.

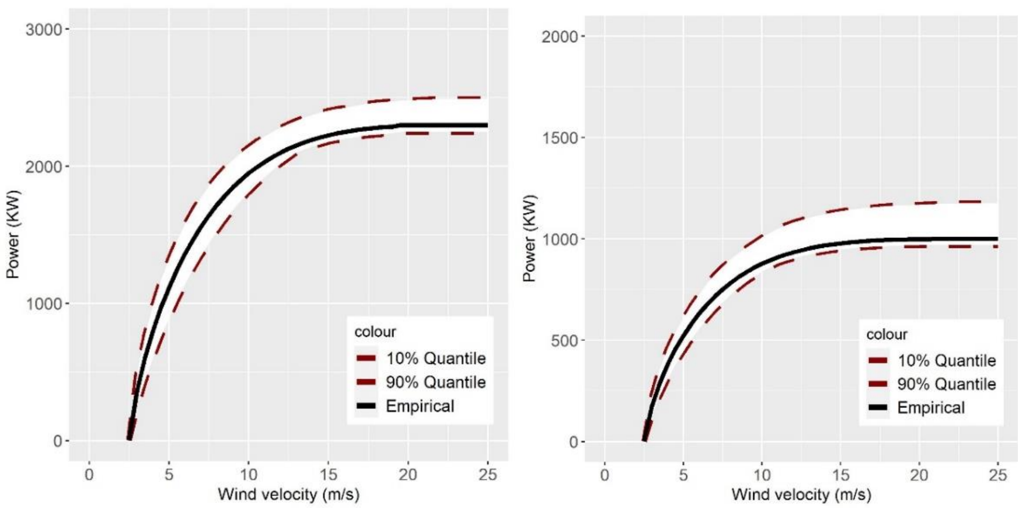


Figure 5.19:: Fitting of power curves to the original prototype for the two wind turbines and associated uncertainty bounds.

The assessment procedure follows in general the same practice with the design proof of concept, thus expressing the internal and external uncertainties settings. However, we adopt a slightly different approach of the modular scheme. Herein, three setting are established, i.e., the first two aim at representing the external uncertainty, by providing 100 ensembles of synthetic hourly wind velocity with 25 years length (i.e., the lifetime of the project). The difference between these settings is that the first setting ignores the dependencies across scales and the effects of seasonality, while the second setting reproduces the full regime of the observed wind velocities, as demonstrated in Figure 5.20**.** The first setting offers the simplicity against the second one, which is a more advanced method, since it accounts for seasonality across two scales, i.e., monthly and hourly. The last setting combines the internal and external uncertainties, by enhancing the second setting with a more detailed approach for the turbine power curve. Specifically, 100 equally probable power curves for the two wind turbines are formulated, in order to express the uncertainty that reveals in their real operation. As shown in Figure 5.19, the uncertainty bounds are negative asymmetrically spread, in order to reflect the observed deviation between the manufacturer's power curve and the output power at the site (Veena et al., 2020). For all settings, the economic performance of the wind power plant is expressed in stochastic terms, by applying a randomly varying energy price, which reproduces the statistical characteristics of the historical timeseries for a 5-year period (2015-2020). As made with the wind velocity process, 100 ensembles of hourly price timeseries for the 25-year period of simulation are generated, via the electricity price generator described in 3.3.3. The timeseries of the actual price data and one out of 100 synthetic samples are illustrated in Figure 5.21**.**

Each simulation results to 100 scenarios of characteristic quantities of interest for assessing the vitality of the RES, e.g., mean annual energy, expected profit, etc. A summary of the key outcomes is demonstrated in Table 9. In order to quantify the predictive uncertainty of the mean annual income, a copula model if fitted with respect to mean annual energy, as demonstrated in Figure 5.22. The practical use of this graph is discussed in next section.

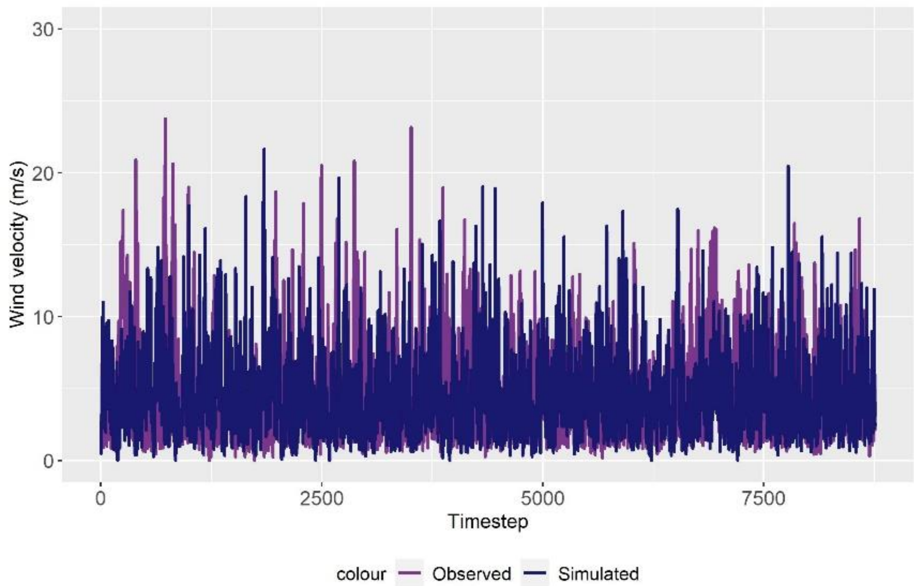


Figure 5.20: Stochastic and observed wind velocity data (randomly selected window of one year length).

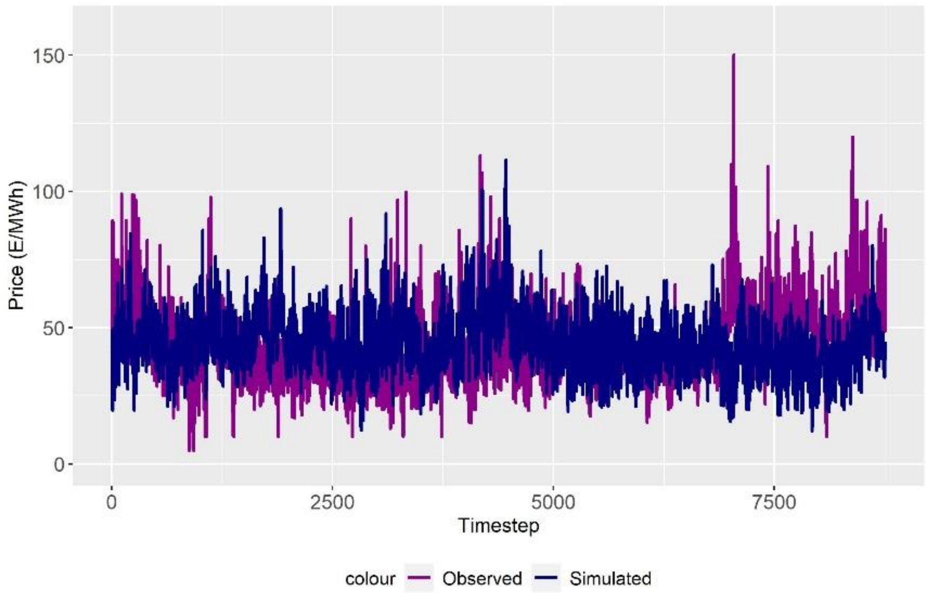


Figure 5.21: Stochastic and observed price data derived by Greek energy market (randomly selected window of one year length).

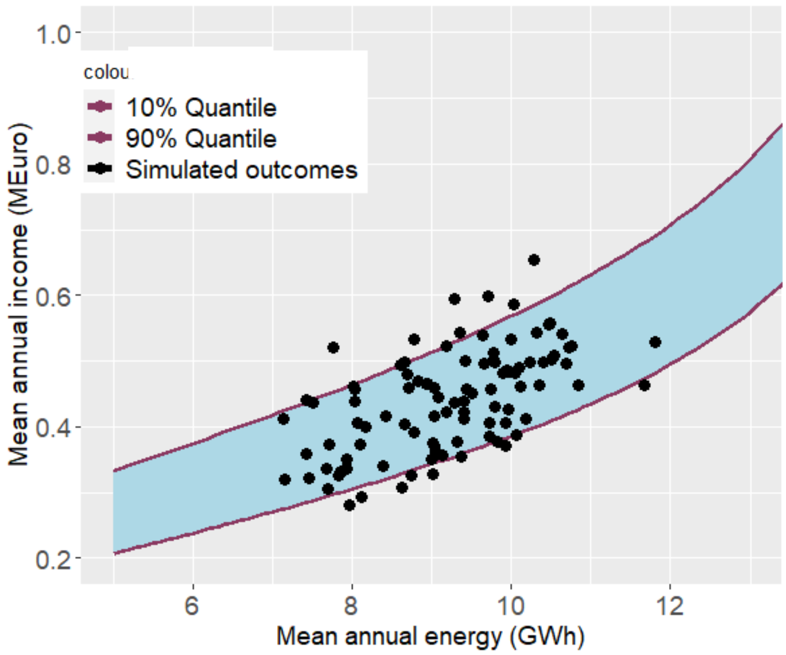


Figure 5.22: Fitting of Gaussian copula to mean annual energy generation and mean annual income (setting C).

Table 11: Summary of results from the alternative assessment approaches.

Assessment approach	Deterministic	Setting A	Setting B	Setting C
Mean annual energy (GWh)	8.97	9.19	9.13	9.19
Minimum annual energy (GWh)	-	9.13	6.96	7.02
Maximum annual energy (GWh)	-	9.25	11.11	11.40
Mean annual income (10^6 €)	0.36	0.38-0.53	0.18-0.63	0.37-0.66

5.6 Discussion: Implication for energy planners, managers and stakeholders

Our analyses indicated that the proper representation of uncertainty is not just a "game for statisticians", but has a significant operational relevance. Besides the pure technical sector, the proposed uncertainty-aware framework involves multiple groups of interest, from energy planners and managers to policy-makers and stakeholders.

From a technical point-of-view, it provides a holistic route to the design and economic assessment of RES, by representing their potential real-world operation through Monte Carlo scenarios. This is a major step forward the running paradigm, hypothesizing a unique future state of the system, under known internal and external conditions (i.e., forcing processes and characteristic properties). The resulting shift from the unique deterministic solution to the ensemble of possible options allows for interpreting the outputs of simulation and optimization in probabilistic terms. Overall, this approach can be the means to estimate the combined risks derived from the multiple sources of uncertainty and thus assist in the decision level. For instance, in the design of small hydroelectric plants, the coupling of Figure 5.14 and Figure 5.15 offers a decision tool for selecting the optimal turbine mixing and quantifying the full range of uncertainty with respect to anticipated performance of the system. Also, in a preliminary study of the associated investment, a stakeholder is able to estimate the optimal capacity and the mix of turbines, as well, by using proposed nomographs of **Figure 5.17** and **Figure 5.18**. These offer a key insight to the policy-maker, since it is a quick yet accurate estimation of the investment scale and the associated incomes.

The embedding of uncertainties can also be incorporated in the evaluation of renewable energy systems at a more macroscopic level. This approach has a twofold value a) for planned projects, it reveals a priori their vitality, and b) for existing systems, it highlights their potential weaknesses. For instance, the graph shown in Figure 5.22 can be used as a strategic management tool for both potential and existing projects. Specifically, in the case of existing projects with already known performance, in terms of mean energy production, we can estimate the anticipated range of associated profits, and thus recognizing whether the system is effective or not. In addition, in the planning context regarding the deployment of potential RES, the stochastic simulation procedure offers a priori the valuable information about not only the mean annual energy per se but also the expected revenues from their long-term operation.

The abstract information and knowledge gained from the aforementioned procedure can be eventually served as a communication channel with investors, stakeholders and local communities, which are the actual beneficiaries from a proper design and effective operation and management of RES.

5.7 Conclusions

An accurate representation of uncertainties is crucial across all aspects of renewable energy. This research presents and discusses the principles of a holistic simulation-optimization approach for such systems, by first recognizing the key sources of uncertainty, external and internal, and by setting them within a probabilistic framework. In this respect, the representation of uncertainties is made through the probabilistic triptych: (a) statistics, accounting for marginal properties of independent variables, (b) stochastics, also accounting for dependencies of hydrometeorological drivers, and (c) copulas, for quantifying the joint uncertainty of simulated outcomes. As the three most widespread RES (wind, solar, hydroelectric) have fundamental similarities, a generic procedure for the related design and long-term performance assessment problems is established, which is a significant novelty of this work.

In the proposed framework, all uncertain components within the design and the long-term assessment of RES are expressed in probabilistic terms, either as stochastic processes or randomly varying quantities (i.e., model parameters). Particularly, the representation of internal uncertainties across the energy conversion phases is simply made by introducing parametric analytical formulas for the system's efficiency and sample their parameters from suitable distribution models. This is a key methodological novelty, which also avoids the application of detailed physical models for capturing complex uncertainties at the microscale. The combined effects of internal and external uncertainties are finally mapped to the outputs of interest, namely the optimized design variables (i.e., power capacity values) and the key performance assessment metrics (i.e., investment costs, expected energy production and revenues, capacity factor). In the context of their post-analyses, we have also developed probabilistic tools, also based on copulas, for quantifying individual and joint uncertainties.

The modular application of the uncertainty-aware framework to the design of small hydroelectric plants as well as to the assessment of a planned wind power park, revealed significant benefits of the proposed approach over conventional deterministic practices.

As a conclusive remark, also derived from the discussion of section 5.6, is that the coupling of uncertainty in the assessment of RES, either existing or planned, also has a practical footprint. In fact, it is crucial for the evaluation of the system's performance under alternative states (hydroclimatic and economic drivers, as well as operational conditions) and the quantification of associated risks. The explicit incorporation of the concept of risk within RES design and planning, which has been the overall outcome of this research, allows decision makers and stakeholders to assess, a priori, whether the investment is effective and sustainable.

6 Water supply systems under the concept of water-energy-society nexus

Preamble

This chapter focuses on mitigating the emerging paradigm in the modelling of water supply systems, under the water-energy nexus perspective. In this vein, we set the specifications for an adjustable framework that couples four modelling subsystems, i.e., physical, technical, economic, and social. Considering as case study the water supply system of Athens, Greece, we reveal the multiple methodological and computational challenges of this implementation in practice. This consists of: (a) a simplified simulation of water-energy processes and associated infrastructures (reservoirs, aqueducts, pumps, etc.), in order to fulfill given water demands, under already optimized operational rules for the long run; (b) a water price model that accounts for simulated energy consumption, electricity prices, and net present fixed costs, and (c) an agent-based context that represents water consumer groups, whose behavior is influenced by water bills, water-saving campaigns, and their social network. The water bills are associated with the varying electricity price and the operational policy of the water utility, while the campaigns are triggered by the reservoir storage conditions. Since the external drivers of the water-energy-society nexus (hydrometeorological processes and energy price) are expressed in stochastic terms, the water supply is sketched as a *sociotechnical system under uncertainty*.

This chapter is based on these publications:

Sakki, G. K. and Efstratiadis, A.: Water supply systems under the sociotechnical context driven by the energy market, Urban Water Journal, 2024 (under review).

G.-K. Sakki, A. Efstratiadis, and C. Makropoulos, Stress-testing for water-energy systems by coupling agent-based models, Proceedings of 7th IAHR Europe Congress "Innovative Water Management in a Changing Climate", Athens, 402–403, International Association for Hydro-Environment Engineering and Research (IAHR), 2022.

A. Efstratiadis, and G.-K. **Sakki**, Revisiting the management of water-energy systems under the umbrella of resilience optimization, Environ. Sci. Proc. 2022, 21, 72. https://doi.org/10.3390/environsciproc2022021072

6.1 Setting the scene

Sustainability has been a highly promoted principle in the last decades and significant efforts have been put to embed it into several aspects of natural resources management and environment protection, with focus to urban systems. While the global economy is driven by the energy and water sector, it is expected that during the 21st century, water will be what oil was in the 20th one. This makes essential to revise the conventional, monomeric, planning and management of water supply systems, which is employed so far from a “water-centric” perspective. In fact, such systems embed multiple energy consumption components across all their processes of interest, i.e., water abstraction, conveyance, distribution, treatment and reuse. They may also facilitate renewable energy production, by means of small hydro power plants that are installed across water conveyance and distribution systems (Sitzenfrei et al., 2014), solar panels installed over aqueducts (McKuin et al., 2021) and biogas retrieve units in wastewater treatment plants (Plevri et al., 2021).

However, the reliability, resilience, economic effectiveness, and, overall, sustainability of both pillars of water supply systems, i.e., water and energy, are also subject to complex social processes. In particular, the human decisions made by citizens and the water utility has a footprint to the natural system, while the natural system responds to these decisions directly by means of freshwater availability (M. Giuliani et al., 2016). The incorporation of the anthropogenic behavior and its multiple interactions and feedbacks within the water-energy nexus, can be considered as a turning point for handling the assessment of technical systems under the crucial social dimension (Molajou et al., 2021). In this vein, water supply systems should be considered as a promising area of investigating synergies and feedbacks across the water-energy-society nexus (Figure 6.1).

Thus, this research aims at providing a tailored made methodology for the assessment of urban water supply systems, by incorporating water, energy, society and the energy market (in terms of electricity prices), as a nexus of synergetic fluxes, and under the prism of uncertain (better referred to as stochastic) sociotechnical systems (Efstratiadis and Sakki, 2024). The generic specifications of this approach, involving the interconnection of four modelling building blocks (physical, technical, economic and social), is provided in section 2. As a proof of concept, we analyze the complex and highly extended raw water supply system of Athens, Greece, to assess its long-term management under different disturbances that arise from the hydroclimatic conditions and the socio-economic environment. For the social factor, we are taking advantage of agent-based models to simulate the water demand behavior, driven by external influences and pressures (water and energy prices, public awareness campaigns). Finally, to overcome the issue of uncertainty we use stochastic models in order to provide synthetically-generated time series for the hydrometeorological inputs and the electricity price, which is embedded within the water cost and price. Before providing the holistic methodology, a proof of concept is described, by revisiting the long-term management under the umbrella of resilience optimization. The resilience of the system is stress-tested under various scenarios, originated from climatic, technical and socioeconomic drivers.

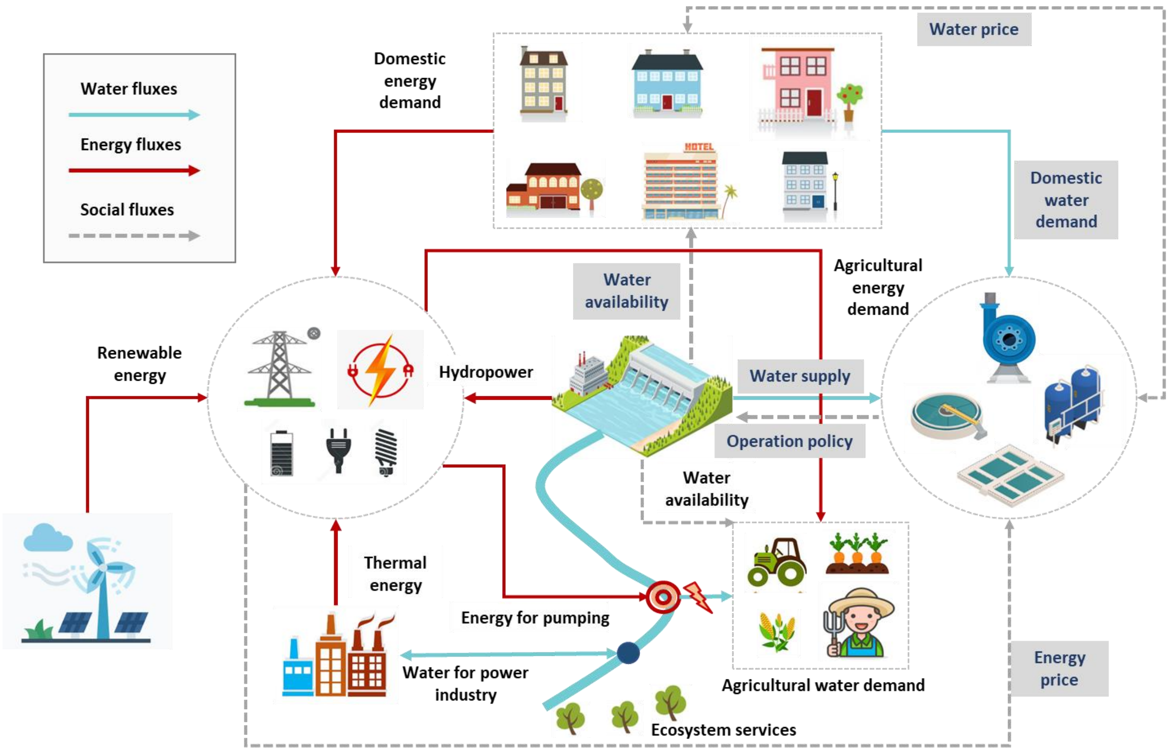


Figure 6.1. The water-energy-society nexus from the water supply perspective, the grey boxes corresponds to the fluxes (drivers) will be discussed.

6.2 The Athens water supply system

6.2.1 Technical system

The Athens raw water supply system, operated by the Athens Water Supply and Sewerage Company (Greek acronym, EYDAP S.A.), is highly extended and complex, since it lies over an area of 4000 km^2 and comprises 350 km of aqueducts (Figure 6.2). Also, it includes four reservoirs (Mornos, Evinos, and Marathon, as well as the natural lake Hylike), 15 pumping stations, several dozens of boreholes and four water treatment plants (WTPs). The external conveyance network is separated in two subsystems, namely the southern branch and the northern one. The southern branch carries water via gravity from the interconnected reservoirs Evinos and Mornos. On the other hand, the northern subsystem transfers water from Hylike and several boreholes through pumping, with considerable cost.

In particular, water from Evinos reservoir is diverted through a tunnel to the neighboring Mornos reservoir, since its inflows are the largest of the whole system, while its storage capacity is quite small. Thus, the major role of Evinos is to support the major regulating infrastructure, i.e., Mornos, by transferring almost the half amount of the Athens' water demand. On the other hand, key characteristic of Hylike lake is the significant leakages due to its karstic underground, which may cause losing half of its storage in one year. We underline that due to quite rich hydrological conditions and the reduction of consumption, until recently, the water utility was not forced to pump remarkable water amounts from Hylike to fulfill the water demand of Athens, thus the associated cost was minimal. Finally, Marathon is the smallest and the oldest reservoir of the hydrosystem and is mainly used as a backup for emergency situations and as a regulator of peak water demands during the summer season.

The overall storage capacity of the four reservoirs reaches 1400 hm^3, while their accumulated mean annual inflow is 825 hm^3 (the groundwater resources, which are mainly activated in case of emergency, can also contribute up to 90 hm^3). While the key objective of the system is to provide raw water to broader Athens Metropolitan area (up to 400 hm^3 per year, as explained herein), it also serves several other uses. In particular, it provides water for irrigation, water supply of nearby domestic and industrial areas, and also environmental preservation downstream of the Evinos and Marathon dams. Furthermore, besides Hylike's losses due to leakages, there are also several other water losses across the aqueduct network and the reservoirs (due to leakages, evaporation and spills).

Due to its complexity and its vital role of Athens, this system should be successful, robust and resilient under external influences and stresses. In this vein, the day-to-day operation and the long-term management of the system are crucial for its reliability, and relies upon several decisions, regarding the allocation of withdrawals to the different reservoirs and the conveyance of water. We remark that the reliability of the system highly depends on the inflows to the Evinos-Mornos complex, which may be too risky, in case of prolonged drought periods. Thus, the optimization of its long-term management is subject to multiple and conflicting objectives, aiming at balancing competitive uses, socioeconomic constraints, and environmental requirements. Specifically, the optimization problem aims to ensure an acceptable tradeoff between two key performance metrics of interest, i.e., the reliability, and the cost/benefit ratio, in order to extract the associated set of operational rules. We highlight that the desirable reliability for the water supply of Athens is set as high as 99% on annual basis (indicating one failure per 100 years), while the minimum acceptable value is 97%.The extraction of optimal operation rules for the water supply system of Athens and their long-term effects have been subject to exhaustive analyses (Efstratiadis et al., 2004).

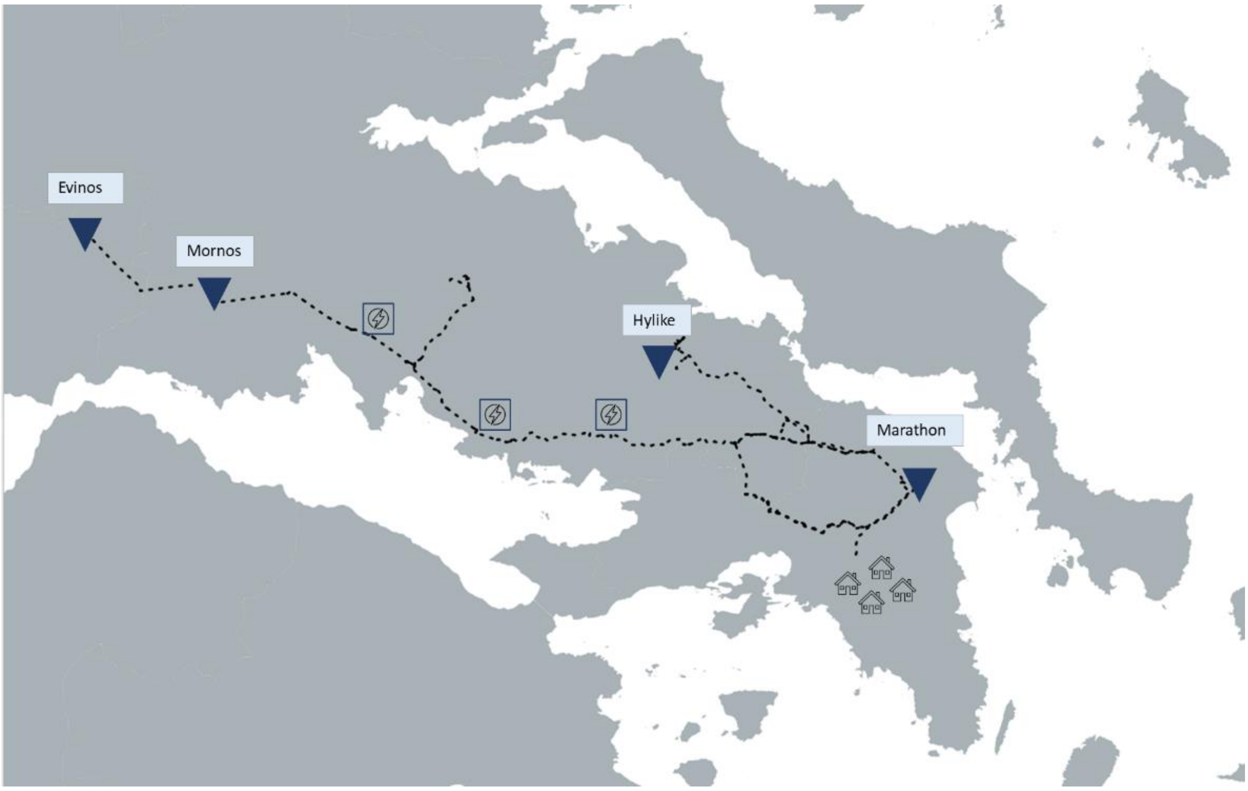


Figure 6.2. Configuration of Athens' water supply system.

6.2.2 Economic System

We argue that cost reduction strategies are always a priority for water utilities. Regarding the management of the Athens' hydrosystem, this objective becomes crucial, particularly under the recent energy crisis. Nevertheless, under stressful conditions, i.e., persistent droughts, limited storages, malfunction of aqueducts etc., this low-cost intention cannot be achieved, as result of increased pumping, which makes the system to be strongly depended on the electricity market price. Figure 6.3 demonstrates the evolution of the energy market price in Greece the last three years, when the price of electricity has almost trebled. However, this trend doesn't result one-to-one response to the water price, given that due to favorable inflow and storage conditions, until recently the water utility was not forced to pump significant amounts of water from Hylike and the boreholes.

The methodology for estimating the cost of raw water production across the Athens water supply system has been subject of former research (Makropoulos et al., 2018). Generally, this approach is based on the combination of the Capital Recovery Ratio (CRR), Capital Accumulation Ratio (CRR) and Equivalent Cost (EC) methods. Essentially, what is sought is to accumulate a certain amount of money at a given future point to cover all the costs of the initial investment, opportunity costs and depreciation, making the capital available to fully replace the depreciated fixed asset if necessary. The above methodology is in the same line with the EU Water Framework Directive and the national law. Thus, the overall fixed cost for the water supply system has been estimated to be approximately 58 M€ per year. On the other hand, the cost of energy was estimated by considering alternative scenarios of the long-term management of the system, since the lower is the acceptable risk of deficits the more intensive should be the pumping from Hylike and the groundwater resources (Efstratiadis et al., 2004). This approach made use of empirical relationships to link the operation of pumping stations with energy costs, retrieved from electricity bills of period 2008-2017. Under this premise, the overall pumping cost was estimated to range from 1.8 to 2.8 M€ per year. However, this expected to change due to high electricity prices.

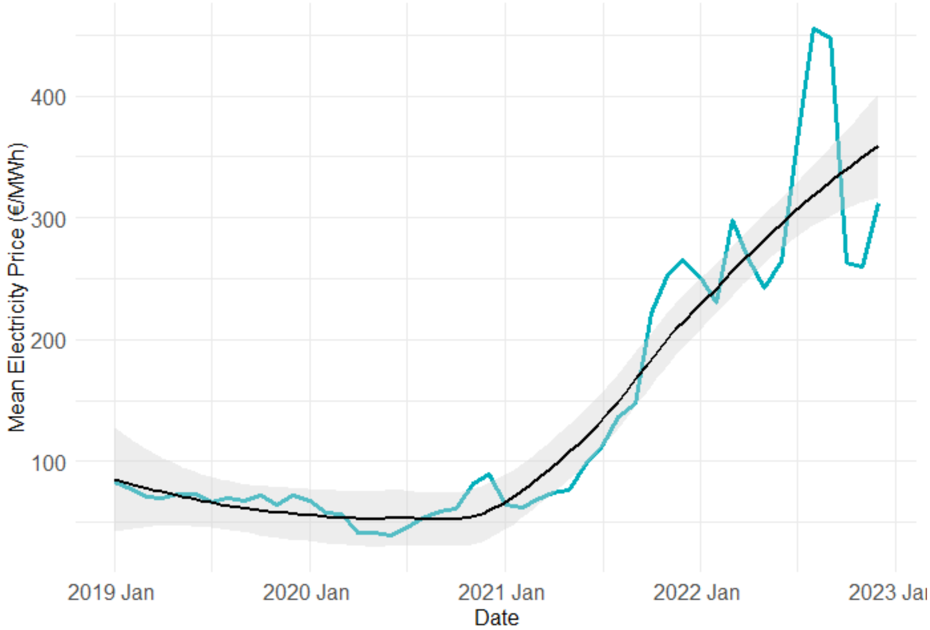


Figure 6.3. Daily evolution of electricity market price from January 2019 to January 2023.

6.2.3 Social System

As already mentioned, the main target of the hydrosystem in study is to provide drinking water to the citizens of Athens (3,738,140 hydrants, according to EYDAP records). Actually, the water consumption is subject to multiple factors, i.e., occupancy rate, family type, householders' age, income, occupational status, and educational level (Mazzoni et al., 2023). For the case of Athens, some key socio-demographic determinants are demonstrated in Table 12. The distribution of water consumption follows the seasonal pattern of Figure 6.4. As expected, during the summer season, this is increased.

Figure 6.5 also illustrates the evolution of population and water consumption during last 50 years. The most impressive feature is the substantial drop of water consumption in the early 90's, by about 30% (from 367 hm^3 in water year 1988-89 to 257 hm^3 in 1993-94), which is further analyzed in next sub-sections. Regarding the recent evolution of Athens water demand, over the last decade this did not exceed 400 hm^3, while in the past the annual consumption has reached 430 hm^3. It is also quite interesting that even through the population is increasing, the annual consumption exhibits a slight reduction. This phenomenon is explained by the recent financial crisis (2008-2018), and also to the reduction of losses across the water distribution network.

Table 12: Demographic data for Athens' citizens (Hellenic Statistical Authority, after processing).

Perc. of population (%)	Income (€)	Perc. of population (%)	Family size
30	0 - 5 000	11	1
28	5 000 - 10 000	23	2
18	10 000 - 15 000	25	3
14	15 000 - 20 000	29	4
9	> 20 000	8	> 5

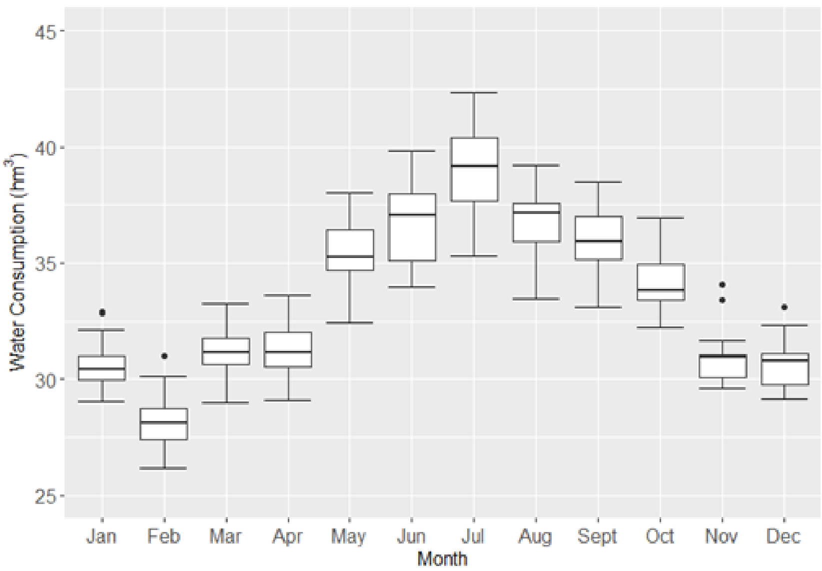


Figure 6.4. Box plots of monthly distribution of water demands in Athens for years 2000 to 2022.

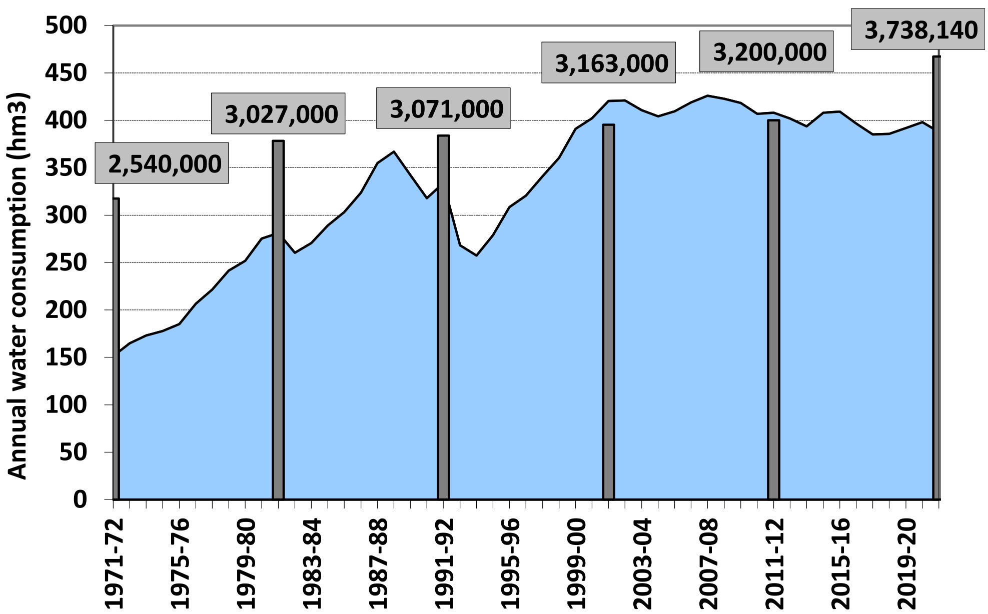


Figure 6.5. The evolution of population and its water demand in Athens.

6.3 Water supply management under the umbrella of resilience optimization

Prior to the establishment of the holistic methodology of the water-energy-society-market nexus under the coupling of different models, we employ a stress-test of the water supply system of Athens under the resilience concept. This better reveals the necessity of holistic and uncertainty aware approaches to the long-term management of critical infrastructures.

In the context of water-energy management, this is usually expressed by means of operational rules, which can be conventionally derived from an optimization procedure, that regards the successful interplay of the water and energy components under a specific set of assumptions. The two elements are highly interconnected and conflicting, since water is the critical ingredient of energy production. On the other hand, energy is needed for the complete water cycle, from water abstraction (through pumping) to water treatment, as well as for recycled water collection and treatment. Following this, we agree that this optimization context is in fact a multicriteria problem, thus leading to multiple rules that are equivalent, from the Pareto optimality perspective (Efstratiadis & Koutsoyiannis, 2010). In this vein, the incorporation of resilience as an overall performance metric may be the turning point for supporting decision-making. In particular, this allows for mining the management rules that remain robust across increasing pressures of the system, and finally detect the best compromise one.

6.3.1 Modelling framework for optimizing the system's management policy

The exploration of the management options and, eventually, the detection of the best-compromise one, is employed through the use of Hydronomeas software, which is the cumber stone of a broader decision support system for the supervision and the management of the water resource system of Athens (Koutsoyiannis et al., 2003). The representation of the physical system as a network model within the graphical interface of Hydronomeas is demonstrated in Figure 6.6.

The methodological framework of the model is based on the triptych:

- Parameterization of the operational policy of the system;
- Stochastic simulation of the system's dynamics;
- Optimization of the long-term performance of the system.

More specifically, the mathematical expression of the operation rules in an extension of the rationale by Nalbantis and Koutsoyiannis (1997), and Koutsoyiannis and Economou (2003). These determine the desirable allocation of abstractions from the system's sources (reservoirs and boreholes), according to its current state (storage, demand), by using only few control variables. In addition, the simulation module comprises two components. The first aims at representing the hydrological drivers of the system as stochastic processes, by means of synthetically-generated time series that reproduce the probabilistic and stochastic regime (auto- and cross-dependencies) of the parent historical data. The data synthesis is employed through the hydrometeorological generator, as proposed in 3.1.3. For given inflows and demands, the simulation of the system's operation is formalized as a stepwise allocation of the unknown water and energy fluxes, which are represented as control variables of a network linear programming problem. This aims at minimizing the total transportation cost across the hydrosystem, by preserving the pre-specified hierarchy of water uses and constraints (Efstratiadis et al., 2004). Finally, the overall optimization of the system's performance is generally expressed as a multicriteria problem. Its components are probabilistic metrics, such as the failure probability (or its complementary metric, i.e., reliability), the mean annual energy production or consumption, the water deficits and their costs, etc.

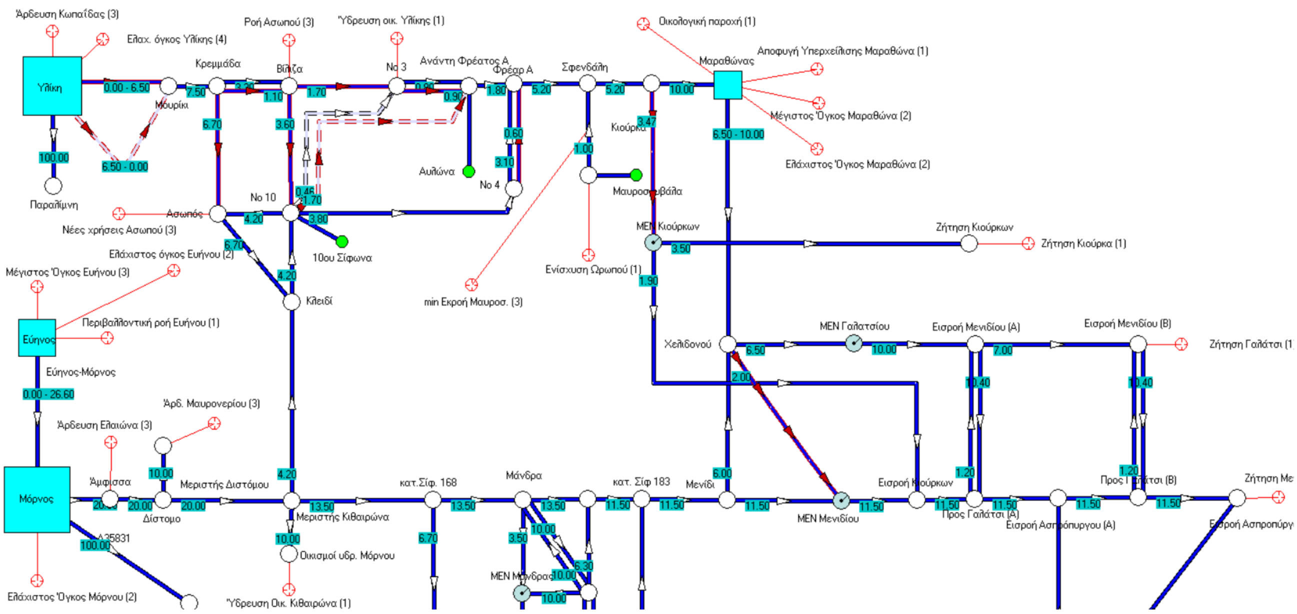


Figure 6.6 Conceptual model of the water resource system of Athens as implemented in the graphical environment of Hydronomeas software.

6.3.2 Resilience-based optimization of the system's management

5.3.3.1. Baseline scenario setting

Based on the schematization of Figure 6.6, we seek for the strategic management policy of the water resource system of Athens, for which we set a plethora of targets and operational constraints, classified in three priority levels. The targets that are set in the highest priority are the water supply of broader Athens. In particular, we consider a total annual demand of 400 hm^3, i.e., close to the current consumption, which is split into five demand zones. Furthermore, we assume all minor water supply uses across the aqueduct network, which are merged as point demands at three nodes, and the two environmental flow demands downstream of Evinos and Marathon dams. In the second hierarchy level, we set the minimum and maximum storage constraints that are assigned to the four reservoirs, as the major components of their operational rules. Finally, the lowest priority is assigned to the three irrigation targets. The system is driven by monthly synthetic rainfall, runoff and evaporation time series of 2000 years length.

Initially, we consider the aforementioned system's state as the baseline scenario, for which we extract the optimal operational rules of the four reservoirs. The optimization problem aims at balancing the two key objectives of the water-energy nexus, namely the fulfillment of water supply uses with very high reliability (preferably, 99% on mean annual basis), and the minimization of pumping cost. In this respect, the performance measure is formalized as a cost function, comprising two elements. The first expresses the mean annual deficit cost of all consumptive water uses, for which we apply different unit penalties, namely 1.0 €/m^3 for water supply and 0.2 €/m^3 for irrigation. The second element is the mean annual cost of electrical energy, due to the use of pumps and boreholes. In order to estimate this cost, we apply piecewise linear functions that are fitted to historical energy consumption and associated cost data, as shown in the example of Figure 6.7.

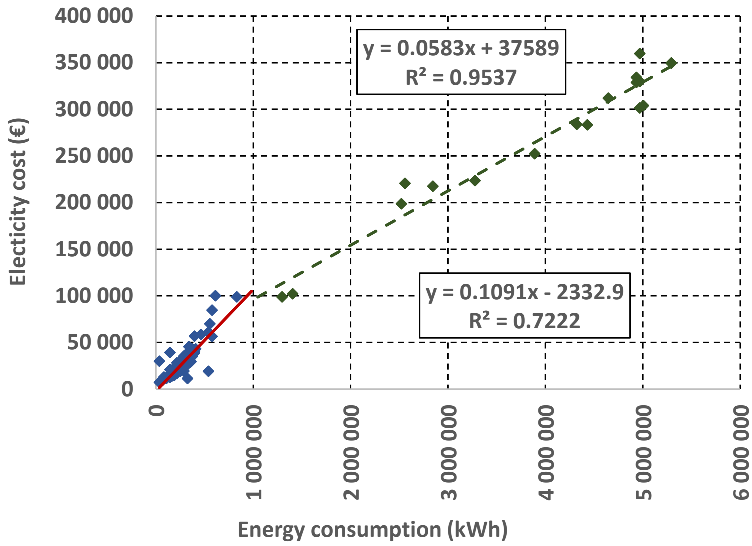


Figure 6.7: Fitting of piecewise linear functions to historical energy consumption and associated cost data at the main pumping station of Lake Hylike.

5.3.3.2. Operation rules

The optimized operational rules for the baseline scenario are illustrated in Figure 6.8a. These specify the desirable storage of each reservoir as function of the expected total storage capacity of the system, which is estimated by accounting for the total storage at the end of previous time step (month), the expected inflows and the total water demand. The optimized control variables that are embedded in these rules are two dimensionless parameters per each reservoir, as explained by Koutsoyiannis and Economou (2003), and the two operational constraints, by means of minimum and maximum desirable storage. This rule is contrasted to a more conservative one (Figure 6.8b), which is adjusted in order to impose a more frequent use of Hylike. As shown in Table 13, from the sustainability perception, both rules are in the safe place, since they guarantee the desirable reliability level of 99%. However, the second rule is sub-optimal, in terms of economy. The question arising is whether this more conservative yet more expensive rule indicates a more resilient management policy. This question is investigated by means of stress scenarios in next section.

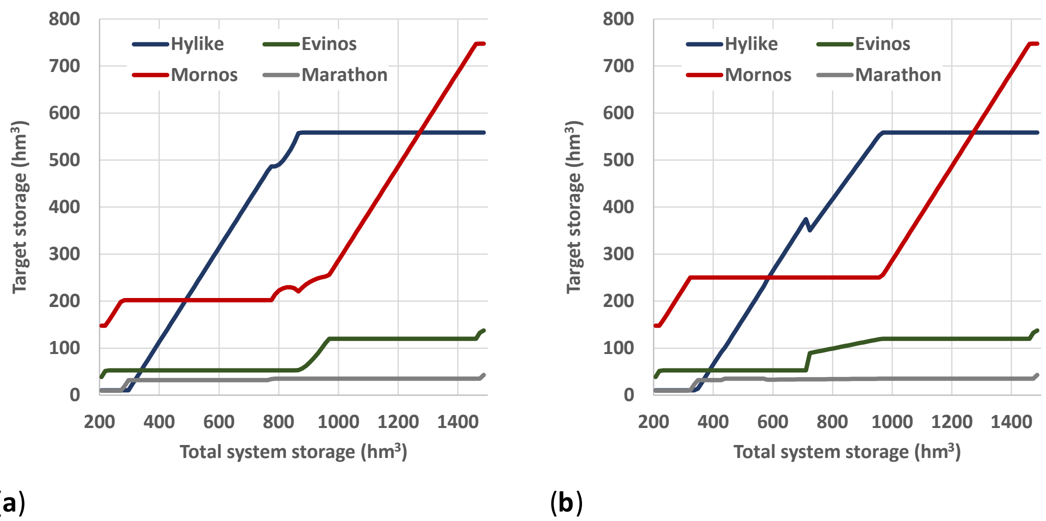


Figure 6.8: Graphical representation of operation rules: (**a**) optimized against the baseline scenario; (**b**) optimal in terms of resilience.

Table 13:**.** Key results for the baseline scenario by applying the two alternative management policies. All water, energy and cost quantities are expressed on mean annual basis.

	Baseline-optimal	**Resilient-optimal**
Reliability of Athens' water supply (%)	99.0	99.7
Abstraction from Mornos (hm^3)	442.92	442.03
Abstraction from Hylike (hm^3)	25.22	29.74
Abstraction from boreholes (hm^3)	10.21	7.26
Energy consumed in pumping stations (GWh)	24.18	30.04
Energy consumed in boreholes (GWh)	9.88	6.84
Total energy consumption (GWh)	34.06	36.88
Total energy cost (million €)	2.73	2.90
Water supply deficit (hm^3)	0.26	0.11
Irrigation deficit (hm^3)	0.76	1.36

5.3.3.3. Stress scenarios

The water resource system of Athens is stressed against six scenarios that reflect different aspects of potential disturbance (socioeconomic, hydroclimatic, technical). We remark that these scenarios represent uncertainties that cannot be formalized in stochastic means, as made with the external drivers (rainfall and inflow). In this respect, the system will be remain resilient under futute uncertainties. A brief summary of them is given in Table 14, while in Figure 6.9 we contrast the performance of the two operational rules, in terms of mean annual cost. We remind that this embeds the energy cost and the cost of water deficits.

Table 14: Summary of stress scenarios.

id	**Description**	**Driver of change**
1	Baseline scenario (cf. section 5.4.3.1)	
2	Setting of irrigation targets in a higher priority level	Social
3	50% decrease of available groundwater resources	Hydroclimatic
4	20% increase of pumping cost	Economic
5	Increase of leakage losses across aqueducts from 5 to 10%	Technical
6	Increase of Athens's demand to 430 hm^3 (max. observed value)	Socio-economic
7	Increase of Athens's demand to 450 hm^3 (long-term projection)	Socio-economic

For the first three stress scenarios (numbered 2, 3 and 4), the optimal rule so far, according to the baseline state (scenario 1), is equivalent or slightly overperforms the conservative rule. However, the other three scenarios highlight that the conventional definition of "optimality" does not promise resilience against situations where the system is pushed beyond of its standards. Using the concept of resilience proposed by Makropoulos et al. (Makropoulos et al., 2018), the area below the two curves represents an overall cost metric. Herein, the smaller is this area, the more resilient is the operational rule. Under this assumption, the second rule should be preferred, as more robust. It is worth mentioning that the conventionally optimal rule for the last scenario ensures an unacceptable low reliability, i.e., 91.3%, while the mean annual energy cost is 4.33 million €. On the other hand, the resilient rule still achieves a marginally acceptable reliability level (96.2%), with a relatively small increase of mean energy cost (4.77 M€).

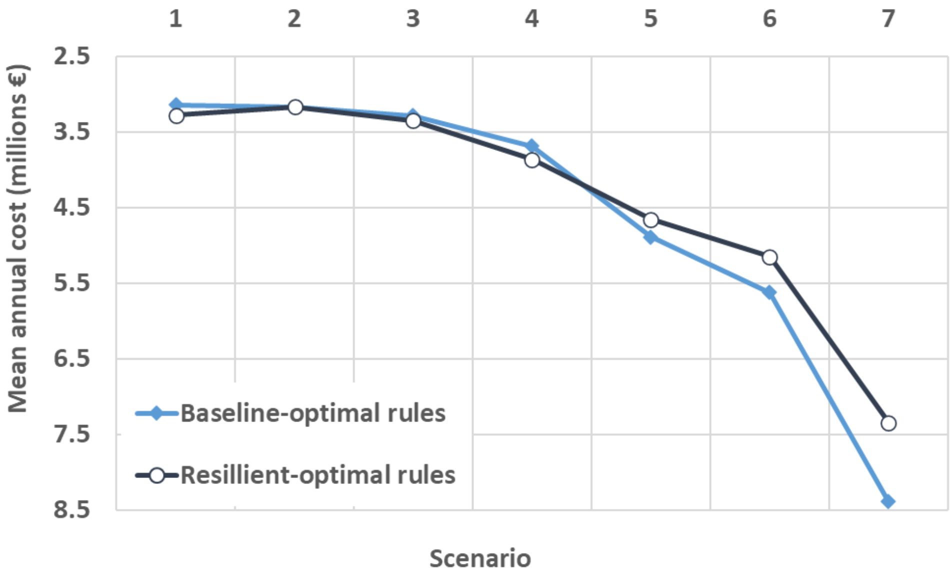


Figure 6.9: Comparison of two operational rules against scenarios of varying stresses.

6.3.3 Conclusions

Triggered by the violent changes that span over all aspects of sociotechnical systems, it is essential to reconsider the far-reaching quest of optimality under the concept of resilience. Taking as example the challenging water-energy system of Athens, we revisit its long-term management policy, which has been conventionally handled as a typical optimization problem under steady-state conditions. By stressing this under a number of plausible disturbances, caused by social, economic, hydroclimatic and technical changes, we reveal the necessity for adopting more conservative (in terms of reliability) although more expensive operation rules than the ones optimized against the baseline scenario. Nevertheless, the stressors scenarios, originating from the socioeconomic unstable environment are the most crucial. In this scene, we manifest the need of *stochastic sociotechnical system*'s approach that incorporates the climatic, social and energy market's dynamic within long-term management of water supply. This approach is next discussed.

6.4 The building blocks of the nexus: Setting the framework's specifications

The assessment of complex water supply systems under the water-energy-society-market nexus requires the coupling of four individual modules and its interactions, also referred to as building blocks, to a unified tool (Figure 6.10). Key specifications of this approach, which will be further analyzed through the real-world case study of the Athens water supply system, are:

Technical system: The representation of water supply systems requires a decision support software to simulate the water abstractions from different sources, their conveyance through aqueducts and pumping stations, and their distribution across different types of users (e.g., water supply, irrigation, industry etc.), as well as all kinds of interactions with energy (hydropower production, pumping, etc.).

Physical system: Water supply systems are driven by randomly varying hydroclimatic processes (e.g., rainfall, runoff, evaporation), which should be preferably described by stochastic models. As mentioned, these have a long history in water resources and other environmental sciences, as the means to generate long synthetic data that reproduce, in statistical terms, the actual regime of the observed processes.

Social system: For the description of the social system and its interactions, we are taking advantage of the proposed human factor model, as described in 3.2.3.

Economic system: Water supply systems are also driven by the electricity market and the pricing policy of water utilities. Specifically, the financial cost of water is associated with fixed costs, i.e., annual depreciation cost, cost of financing, expected return on equity and taxes, which are reflected to the water price, in order to ensure sufficiency of revenue (Aggarwal et al., 2013). However, water utilities are also forced to fulfill the expenditures that are associated with the operation and maintenance of their systems. Following this, the operation cost is strongly related with electricity market and the fluctuations of energy price during each day and across seasons. Similar to hydroclimatic processes, stochastic models can be applied for generating synthetic economic data, e.g., by means of energy price, which can be further translated into water price.

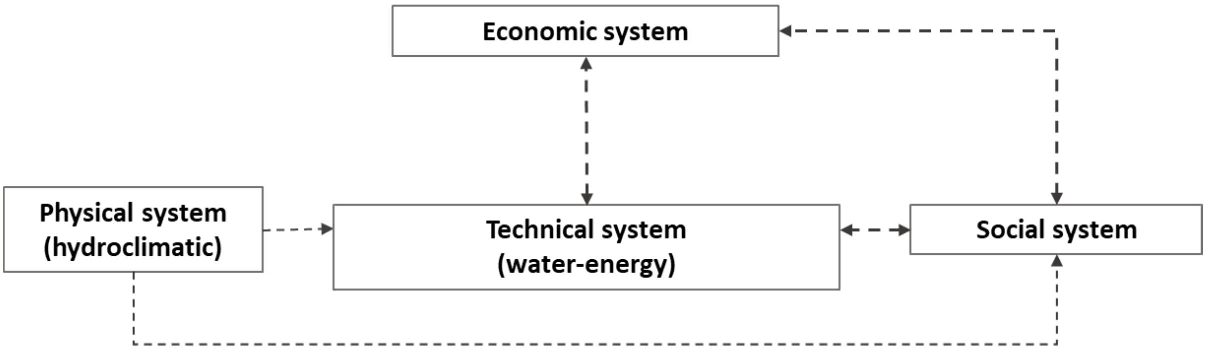


Figure 6.10: Outline of modelling building blocks and their interactions.

The structural challenge of this customization is the need of handling a very large number of heterogenous inputs, control variables, constraints and objectives, due to the simultaneous modelling of the four parallel systems and their interactions. Past research in this area has only provided rather simplified and fragmented formulations that misrepresent important systemic complexities and intersectoral interactions (Giudici et al., 2021). Apart from this structural complexity, there is also a hidden challenge, since the link of sub-systems across varying scales imposes coupling of different modelling philosophies, e.g., agent-based models (for the social system), following a bottom-up approach, with top-down models for water-energy simulations. Nevertheless, the final approach should be generic, flexible, computationally efficient and accessible by different groups of interest, and overall able to solve real-world problems.

6.5 Building the simulation procedure

The overall simulation procedure of the Athens hydrosysytem, under the water-energy-society-market nexus, follows the generic modelling specifications that are outlined in section 6.4. For convenience, the physical, technical and economic building blocks are presented together (section 6.5.1). On the other hand, the social element, which is formalized as an ad-hoc built agent-based model, is described in more detail, in section 6.5.2.

6.5.1 Water-energy modelling under a technical and economic context

For the representation of the water supply system of Athens and its interactions with energy (technical, involving water-energy conversions, and economic, by means of cost of energy and its footprint to water price), the conceptual structure of Hydronomeas is used. As already mentioned, the underlying methodological framework follows a parameterization-simulation-optimization scheme, allowing for: (a) network-type schematization of the water and energy fluxes, in terms of nodes, corresponding to sources and sinks (i.e., demands), and links, representing water transfers and exchanges; (b) formulation of operation rules, in terms of parametric mathematical expressions, with regard to major control components, both hydraulic (e.g., reservoirs, diversions) and power (hydropower stations, pumping stations, pumped-storage stations); (c) step-by-step representation of the real-world system operation, under multiple targets and constraints, through advanced simulation techniques; (d) evaluation of the system's performance under multiple criteria, including economy, efficiency, reliability and resilience; (e) derivation of best-compromise planning and management solutions, at both the short and long-term horizons, through robust optimization approaches.

However, Hydronomeas cannot represent dynamic inputs, i.e., water demands and energy prices, since both elements are built upon the steady-state hypothesis. Under this premise, the model only accepts constant or seasonally varying inputs for the two components, which hides significant aspects of the perpetually changing socio-economic environment.

To overcome this constraint, we developed a surrogate model of Hydronomeas that is able to account for the socioeconomic variability and is much more efficient computationally, since the module of the optimization to extract the operational rules is not available. Thus, the operational policy of the system is expressed in terms of the so-called "resilient-based" rules, which are depicted is Figure 6.8b. The surrogate tool also implements a simplified representation of the total power consumption. This relationship has been established by compiling discharge and energy consumption data from the main pumping stations during last 15 years.

As mentioned, the technical system is driven by monthly rainfall, runoff and evaporation time series, while the economic system is driven by the energy market price to extract the associated water price. Since this system is a key asset for the sustainable development of the capital city of Greece, its long-term assessment procedure should include multiple equally probable scenarios for all key drivers, in order to reflect a wide number of potential states of the hydrosystem (in terms of storages, inflows and demands). As implied by the specifications, the randomly varying characteristics of hydroclimatic processes and energy costs are properly represented through stochastic models. Thus, synthetic time series of 2000 years of monthly rainfall, runoff and evaporation, as well as electricity prices (Figure 6.11), are generated, based on associated historical data. The data synthesis is employed via the hydrometeorological and electricity price generators, as described in sections 3.1.3 and 3.3.3, respectively.

Following this, the water price is function of the overall energy cost, which is in turn function of the energy consumption across the hydrosystem, which is eventually associated with its long-term management policy, expressed in terms of operational rules. In contrast with energy price, which is an external information to the water utility, the energy consumption is highly dependent to the past, present and future operational policy by the water utility. For the case of water supply system of Athens, we follow a low-cost policy and the resilience-based operational rules, that set as priority the water abstraction from Evinos and Mornos.

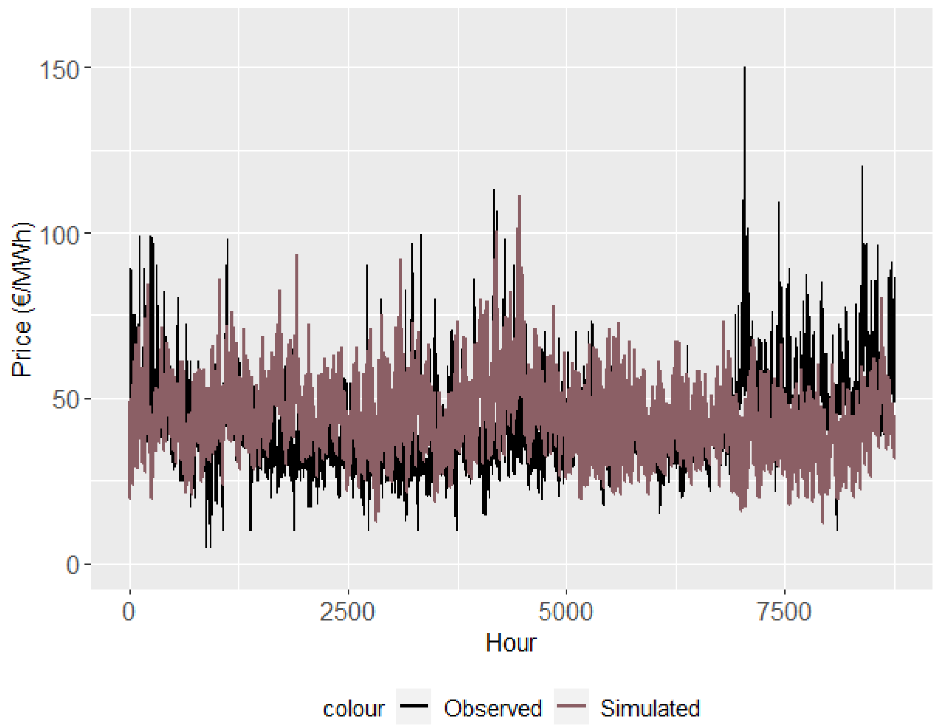


Figure 6.11: Time window of synthetic electricity prices contrasted to historical data.

6.5.2 The social system as an agent-based model

5.6.2.1 Model architecture

An agent-based model for Athens' consumers is developed by using the Mesa framework, i.e., an Apache2 licensed agent-based modelling framework in Python (Kazil et al., 2020), in which the household reflects the heterogeneous and adaptive nature of the water use behavior. All households are spatially distributed in the urban boundary (which is configured as a grid), and they can move by following a random uniform distribution in order to interact with their immediate neighbors and influence each other's water consumption attitude. The conceptual methodological framework is described in section 3.2.3.

5.6.2.2 Entities and state variables

As already mentioned in section 3.2.3, each household agent consists of three essential parts, i.e., attributes, behavioral rules, and memory, which vary across households in the initial set up of the model, and they change during the simulation, due to both external and internal influences. In the model, we consider two entities, i.e., the Households and the Water Saving Campaigns, the interactions of which are assumed independent, while their further taxonomy is described below.

In particular, the Households are classified into five categories according to their income (Hussien et al., 2016) and their environmental consciousness, in order to describe the range of their water consumption. The consciousness is further distinguished into three sub-categories, namely low, moderate, high. Thus, their behavior/adaptation is depended on all these characteristics and their tendency to be influenced by their social network.

The five distinct Household categories are:

Category 1: Their annual income is up to 5,000 € and their daily water consumption is in a range of 100-120 L/capita, according to their environmental consciousness. These households cover the 30% of the available grid;

Category 2: Their annual income ranges from 5,000 to 10,000 € and their daily water consumption is in a range of 120-140 L/capita, according to their environmental consciousness These households cover the 28% of the available grid;

Category 3: Their annual income ranges from 10,000 to 15,000 € and their daily water consumption is in a range of 140-160 L/capita, according to their environmental consciousness These households cover the 18% of the available grid;

Category 4: Their annual income ranges from 15,000 to 20,000 € and their daily water consumption is in a range of 160-200 L/capita, according to their environmental consciousness These households cover the 14% of the available grid;

Category 5: Their annual income exceeds 20,000 € and their daily water consumption is in a range of 180-250 L/capita, according to their environmental consciousness. These households cover the 9% of the available grid.

The Water Saving Campaigns are also distinguished in three categories, according to their type, namely physical, media and social media based. The physical campaigns reflect the messages on newspaper, leaflets, workshops in schools, universities, jobs etc. On the other hand, media and social media campaigns represent the messages on TV and the Internet, and on the platforms of social media (Borawska, 2017). Their distribution in the grid is 20%, 50% and 30%, while their influence, by means of "intensity", follows a uniform distribution in a range 1-5 as below:

Physical campaigns: random sampling between 1-2;

Media campaigns: random sampling between 2-4;

Social media campaigns: random sampling between 2-5.

However, when the total reservoir storage is lower than a specific threshold (400 hm^3, corresponding to about 25% to their total capacity), the campaigns are potently activated.

5.6.2.3 Process overview

The modelling of the Athens' society is based on the simultaneous interaction between the Households and their external influences. The description of the process is presented in section 3.2.3.

6.5.3 Model coupling

The modeling of a sociotechnical system presupposes the coupling of the four building blocks, i.e., physical, technical, economic and social. The computational procedure is outlined in the conceptual flowchart of Figure 6.12, while its description is as follows (in the parenthesis are the associated fluxes):

For the representation of the physical system in stochastic means, we generate correlated time series of rainfall, evaporation and runoff (1b) as inputs to the technical one (in particular, we assign three input time series to each reservoir). Additionally, we consider a predefined seasonal pattern of water consumption (1a), while the energy price is also handled as a stochastic process (1c) that reproduces the probabilistic behavior and autocorrelation structure of the historical data. Then, the model of the technical system runs, providing as outputs the water price (2a) and the total system's storage (2b). We remark that the water price is estimated by combining the energy price, the fixed cost and the energy consumption across the water supply system.

Following this, the social system, i.e., the ABM runs by taking as inputs the simulated water price data (3a, bills), and, indirectly, the accumulated storage data of the water supply system (3b). Specifically, the information about the available water storage is depicted in the frequency and intensity of the water saving campaigns. Eventually, the technical system re-runs, by replacing the steady-state hypothesis of water demands with the dynamic demands (4), as extracted from the ABM. The final output is a new, more realistic, allocation of all water and energy fluxes, including the simulated storages (6).

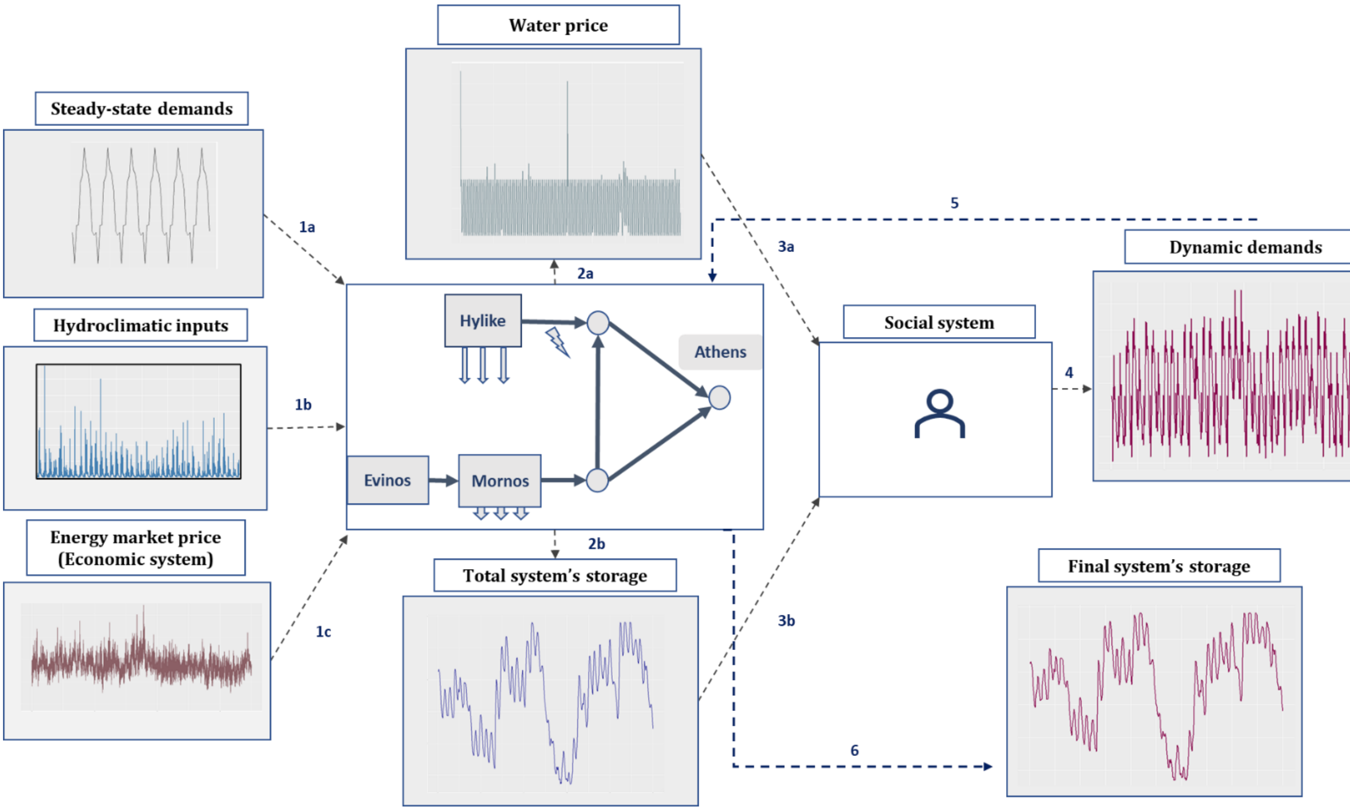


Figure 6.12:: Conceptual flowchart of the overall modelling framework. Fluxes (1a), (1b) and (1c) are the inputs of the technical system, while its outputs are fluxes (2a) and (2b). Fluxes (3a) and (3b) represent the essential inputs for ABM that results to path (4). Finally, the technical system re-runs with inputs (1b), (1c) and (5), and its output is the revised water balance (6).

6.1 Insights to the persistent drought of 1988-1994

During years 1988-1994, the water supply system of Athens has been substantially stressed by a persistent drought, thus forcing the water utility to apply both structural and non-structural measures (Karavitis, 1998). These included large scale improvements of the water distribution network, on the one hand, and extended water saving awareness campaigns, together with effective pricing policies, on the other.

Figure 6.13a, illustrating the evolution of the total storage of Mornos and Hylike from 1981 to 1996, reveals the emergency of the system, which reached twice its dead volume. We remark that during the aforementioned 15-year period, the water supply system of Athens system comprised only these two main reservoirs, since the Evinos dam and the diversion tunnel were constructed after 1996. Similarly, Figure 6.13b, shows the evolution of the average price of drinking water during the same time window. This has been approximately estimated on the basis of the tariff data of Focusing on sub-period 1988-1996, we employed a correlation analysis, by considering the water consumption as dependent variable, and using as predictors the reservoir storage and the mean water price, for different time lags. We underline that from the water utility perspective, the storage is a signal for launching water saving campaigns, and may also utilized as an easily retrievable information for the stakeholders and the media. We also highlight that the use of lags is necessary, since the water bills are quarterly, while they allow to establish a reasonable period of response to the campaigns that are associated with the available storage. For both predictors, the optimal lag was found to be three months.

In order to account for the combined response of the two variables, we established a simple regression model of the form:

$$D_t = w_j \; a \, V_{t-3}^{b} \, C_{t-3}^{c} \tag{6.81}$$

where D_t is the consumption, w_j is an adjusting factor, which is periodic function of month j (in order to describe the seasonal variation of demands), while V_{t-3} and C_{t-3} are the reservoir storage and water price with a three-month lag. The above relationship was calibrated exclusively for the dry period (1988-1994), exhibiting a Nash–Sutcliffe efficiency (NSE) up to 36.5%. Yet, outside of this period, the model performance is rather unacceptable (Figure 6.15). It is clear that such simple statistical tools that ignore the complexities and uncertainties of the water-energy-society-market nexus are unable to represent properly the water consumption for all potential system's states. In this vein, we next demonstrate a more sophisticated context, key element of which is an agent-based model (ABMs) that represents the Athens's consumers. The predictive capacity of the ABM component is evaluated by using as benchmark the same historical period.

Table **15** summarizes the progressive pricing policy by the water utility. For convenience, at the beginning of the period of interest (1/1/1981), we assumed an average price of 0.10 €/m^3.

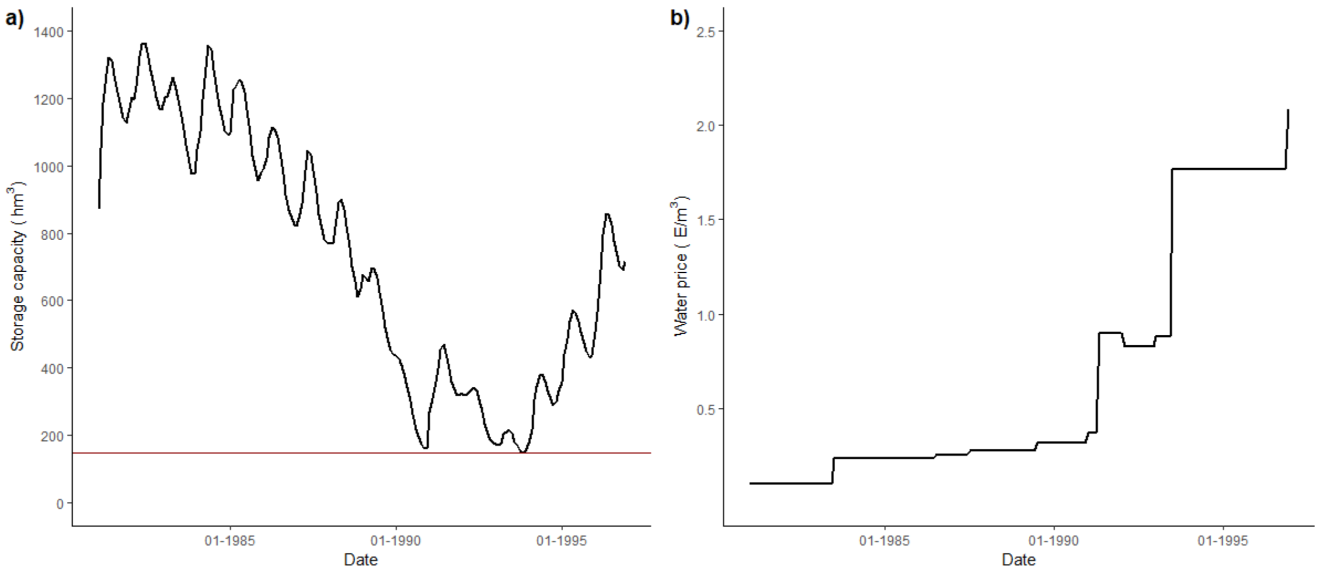


Figure 6.13 :(a) Observed storage capacity during years 1981-1996 (black line) compared with the dead volume of the system (red line), and (b) average price of drinking water.

Focusing on sub-period 1988-1996, we employed a correlation analysis, by considering the water consumption as dependent variable, and using as predictors the reservoir storage and the mean water price, for different time lags. We underline that from the water utility perspective, the storage is a signal for launching water saving campaigns, and may also utilized as an easily retrievable information for the stakeholders and the media. We also highlight that the use of lags is necessary, since the water bills are quarterly, while they allow to establish a reasonable period of response to the campaigns that are associated with the available storage. For both predictors, the optimal lag was found to be three months.

In order to account for the combined response of the two variables, we established a simple regression model of the form:

$$D_t = w_j \, a \, V_{t-3}^{b} \, C_{t-3}^{c} \tag{6.81}$$

where D_t is the consumption, w_j is an adjusting factor, which is periodic function of month j (in order to describe the seasonal variation of demands), while V_{t-3} and C_{t-3} are the reservoir storage and water price with a three-month lag. The above relationship was calibrated exclusively for the dry period (1988-1994), exhibiting a Nash–Sutcliffe efficiency (NSE) up to 36.5%. Yet, outside of this period, the model performance is rather unacceptable (Figure 6.15). It is clear that such simple statistical tools that ignore the complexities and uncertainties of the water-energy-society-market nexus are unable to represent properly the water consumption for all potential system's states. In this vein, we next demonstrate a more sophisticated context, key element of which is an agent-based model (ABMs) that represents the Athens's consumers. The predictive capacity of the ABM component is evaluated by using as benchmark the same historical period.

Table 15: Percentage variation of water prices for different levels of consumption (m3).

DATE/CONSUMPTION	10	15	20	30	40	50	60	81	105	200
01/07/1975	202	158	141	134	131	129	128	126	125	124
01/07/1982	133	148	197	234	251	261	268	277	282	291
01/07/1985	0	0	5	8	9	10	11	11	11	12
01/07/1986	24	22	13	7	5	4	3	2	2	1
01/07/1988	21	19	5	12	15	17	18	19	20	21
01/01/1990	-8	-11	-13	6	18	25	29	34	37	41
01/05/1990	159	176	184	202	237	265	281	298	309	323
01/01/1991	-20	-20	-20	-8	-5	-3	-2	-2	-1	-1
01/01/1992	7	7	7	7	7	7	7	7	7	7
01/07/1992	100	100	100	100	100	100	100	100	100	100
01/12/1995	15	15	15	18	19	19	20	20	20	20

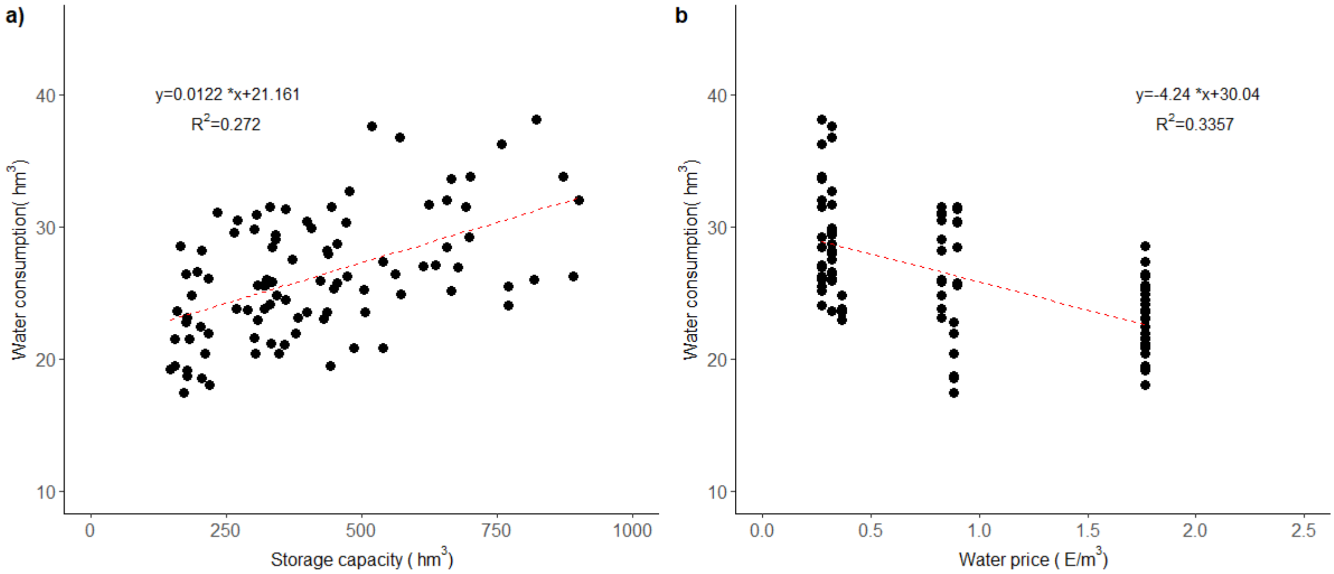


Figure 6.14:. Scatterplots of historical water consumption, storage capacity, and water price for the drought period (1988-1994).

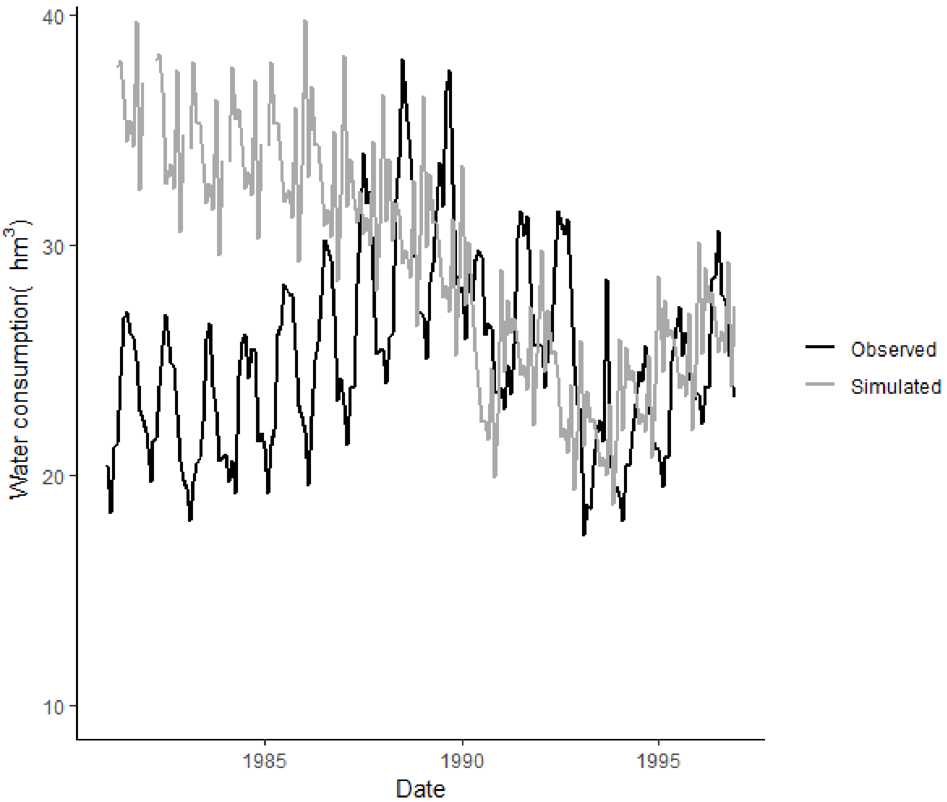


Figure 6.15:. Comparison of observed monthly consumption data with calibrated ones for period 1981-1996.

6.2 Applications: Learning from history to employ long-term management policies

6.2.1 Representation of historical consumptions (1981-1996)

As mentioned, we initially use as benchmark the period 1981-1996 that also includes the persistent drought of years 1988-1994, which pushed the water supply system beyond of its standards. In this case, we only consider the ABM component, which is driven with historical storage and water price data.

In order to obtain safe conclusions, an essential task is to provide a realistic representation of the Athens's consumers during the 80's and early 90's. In this context, we adjusted the ABM to the corresponding social characteristics, when the consumers were about 3.05 million, substantially less environmental aware than today, while the price of water was very low with respect to the average purchasing force. Also, four decades ago, the information means were very limited, with respect to the current expansion of social media. Thus, in the current analysis, the coverage of the consumers categories in the grid is changed, and the social media campaigns are ignored. Specifically, categories 1 to 5 cover the 15%, 30%, 25%, 20% and 10%, accordingly.

Figure 6.16 demonstrates the comparison of the simulated water consumption, through the ABM, and the historical one. We remark that, on an annual basis, the maximum observed reduction of the water consumption was 23.6%, while the simulated one is 23.3%. For the full time period (1981-1996), the NSE is 0.350, while for the dry sub-period (1988-1994) rises to 0.501.

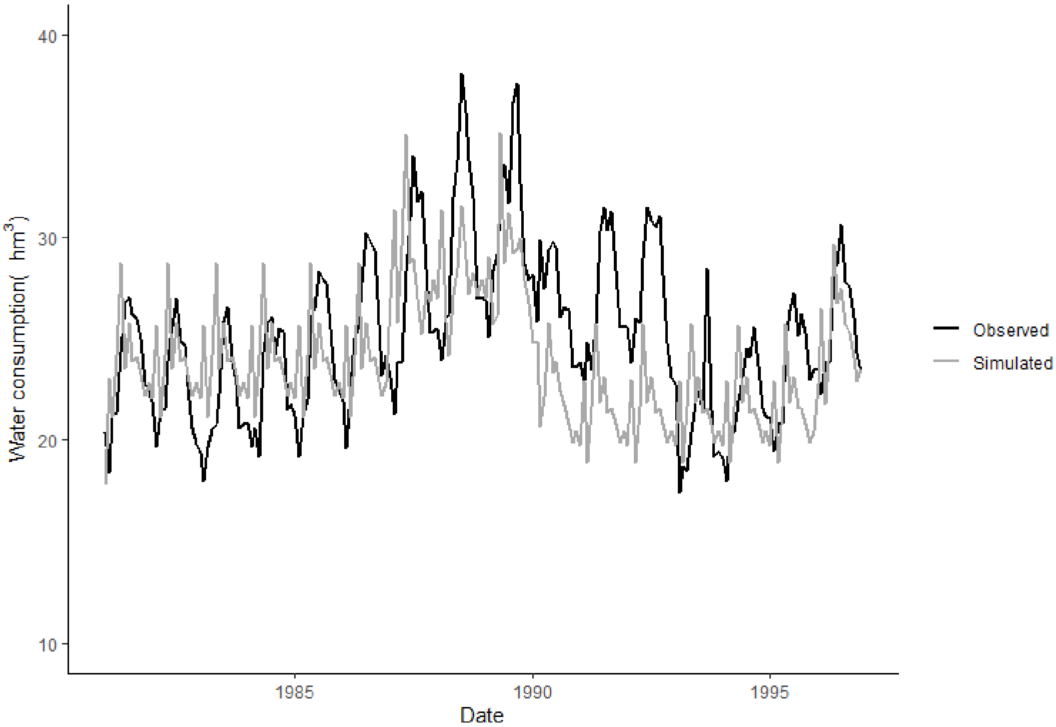


Figure 6.16: Comparison the historical water consumption data against the ABM approach.

6.2.2 Long-term simulation scenarios

After validating the predictive capacity of the ABM component against historical data, we reveal the advantages of the full modelling framework in a stochastic simulation context, where the water demands and electricity costs are dynamic elements, that are interacting with the technical and the social system. In this vein, three ABM settings are adopted:

ABM setting A: Baseline setting, in which we consider that the agents are influenced by their network and the public awareness campaigns.

ABM setting B: The households are only affected only by their network, while the aforementioned campaigns don't exist.

ABM setting C: The households are further motivated by the external environment (including campaigns and social network), considering a 10% increase with respect to setting A.

A key question of such analysis is the effect of influencing tactics in water consumption and eventually in the reservoirs' storage under different conditions in the long term. In Figure 6.17 we compare the constant annual demand, imposed by the steady-state hypothesis, with the dynamic demands obtained by the ABMs (extremes settings B and C), for the first 40 years of simulation. These are also contrasted to the simulated storage data, derived from the steady-state model. As expected, under the steady-state hypothesis the modelling procedure ignores the impacts of persistent droughts to the society's response, in terms of consumption, thus the demand remains constant although the system's storage is systematically dropping. On the other hand, when the influencing tactics are adopted, through the ABMs, the unified, i.e., sociotechnical system, is well-responding to such unfavorable hydroclimatic conditions because of the household's adaptation. Koop et al. (2019) concluded that a combination of price incentives, water use restrictions and knowledge transfer is claimed to lead to roughly 10–25% savings, in particular during drought periods and predominantly in lawns and gardens. This outcome is reasonable, due to the anelasticity of domestic water demand. It is also in line with our experience with regard to the water supply system of Athens during the persistent drought from 1988 to 1994, where the overall drop of water consumption due awareness campaigns and pricing policies reached about 23% (Figure 6.3). This key historical feature is well represented by the proposed modelling framework, in which the decrease of water consumption during a similar period is about 18-23%.

The difference of the two approaches in terms of simulated storages for the 40-year period are demonstrated in Figure 6.18. Under the ABM approach, the reservoirs usually retain larger amounts of water, thus they are able to respond more effectively during persistent droughts, thus generating smaller water deficits. For, during this period, these are 4.25% less than the steady-state scenario.

A clearer picture is obtained by plotting the cumulative storage data by the steady-state hypothesis and the ABM setting C. At the end of 40-year period, the two lines differ by 32,774 hm^3, that equals to 65.5 hm^3 per month (Figure 6.19). Actually, this difference is not only due to the water consumption per se but is the aftereffect of multiple and complex processes. Interestingly, a systematic reduction of water demands leads to larger reservoir storages and, eventually, water levels, which in turn may result to increased water losses due to leakage and spills. On the other hand, since smaller amounts are released to the conveyance network, the water losses across the aqueducts are decreasing.

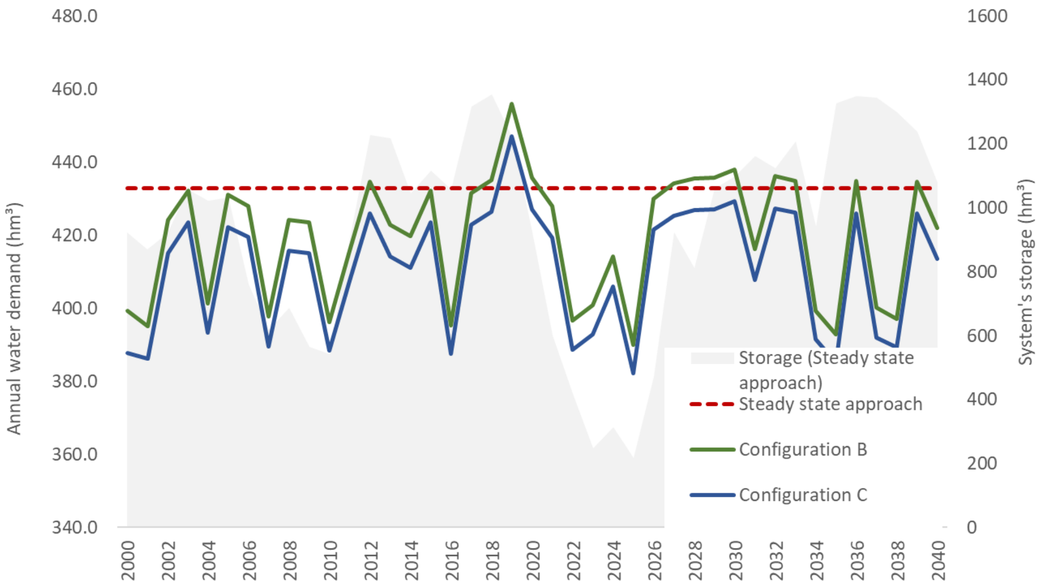


Figure 6.17: Comparison of steady-state (thus constant) annual demand against the two extreme ABM settings, where demands are evolving on the basis of simulated social behaviors. The simulated storage under the steady-state context is shown in the background.

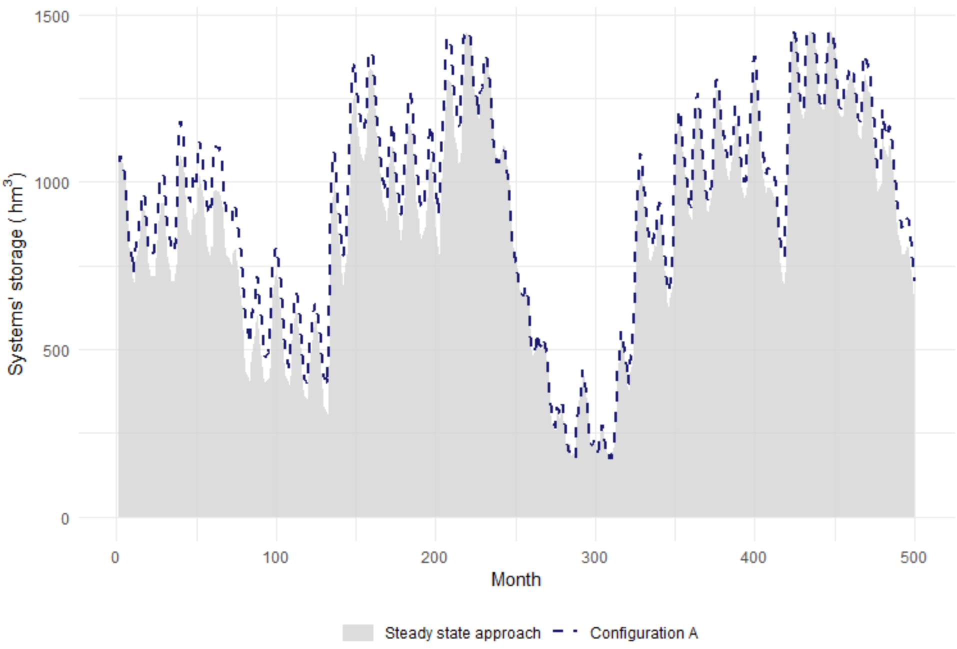


Figure 6.18: Comparison of steady-state hypothesis against ABM setting A in the resulting evolution of total reservoir storage.

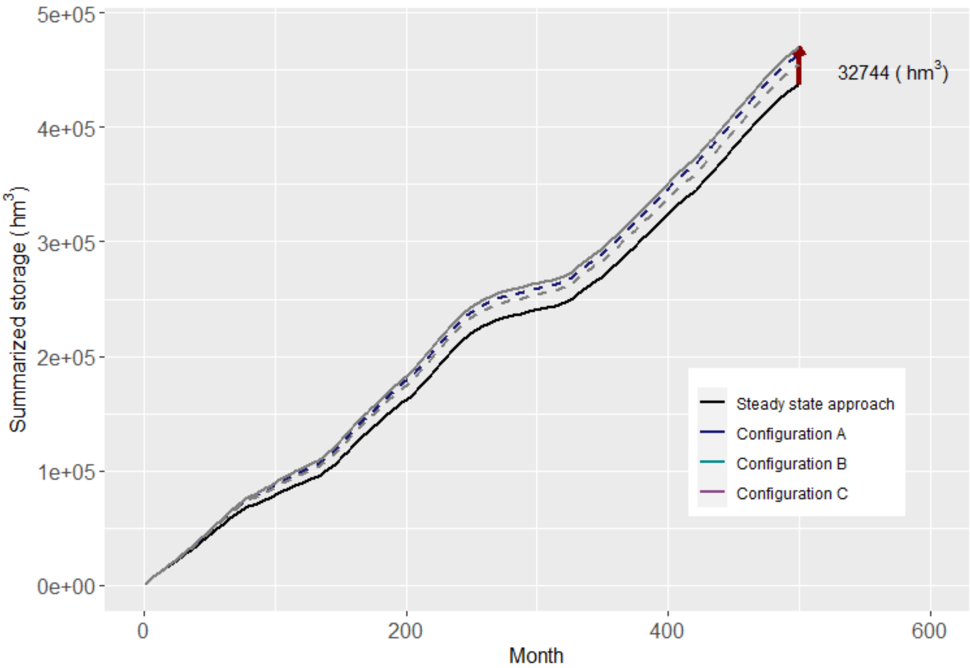


Figure 6.19:: Comparison of steady-state hypothesis against ABM settings in terms of accumulated storage.

6.3 Conclusions

The rapidly increasing water demand and the recognition of the vital role of water resources to sustainable development impose a new view to the so far practices of integrated water resources management. According to its widespread definition, this concept promotes the coordinated development and management of water, land and related resources to maximize economic and social welfare in an equitable manner, without compromising the sustainability of vital ecosystems (Agarwal et al., 2000). While the above declaration makes indirect reference to energy ("related resources") and society (by highlighting the overall objective of social welfare), it fails to reflect the complex and multidimensional interactions between water, energy and society, and also ignores the key role of energy market, as an overall driver of water costs, prices and demands.

This research attempts to provide a tailored-made methodology for evaluating water supply systems by representing them under the prism of the water-energy-society-market nexus and under the uncertain conditions. While the individual representation of these four elements is a challenging task per se, it becomes even more demanding if they are accounted for as a dynamically changing nexus. In this vein, we initially set the specifications for a macroscopic, unified and easily adjustable stochastic simulation framework. The adaptability is key question, particularly when dealing with large-scale systems, since these are followed by computational burden and large amount of data. Other issues that have been addressed are: (a) the definition of the boundaries of the socio-technical system, (b) the description of interactions between the technical and social components, and (c) the unified representation of four building blocks, in terms of natural, technical and economic processes, and their feedbacks to the social behavior as well.

A first essential step to this objective was to level up from geography to anthropogeography, in order to expand the spatial boundaries of water supply systems, thus incorporating the structural limits of society. The conventional determination of such systems is dictated by the extent of associated infrastructures, which link water resources with water demand nodes, under steady-state approaches for the representation of the social footprint. On the other hand, the nexus-based approach seeks for substituting the oversimplified and static concept of the entire urban area as a "node" by a dynamic social sub-system, which interacts with the technical one, and reflects the behavioral rules of society. For the swift from the steady-state hypothesis to a dynamic social subsystem, we took advantage of agent-based models, which is the sole approach that explicitly accounts for internal interactions across the social network, in order to represent the household's behavior with respect to water consumption.

Another significant contribution of the proposed framework is the indirect incorporation of the energy market (which is the cornerstone of our era) and its uncertainty, within the water supply system. As indicated by the literature review, the building block of energy is simply handled in terms of power generation and consumption (namely, as a flux). Here, apart from the energy fluxes, we also consider the energy price as a stochastic component, driven by the energy market, which is linked with the full water-energy-society cycle, i.e., the water price, the associated social response, the water consumption, and, eventually, the water management.

As a demo study, we built and evaluate our framework upon the water supply system of Athens. Due to its complexity and scale, and the experience of the persistent drought that has substantial impacts to the consumer's behavior, this system is ideal for revealing the importance of the nexus approach, as well as the multiple modelling challenges. We underline that in this case, the water price is strongly associated with the running energy prices and the long-term management policy (intense use of pumps in case of unfavorable hydroclimatic conditions), while the water saving campaigns are mainly driven by low reservoir storages. Our long-term simulations indicated that after influencing tactics, including changes to water price and public awareness campaigns, the households can adapt their consumption. Specifically, this practice reduced the deficits by 4.5% along with a water saving of 65.5 hm^3 per month (about 15% of the annual consumption of Athens for the projection scenario).

7 Dealing with the conflicts of the water-energy nexus: the case of multipurpose reservoirs

Preamble

This chapter deals with the ongoing debate about hydropower in the energy transition, which is strongly associated with its sustainable character, social and environmental footprint, and potential benefits. Since their operation and management policies are subject to inherently uncertain processes, we contribute an uncertainty-aware optimization methodology that supports operators in accounting for the cascade effects of three main uncertain drivers, i.e., rainfall, water demands, and energy scheduling. To describe climatic and energy-market uncertainties, we follow the generators described in **Chapter 3**. In addition, for the human-oriented procedures, i.e., water and energy targets, we employ statistical analyses of historical abstractions to fit copula-based relationships, in which the desirable releases for energy production depend on day-ahead electricity prices, as described in **Chapter 3** and **4**. Eventually, we establish a toolbox that offers insights for decision-making regarding the estimated profits, their expected changes and the associated risk due to climate or market-oriented shifts. Our approach is demonstrated in a multipurpose reservoir in Greece, Plastiras, which is affected by highly increasing socioeconomic conflicts. This chapter is based on:

Sakki, G. K., Castelletti, A., Makropoulos, C., and Efstratiadis, A.: Unwrapping the triptych of climatic, social and energy-market uncertainties across multipurpose hydropower reservoirs, Journal of Hydrology, 628, 2025, 10.1016/j.jhydrol.2024.132416

Sakki, G. K., Castelletti, A., Makropoulos, C., and Efstratiadis, A.: Trade-offs in hydropower reservoir operation under the chain of uncertainty, EGU General Assembly 2024, Vienna, Austria, 14–19 Apr 2024, EGU24-3487, https://doi.org/10.5194/egusphere-egu24-3487, 2024.

7.1 Setting the scene

Hydropower reservoirs are keys to both water and energy security at the national level. As water elements, they serve multiple consumptive and environmental uses, while as energy elements, they determine the stability and reliability of interconnected grids (Llamosas & Sovacool, 2021). In this context, their planning and management should consider water resources protection, energy transition concerns, economic growth, environmental improvement, and social prosperity.

Since hydropower systems, as a typical water-energy nexus paradigm, are driven by inherently uncertain hydroclimatic processes and multiple human-induced procedures (e.g., legal regulations, strategic management policies, real-time controls, market rules), their operation is highly exposed to emerging climatic (e.g., Wasti et al., 2022), social (Bazzana et al., 2020; Hurford et al., 2020) and energy-market pressures (e.g., Luo et al., 2019). For instance, Sovacool and Walter (2019) investigated the ongoing debate about the future role of hydropower in the energy transition, highlighting the main policy issues. Recent studies reveal that the shifts of energy policies and the social pressures are eventually more impactful than climate change itself (Anghileri et al., 2018). Nevertheless, this triptych of stresses requires revisiting and adapting conventional planning and management practices to ensure adaptability against future risks and potential violent changes. The redefinition of its management is becoming even more urgent in the aftermath of the energy crisis, whether a dilemma arises between security and transition (Joița et al., 2023).

The optimal design of reservoir operation accounting for time varying demands and other sources of uncertainty has been largely addressed by multi-objective optimization approaches (cf. recent state-of-the-art review by Giuliani et al., 2021). Focusing to hydropower reservoirs, Wyrwoll and Grafton (2022) propose a resilience framework to reform hydropower governance and support the design of multipurpose operations under water and energy risks. On the other hand, Yazdi and Moridi (2018) manifest for a synergetic perspective across the water and the energy sector by applying operational rules to overcome the conflicts and balance the trade-offs to a wider set of stakeholders whose interest lies in the water supply and energy production. Nevertheless, the optimal water allocation among users (energy and water demands) relies on the proper economic representation of the effects of alternative allocations. This option is also offered by hydro-economic models, which can be the basis for water decision-making (Arjoon et al., 2014; Harou et al., 2009). These are based on the concept of opportunity cost, where the objective is to maximize the profits from power sold to the day-ahead market and the profits from water supply and irrigation while minimizing the penalties of non-fulfilling the water and energy demands.

Nevertheless, from their early steps of systems analysis approaches in reservoir modelling, the steady-state hypothesis is adopted, where water and energy demands are considered time constants (or following seasonally varying patterns). In this respect, more advanced methods should be established to account for the joint fluctuations of the market price, the uncertain human factor, and the hydroclimatic variability as well.

According to the uncertainty's architecture, as described in section 2.1, two kinds can be discriminated, i.e., the aleatory, which is caused by random phenomena that can be described in probabilistic means, and epistemic, which is mainly caused by a lack of knowledge or data (Kiureghian & Ditlevsen, 2009). In the modelling procedure of complex engineering systems, this discrimination and a proper representation are crucial since the epistemic uncertainty is theoretically reducible, while the aleatory is intrinsically not (Caputo et al., 2023). This chapter is focused on hydropower systems that are driven by both kinds. In particular, the aleatory uncertainty refers to climatic, energy-market, and social processes, while the epistemic one regards all steps of the modelling procedure (from the overall configuration to the estimation of its parameters).

In the literature, the hydrological and the social uncertainty has been widely studied within hydropower systems and its applications, as described in section 2.4. In contrast, the uncertainty of the energy market is not broadly explored since this is the aftereffect of the recent deregulation and liberalization. Specifically, its variation is the indirect effect of social uncertainty since the electricity price process now enables the determination of competitive prices according to supply and demand market forces. The research on this uncertainty mainly focuses on forecasting (Kostrzewski & Kostrzewska, 2019) and market structures (Papavasiliou et al., 2015). However, an effort for stochastic reproduction of electricity price processes has been made, but the representation of its critical characteristics, i.e., double seasonality and abnormal, yet persistent, changes are ignored (Borovkova & Schmeck, 2017; Hou et al., 2017).

Even if a scientific effort has been made to investigate the uncertainty and its effects on the operation of multipurpose reservoirs, there are still open questions about a holistic approach. In particular, the exploration, representation, and eventually the simultaneous incorporation of multiple sources of uncertainty, i.e., epistemic, hydroclimatic, social, and energy markets in the management of reservoirs, are unexplored. Gaudard et al. (2016) and Anghileri et al. (Anghileri et al., 2018) studied the combination of climate change scenarios and the variability of electricity prices within the assessment of hydropower systems . Along the same line, Ray et al. (2018) examined climate change scenarios under financial risks to stress-test hydropower resilience. Further to long-term assessment studies, the incorporation of uncertainty within the optimization of hydropower production has also been investigated by means of climatic projections and social uncertainties that refer to land use projection and operation policies (Y. Guo et al., 2021).

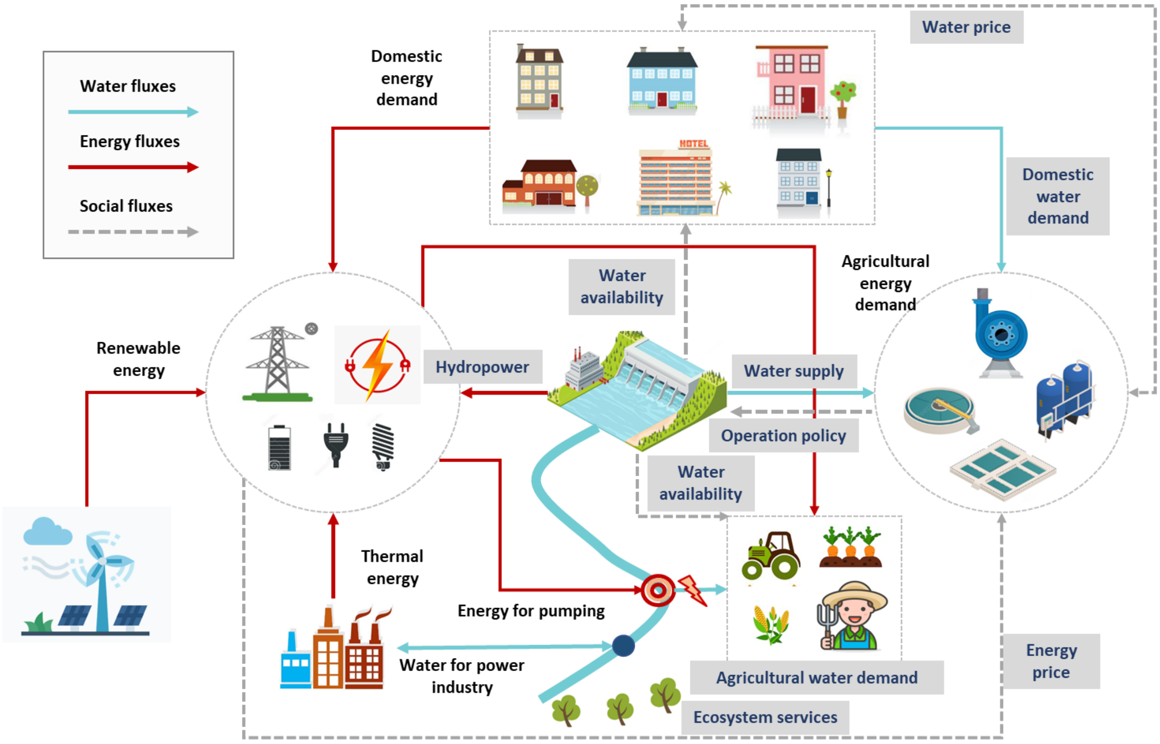


Figure 7.1: The water-energy-society nexus from the multipurpose hydropower perspective, the grey boxes corresponds to the fluxes (drivers) will be discussed.

All these approaches investigated individual or limited sources of uncertainty. Our approach is called to fill this gap by adapting the already introduced *uncertainty-aware simulation-optimization framework,* tailored for multipurpose hydropower reservoirs. This sets the specifications for handling the different facets of uncertainty and then formalizes them into robust and generic tools. Specifically, stochastic models are employed with different structures adapted to each process to represent climatic and electricity price uncertainty. For the direct social uncertainty, i.e., the social response, we use statistics to express the water demands as dependent random variables against climatic processes and the reservoir state. For the indirect social uncertainty, namely, the operation policy of the hydropower station, copula-based tools are developed that predict the energy target according to day-ahead energy prices and the operator's willingness. Finally, for the epistemic uncertainty, the emphasis is given to the inference of rainfall-runoff model parameters through calibration. To reveal the advantages of this framework, a modular procedure is employed, initially for assessing the current operation policy of the water-energy system and next for optimizing its operational rules under all examined aspects of uncertainty. This is stress-tested in a multipurpose reservoir in Greece, Plastiras, that fulfils energy (covers 5% of the hydropower production in Greece), water supply, and irrigation uses.

7.2 Uncertainty-aware framework for hydropower reservoirs

7.2.1 Holistic description of hydropower reservoir system

Let us consider a hydropower reservoir that fulfils water supply and irrigation demands. This is driven by hydrometeorological processes (precipitation, temperature, etc.), energy market fluctuations, and human-induced procedures (water demands, management policies). All these are inherently interconnected, thus forming complementarities and conflicts. In this respect, modelling the holistic water-energy system as a unified tool that accounts for all uncertainties is demanding. To untangle this, and following the generic principles discussed so far for water-energy systems, a specific framework is developed that includes several models, io order to incorporate both epistemic and aleatory (i.e., climatic, social, and energy-market processes) uncertainties within the optimization of hydropower reservoir management.

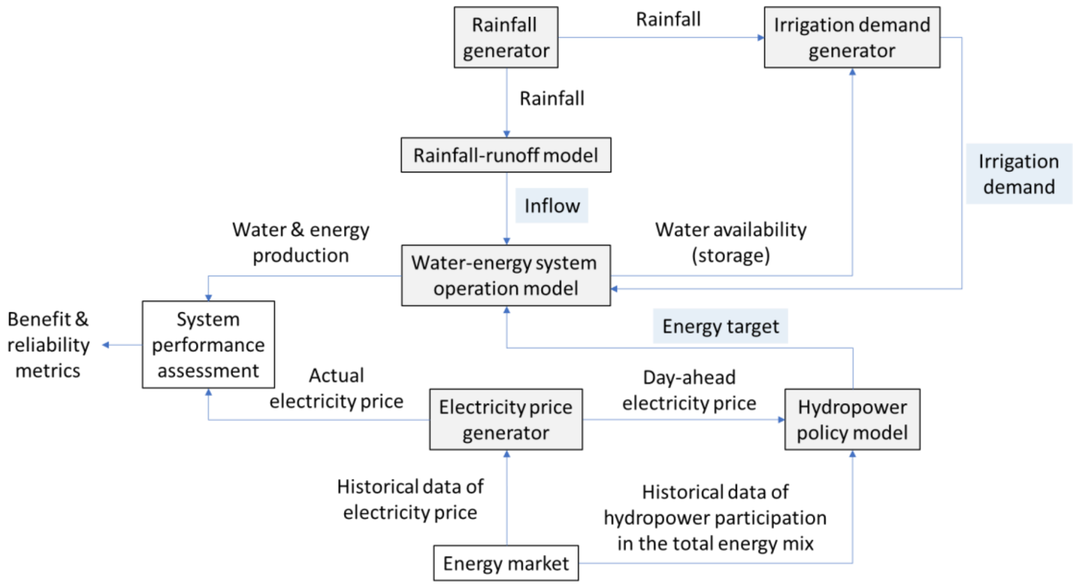


Figure 7.2: Schematic layout of models (light grey filled) and their interlinkages (blue lines).

Specifically, there is a need of the combination of six highly interlinked models, as represented in Figure 7.2**.** In particular, the two first models represent the overall drivers of the system, i.e., rainfall and electricity prices, as random processes. Their outcomes are synthetic time series, accounting for the stochastic regime of the observed processes across seasons and three scales of interest (daily, monthly, and annual). The rainfall time series (output of the first model) is input to the second one, i.e., rainfall-runoff, and is also used by the irrigation demand generator. Specifically, to account for the variability of irrigation uses, this model is also fed by the water-energy system operation model by means of water availability. In this respect, the water abstractions, which are in fact social pressures to the operator's system, are dependent on the actual climatic conditions (i.e., precipitation) and the actual system's state (i.e., reservoir storage). In addition, the electricity price time series (outcome of the first model) also has a twofold role since it is used to determine the hydropower production policy and the system's economic performance. Following this, all aforementioned models (rainfall and electricity price generator, rainfall-runoff, irrigation demand generator, hydropower policy model) feed the water-energy system operation model with three dynamic inputs, i.e., reservoir inflow, target energy, and irrigation demand. Eventually, a post-process assessment is employed that summarizes the system's performance in terms of economy and reliability, as well.

7.2.2 Handling uncertainties

The conventional practices for designing and managing multipurpose reservoirs ignore or misuse the combination of all facets of uncertainty. The aforementioned models can be easily adjustable in order to account for the uncertainty of their processes, i.e., inflow, energy target, and irrigation demand, which are also the key inputs to the operation model of the water-energy system. In this respect, three different approaches are adopted for each component to represent them as dynamic variables. Specifically, for the generation of inflows, the emphasis is given to the configuration of both climatic and epistemic uncertainty by employing stochastic generation of synthetic rainfall and randomly-varying parameters of a rainfall-runoff model (Figure 7.3). As explained in section 5.3.1, this model is essential, since it offers a large sample of data and account for the changing hydroclimatic conditions. Furthermore, the estimation of the energy target includes the incorporation of the energy market and social uncertainty that refer to the generation of electricity price time series through a stochastic model and the operation policy as an operator's decision, respectively (Figure 7.3). Finally, the irrigation demand is driven by climatic and social uncertainties since it depends on the hydrometeorological conditions and human perception (Figure 7.3). The proposed implementation of the individual procedures, also associated with their uncertainties, is further described.

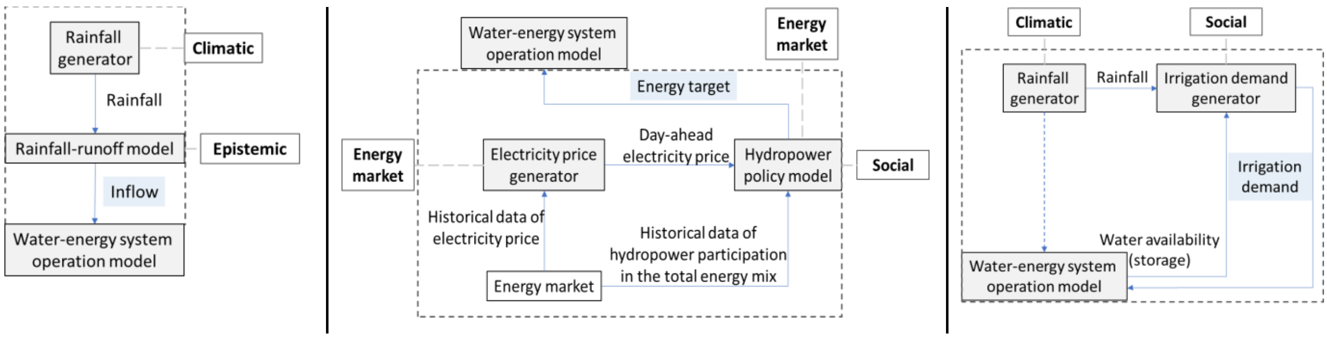


Figure 7.3:: Incorporation of different facets of uncertainty in the three input processes.

For the generation of inflows:

Epistemic uncertainty: Extraction of m parameter sets by calibrating the rainfall-runoff model across different windows of historical data, and by simultaneously applying randomly varying weights to the multi-objective performance measure, as described in section 3.4.3. The outcomes of this procedure are m ensembles of reproduced past inflows that are considered equifinal. We remind that the conventional calibration approach that ignores uncertainty implies extracting a unique set of parameters by assigning the full set of historical data and a specific formulation of the objective function. Hereafter, this will be referred to as the "original" parameter set.

Climatic uncertainty: Generation of m ensembles of synthetic precipitation time series (the primary climatic drivers of all hydropower systems) through the stochastic model, presented in section 3.1.3. Next, these are used as inputs to the rainfall-runoff model by considering the "original" set of optimized model parameters, thus providing m ensembles of simulated inflows.

Combination of climatic and epistemic uncertainty: Combination the m ensembles of synthetic precipitation data with the m sets of equifinal model parameters to account for both kinds of uncertainty.

For the estimation of the energy target and the generation of electricity prices:

Energy market uncertainty: Generation m ensembles of synthetic electricity price time series through the associated stochastic model.

Social uncertainty: Estimation of the actual target energy, according to the operator's desirable policy, by using as explanatory variables the m ensembles of synthetic day-ahead electricity prices.

For the generation of synthetic irrigation demands:

Social uncertainty: Generation of m ensembles of dynamically changing irrigation demands, which are inherently driven by the actual precipitation, yet they may also depend on the system state, i.e., the reservoir storage. We highlight that the farmers and other stakeholders often force the operators to release more water under high water availability conditions, which is yet an irrational and sub-optimal practice, in contrast to the main role of reservoirs as regulators in the long term. Eventually, this allows for embedding social uncertainty into the reservoir operation.

Following the above, different settings are built around the operation model of the water-energy system through a modular assessment procedure to quantify all aforementioned aspects of uncertainty:

Setting 1: Combination of historical inflows with the m ensembles of synthetic electricity prices to account for the energy market uncertainty per se.

Setting 2: The rainfall-runoff model is driven with historical precipitation data and m equifinal parameter sets to derive m ensembles of simulated inflows, which are next combined with m ensembles of synthetic electricity prices to account for both the epistemic and energy market uncertainty.

Setting 3: The rainfall-runoff model is driven with m ensembles of synthetic precipitation data and the original parameter set to derive m ensembles of simulated inflows, which are next combined with m ensembles of synthetic electricity prices to account for both the climatic and energy market uncertainty.

Setting 4: The rainfall-runoff model is driven with m ensembles of synthetic precipitation data and the m equifinal parameter sets to derive m ensembles of simulated inflows, which are next combined with m ensembles of synthetic electricity prices, to account for climatic, epistemic and energy market uncertainties.

Setting 5: Similar to setting 4, by also assigning dynamic irrigation demands, thus accounting for the climatic, epistemic, energy market and social uncertainties under a common context.

These settings are next applied to two practical problems, namely the assessment of existing reservoir policies and their optimization.

7.2.3 Modelling specifications

This section describes the proposed framework's modelling challenges and associated assumptions and objectives. An overall assumption involves the time step of the simulation. In particular, all models are built upon the daily scale since, from a hydrological point-of-view, this ensures very good accuracy with respect to the long-term operation of the water-energy system, while from the energy market perspective, it is the minimum acceptable resolution for representing the hydropower scheduling (Shen et al., 2020).

6.2.3.1 Rainfall and electricity price generators

Both models are based on stochastic theory, thus providing the ability to account for the uncertainty in modelling physical (e.g., precipitation) or non-physical processes (electricity price, driven by the energy market uncertainty). However, different approaches should be followed for the two processes since their probabilistic properties and dependence structure exhibit significant differences across all temporal scales of interest. The methodological frameworks of the rainfall and electricity price generators are described in section 3.1.3 and 3.3.3, respectively.

6.2.3.2 Rainfall-runoff model

To estimate the runoff generated over the upstream catchment, a flexible, parsimonious, and easily adjustable model should be selected. This must combine the ability to run long-term simulations daily with minimal computational burden. In our case, we are taking advantage of the lumped scheme as described in section 5.3.1, which is applicable for long-term simulations accepting stationarity of input processes and both steady-state and changing basin properties. To calibrate the model and extract the optimal set of parameters (totally eight), the use of the multi-objective performance measure is necessary, since it aggregates three typical goodness-of-fitting metrics (NSE, KGE, bias). The outcome of this model, i.e., the daily runoff, will next feed the water energy system operation model.

6.2.3.3 Hydropower policy model

The participation of a hydropower plant in the daily energy mix is a demanding task since it depends on the available reservoir storage, the possibility of spilling, and the energy market's trend. In particular, under flooding conditions, hydropower is set as the higher priority in the mix to produce energy, while it is also used in peak hours to reduce the energy price and maintain the stability of the electricity system. However, under normal operation conditions, the estimation of its participation is doubtful and uncertain.

The conventional practice for the operation of multipurpose reservoirs, and consequently, the estimation of the energy scheduling, are mainly based on steady-state methods. Specifically, it is considered a-priori, a constant or seasonally constant target energy production in order to achieve a desirable capacity factor for the power plant (Cordova et al., 2014; Ghimire & Reddy, 2013). This research aims to move forward with this simplified approach by using state-of-the-art probabilistic tools to predict the participation of hydropower plants in the energy mix. These refer to copula models that are able to describe dependent random variables. In hydropower reservoirs, these could be the observed day-ahead energy prices and operational data with respect to hydropower scheduling, e.g., the participation of the power plant in the energy mix, the frequency of activation of the power station, etc.

Here, we use copulas to develop conditional quantile functions of the response variable, i.e., hydropower sharing, with respect to a vector of regressors, namely potential day-ahead energy prices. Thus, each quantile function represents an operation policy since the hydropower plant follows a consistent approach regarding energy production within a range of electricity prices. In order to incorporate the social uncertainty with respect to the operation policy, three quantiles of interest are denoted that correspond to conservative, median, and energy-centric management policies.

6.2.3.4 Water consumption uses

A multipurpose hydropower reservoir is usually called also to fulfil consumptive water uses, i.e., water supply and irrigation. For estimating the energy demand, the methodology of section 6.2.3.3 will be used, while for the water uses, a statistical analysis should be employed to embed the hydrometeorological drivers. This research aims at estimating the monthly water demand as a dynamic input for the water-energy system operation model that accounts for the monthly precipitation. This allows to follow a rational management policy, in which the released water for water-related uses corresponds with the hydroclimatic conditions of the area of interest. This model will be further expanded to account for the climatic and social uncertainty by means of rainfall variability and irrational practices in the irrigation demands, respectively. In our case, the focus is given to the irrigation demand, since contrasting to water supply demands, these are large amounts of water and fluctuate across seasons.

6.2.3.5 Water-energy system operation model

To assess and optimize the management policy of the reservoir, the daily operation of the water-energy system should be represented by means of a simulation model implementing the reservoir mass balance as well as the technical characteristics of the entire system (regulatory tank, penstocks, water inlet, etc.). As already mentioned, this model is fed by the outcomes of all other modelling components. Specifically, the outcome of the rainfall-runoff model is the inflow to the reservoir, while the energy target estimation model determines the long-term policy of the operator regarding a desirable trade-off between water and energy demands, i.e., conservative, median, and energy-centric.

Next, to define the operational rules of the multipurpose reservoir, an optimization procedure is employed in the long run. The rationale is to maximize the benefits of the water-energy system without substantially changing the existing water allocations. In this vein, the optimization problem lies in the maximization of profits derived from water and energy delivery, simultaneously ensuring a high reliability level for the two consumptive uses (water supply and irrigation). The model should describe the strategic management policy of the reservoir in a systematic matter, e.g., using hedging rules (You & Cai, 2008), that will next be control variables (parameters) to optimize.

In our case, and in order to ensure a parsimonious formulation of the optimization procedure, these rules are denoted through two characteristic reservoir levels, z_{irrig} and z_{energy}, below which the releases for irrigation and energy production, respectively, are prohibited.

7.3 Case study

7.3.1 Layout

The proposed uncertainty-aware simulation-optimization framework for hydropower reservoirs is employed in the case study of Plastiras, which was constructed at the end of the 1950s. Plastiras dam and the associated engineering works, as demonstrated in Figure 7.4, belong to the first hydroelectric projects in Greece. It is a diversion dam, located in Tavropos, a tributary of river Acheloos. The reservoir has a useful capacity of 286.3 hm^3, while its level ranges from +776.0 (intake level) to +792.0 m (spill level). The total drainage area is 161.3 km^2, where 24.7 km^2 is the maximum area captured by the lake. Based on hydrometeorological during the years 1980 to 2020, the mean annual precipitation over the watershed is 1609 mm, and the mean potential evapotranspiration is estimated to be up to 838 mm, thus resulting in 967 mm of runoff (corresponds to a mean annual inflow of 155.9 hm^3).

The electric power station has an installed capacity of 129.9 MW (3 Pelton turbines of 43.3 MW), representing 4.3% of the total capacity of the large hydropower projects in Greece. The station is located on the west side of the Thessaly plain, 577 m lower than the abstraction level (+776 m), thus framing an ideal system for hydroelectric production. After passing through the turbines, the outflows are conveyed to a regulating tank, downstream of which they are distributed for irrigation and water supply of human settlements in the plain. The regulating tank has a capacity of 600,000 m^3, while the irrigation channels and the drainage system cover 887 km and 823 km, respectively. The water abstraction project includes a tunnel of 2,625 m in length with a diameter of 3.5 m. The capacity of the penstock is 33.5 m^3/s, while the water intake capacity is 26.4 m^3/s. Its layout is depicted in Figure 7.5.

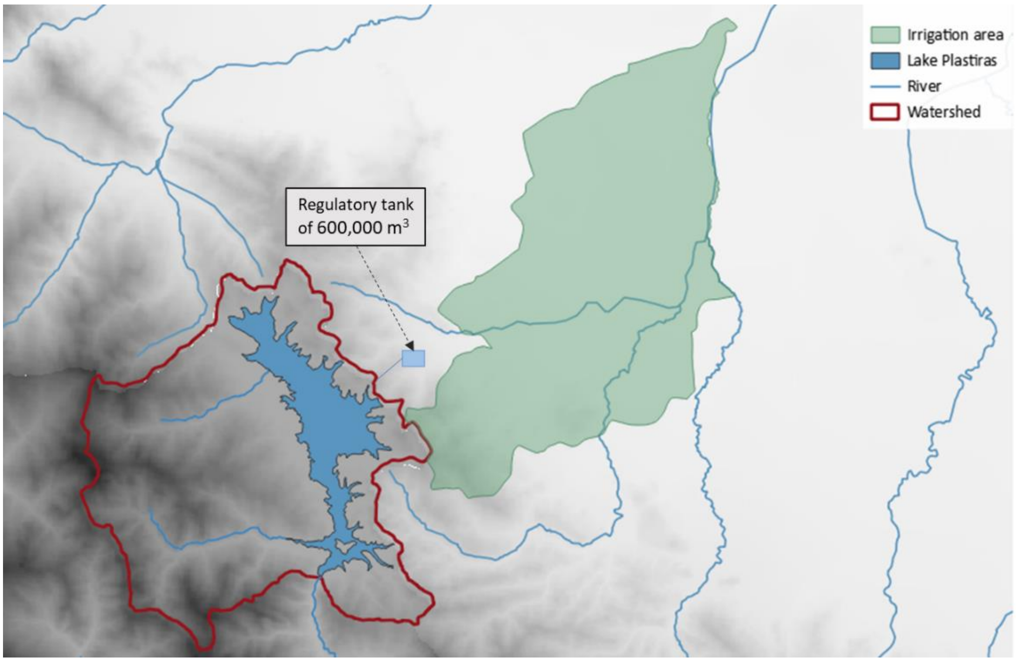


Figure 7.4: The Plastiras Lake, its watershed, and the irrigation area

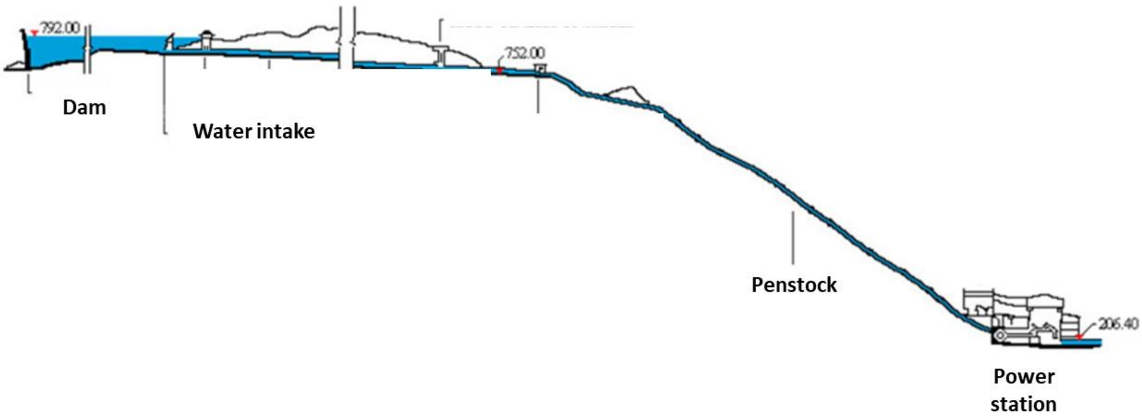


Figure 7.5: The layout of the dam and the associated works.

7.3.2 Operational history

This hydropower reservoir was chosen due to its historical evolution and associated conflicts. In particular, the initial design was dedicated to energy production, but this has been changed, and for a long time, hydropower production has been dictated by irrigation and water supply needs. Specifically, the shift from the energy-centric operation policy occurred in the mid-1980s, as demonstrated in Figure 7.6, when the irrigation needs were increased. On top of that, additional operational pressure for reservoir management was raised due to the touristic development. Specifically, the natural scenery attracted visitors, and numerous resorts were created. As a result, the lake's landscape strongly affects the area's economic development, and thus, the reservoir's level should be maintained high. These conflicting objectives of the different groups of interest, i.e., farmers, energy stakeholders, and hotel owners, further stress the successful management of this reservoir. For these reasons, several studies have been implemented to achieve a satisfactory trade-off between these conflicting targets (e.g., Christofides et al., 2005; Efstratiadis & Hadjibiros, 2011).

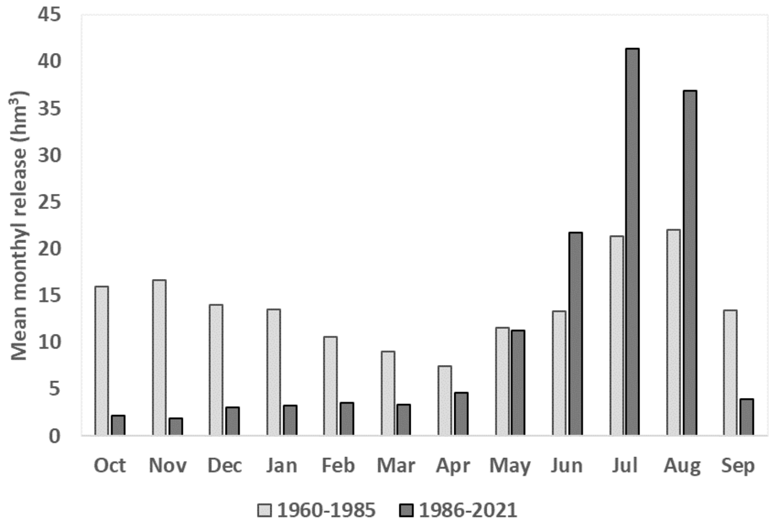


Figure 7.6: Historical evolution of monthly releases.

7.3.3 Modelling assumptions and estimation of the system's drivers

The implementation of the proposed framework requires the representation of the main system's drivers, i.e., precipitation, runoff, water and energy demands, as well as electricity prices, in stochastic-probabilistic means. In particular, the hydrometeorological inputs are the historical data of precipitation, evapotranspiration, and runoff from 1980-2021. Next, for the energy market processes, the historical data are used on electricity prices and participation of hydropower at the hourly scale in Greece. Also, the water releases for irrigation and water supply are used for the social-associated processes. In order to provide a large sample for the uncertainty-aware procedure, we employ the individual settings of the framework for 1000 scenarios (ensembles) of precipitation, inflow, and electricity prices, considering a time horizon of 20 years (7305 days, in total).

7.3.4 Operational policies – Target energy

Taking advantage of a probabilistic tool, i.e., the copula model, we can predict the hours of operation of a hydropower plant based on the day-ahead energy price. To formulate this model, the energy market data are used for a period of seven years, i.e., 2015-2022, regarding the share of hydropower and the day-ahead energy price in Greece (only this short period can be considered representative of the current status of the Greek electricity system). As demonstrated in Figure 7.7 and Figure 7.8, the energy price and the participation of hydropower are highly correlated. Particularly, in 2022 the incorporation of hydropower in the energy mix is identifiably increased, mainly due to the energy crisis. This tactic contributes to decrease the energy price, if possible, or to maintain the energy prices low.

Our statistical analysis is employed after applying a classification to the dataset since no correlation was detected in low and median range values due to the inherent complexity of multipurpose reservoirs. For instance, the operation of a hydropower plant may be dictated by reasons different from the energy price (e.g., to avoid spills). Figure 7.9 shows the scatter plot of the day-ahead energy price and the participation of hydropower plants in the Greek energy mix, in terms of power production. This analysis regards the electricity prices above 200 €/MWh, and the coefficient of correlation of the two variables is 0.392.

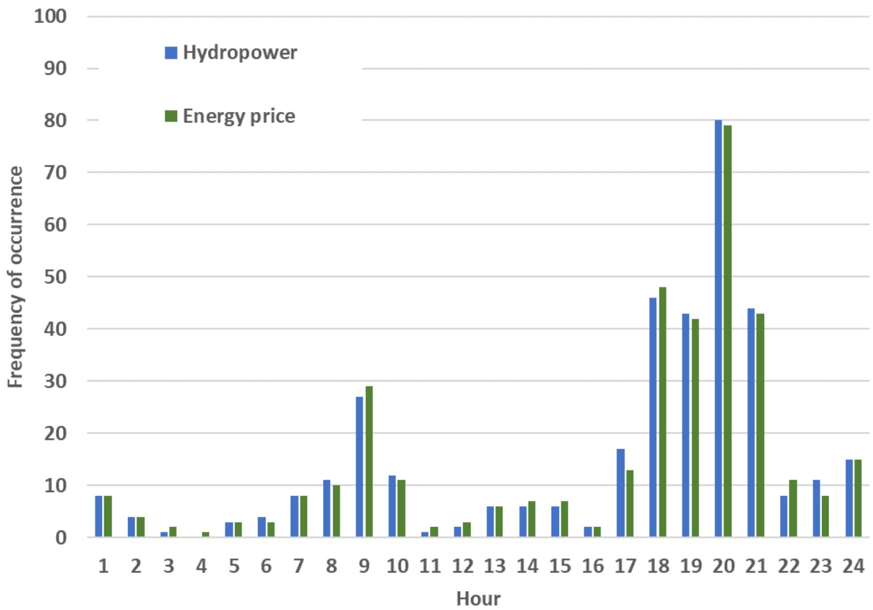


Figure 7.7: Frequency of occurrence of the maximum participation of hydropower in the mix and the energy price per hour, for year 2021.

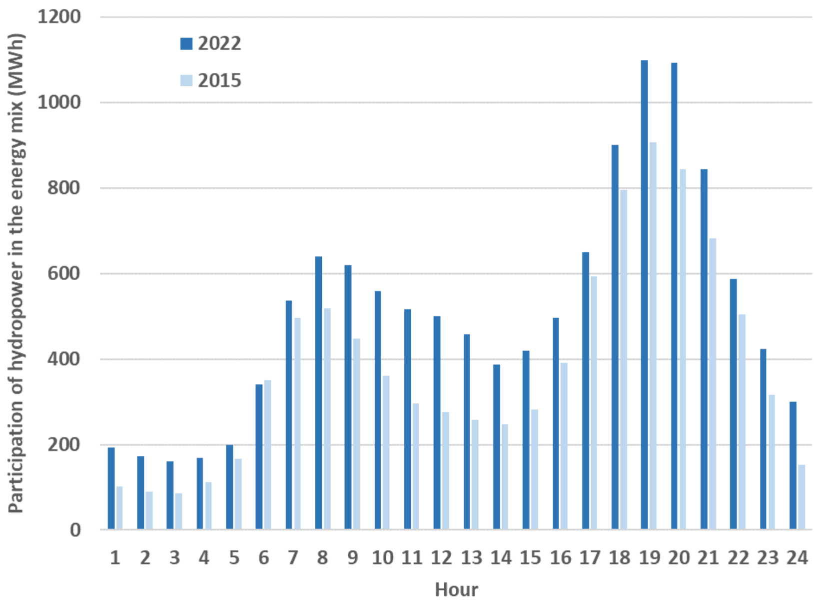


Figure 7.8: Mean values of hydropower sharing in the mix and energy prices per hour, for years 2015 and 2022.

To predict the daily participation of hydropower in the energy mix, a copula model is fitted with respect to day-ahead energy prices, as demonstrated in Figure 7.10. A Gaussian copula is constructed as the most suitable due to the small data sample and its structure. The modelling procedure of copulas is given in section 3.5. To account for the uncertainty in the operation of the hydropower plant induced by socioeconomic and other factors, three quantiles are selected, i.e., 95%, 50%, and 5%, that represent the operation policy of the stakeholder. Specifically, these refer to conservative, median, and energy-centric operation policies. This operation policy's discrimination will further allow us to build the assessment and optimization analysis and, eventually, the post-process to support decisions.

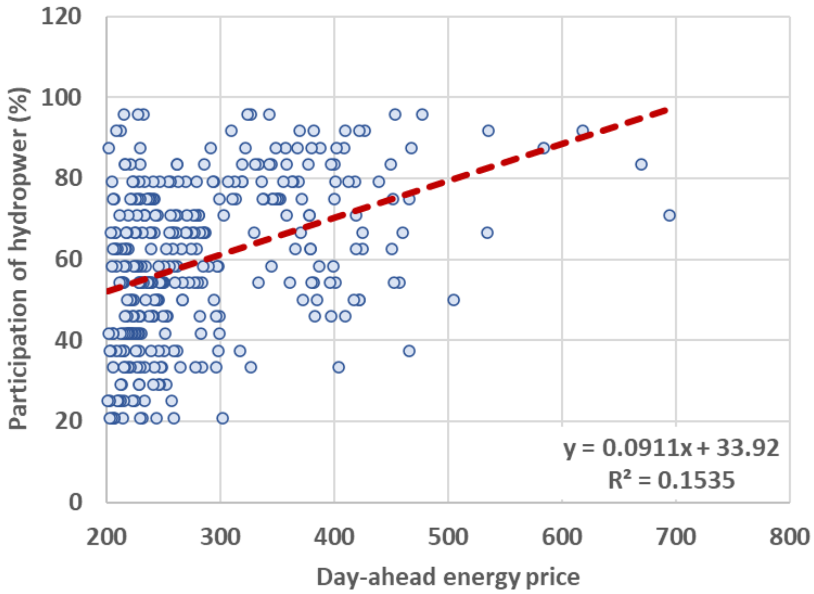


Figure 7.9: Scatter plot of day-ahead energy price and participation of hydropower plants.

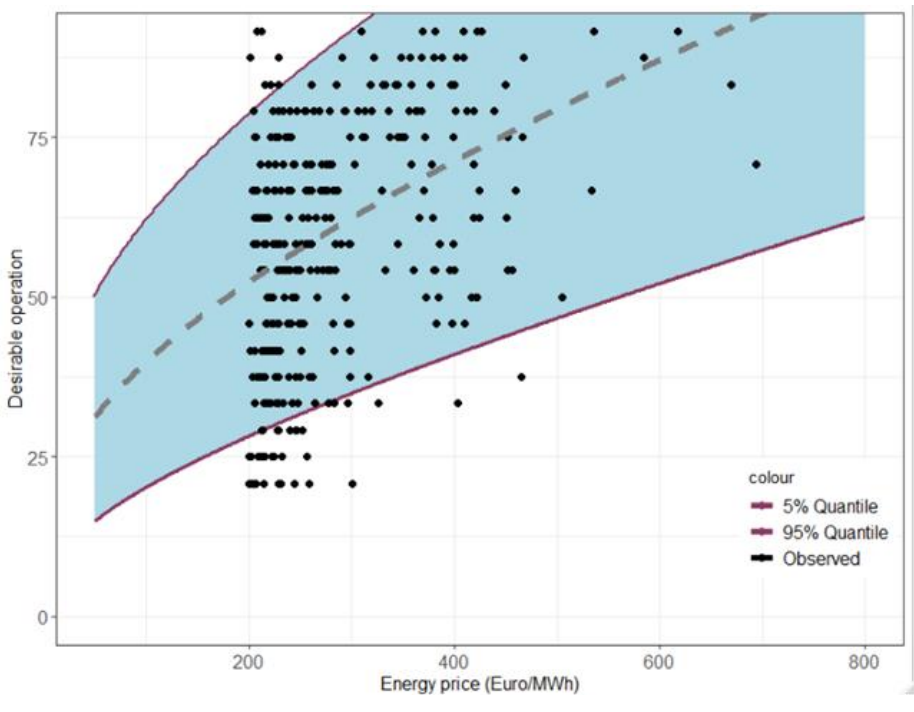


Figure 7.10: Fitting of Gaussian copula in the percentage of participation of hydropower plants in energy mix across Greece.

7.3.5 Estimation of water demands

Plastiras reservoir is a multipurpose system that fulfils water supply, irrigation, and hydroelectricity uses. As indicated by the analysis of historical data, the pivotal factor associated with water demands is irrigation. However, this amount is implemented in high priority and the desirable reliability should be around 97%. The available historical data for the water supply covers a period of 2003-2021 and it is in a monthly scale (Figure 7.11). The average monthly demand is 2.0 hm^3, while the minimum and the maximum observed values are 1.5 and 2.8 hm^3. On a mean annual basis, water supply uses are a small percentage of total releases, also exhibiting relatively small seasonal and overannual fluctuations, and thus, a constant monthly pattern is applied.

In contrast, the irrigation uses, taking place from April to September, are crucial for the operation of the reservoir. For the estimation of the associated demands, two approaches are followed, namely the rational one, which uses the monthly precipitation as an explanatory variable, and the irrational one, which also accounts for the available reservoir storage. The second approach describes the social uncertainty that usually forces the reservoir operator to violate the established management rules. In Figure 7.12, the rational practice is depicted, in which the monthly demand for irrigation is a function of the actual precipitation. It is worth mentioning that the water demands are not correlated with precipitation for the months of May and September. Thus, we apply the average observed values for the simulation, i.e., 9.9 and 2.1 hm^3, respectively.

The rational practice in this case study is rather than an ideal condition for the system. In this vein, we embed the uncertainty induced by the social factor within the assessment and optimization procedures, thus introducing the irrational practices. These consider the irrigation demand as a dependent variable of the reservoir storage, thus resulting in a dynamic modelling procedure. In this respect, a cross-correlation analysis is deployed for the irrigation season (May to August), revealing a satisfactory correlation between the reservoir level at the beginning of each month and the water released for irrigation (Figure 7.13). The functions of Figure 7.13 will be followed to re-estimate the irrigation demands in the modular analysis, i.e., in setting 5 and in the uncertainty-aware optimization of the reservoir's management.

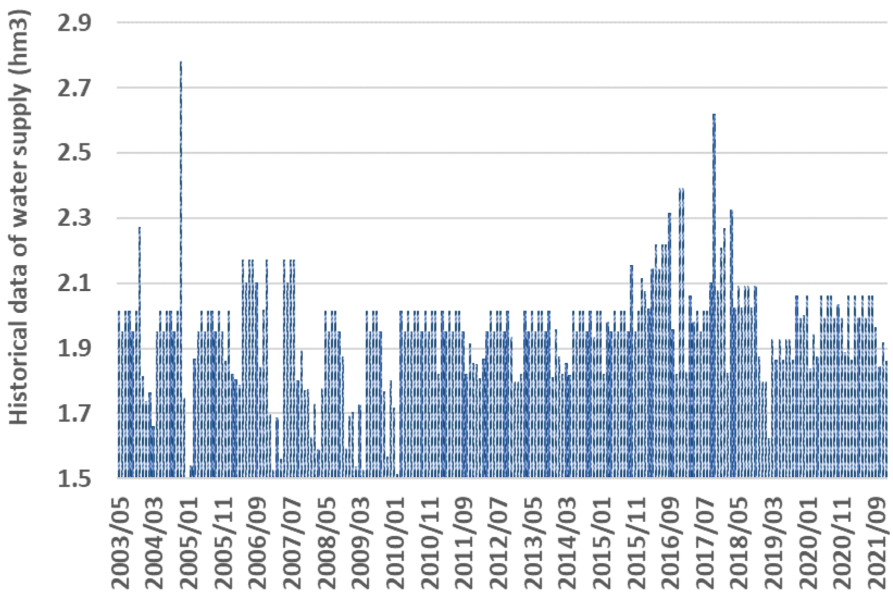


Figure 7.11: Historical data of water supply during 2003-2021.

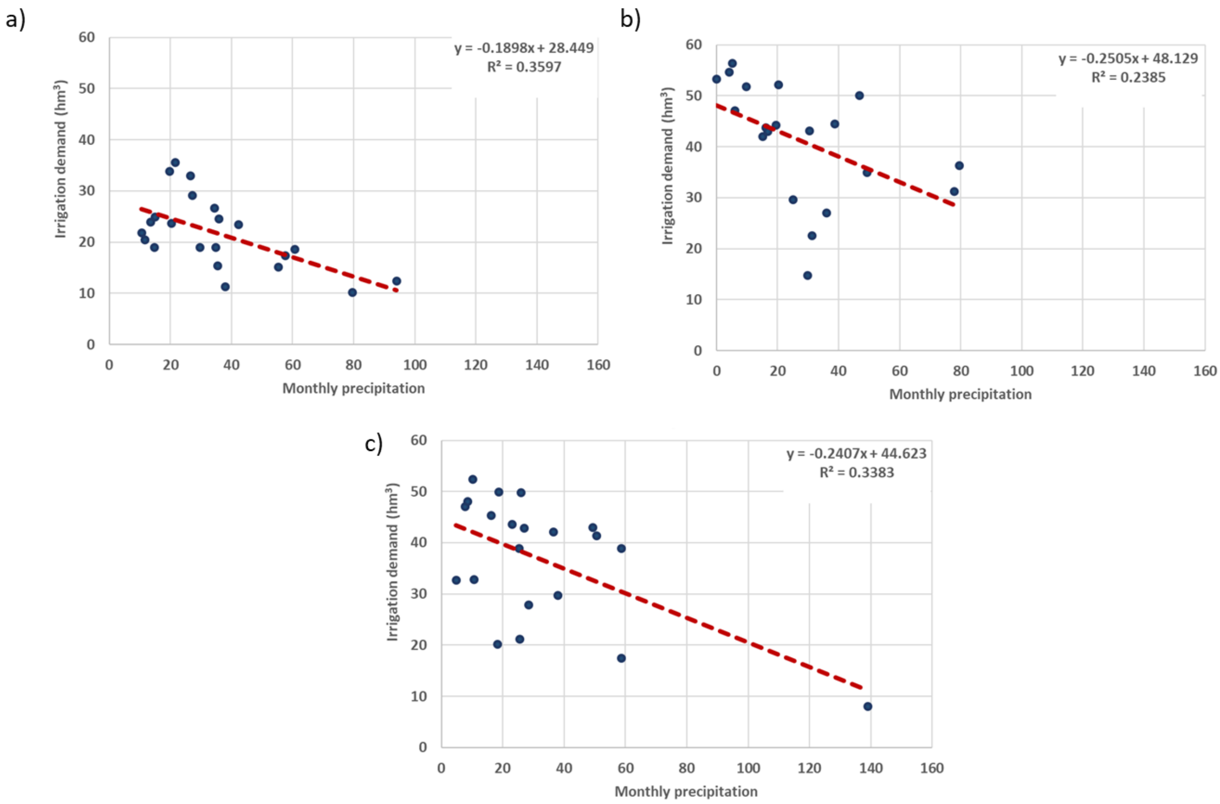


Figure 7.12: Estimation of irrigation demand as a function of monthly precipitation (rational practice) for a) June, b) July, and c) August.

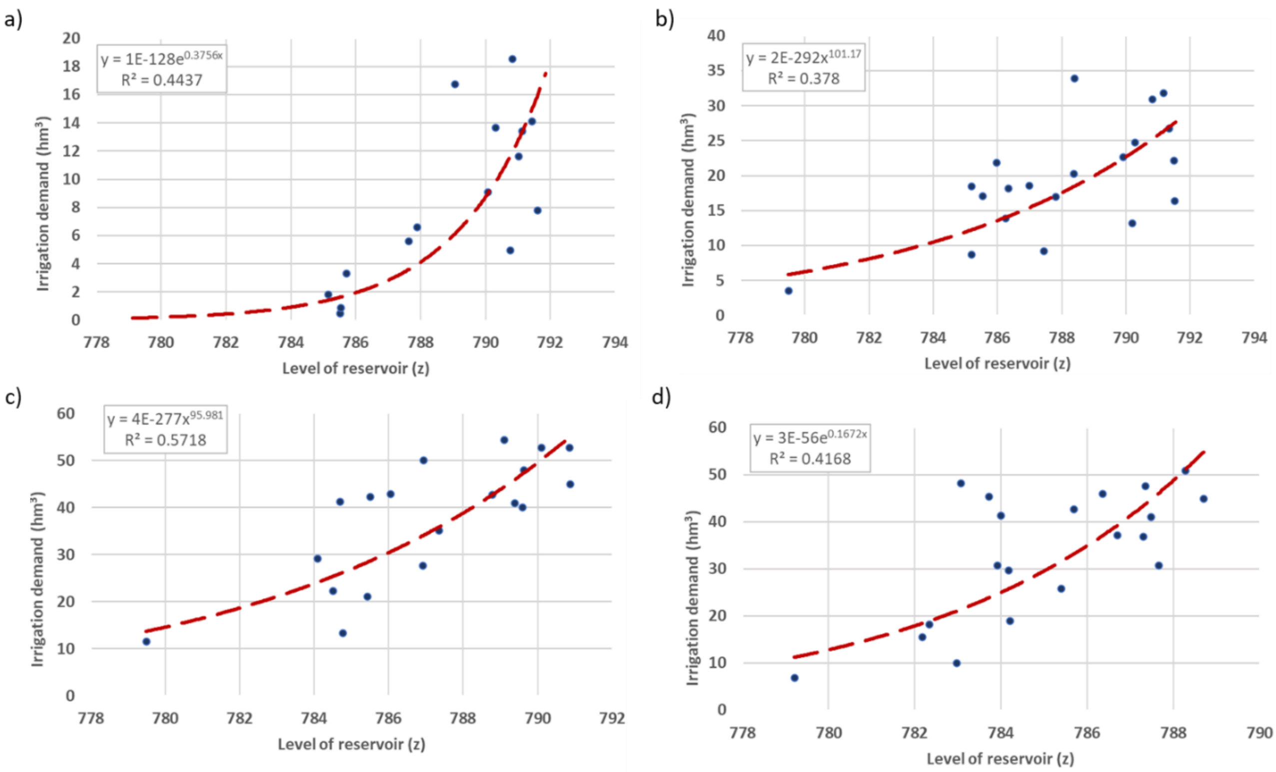


Figure 7.13: Estimation of irrigation demand as a function of reservoir level (irrational practice) for a) May, b) June, c) July, and d) August.

7.3.6 Uncertainty-aware assessment: inside the modular building process

As mentioned, the assessment of the current reservoir management under uncertainty is built in two steps. Initially, a conventional practice is followed, by optimizing the operational policy of the reservoir by means of the two levels of interest, z_{irrig} and z_{energy}, on the basis of the historical data for precipitation, runoff, water supply, and energy price. The energy target and the irrigation demand are estimated as dynamic variables. In particular, for the energy target, three policies are adopted, i.e., conservative, median, and energy-centric, that refer to 95%, 50%, and 5% quantiles of Figure 7.10. On the other hand, the irrigation demand is estimated as a function of precipitation (rational approach; Figure 7.12). The optimal parameters for the three operational policies and associated performance metrics (profits and reliability) are given in Table 16.

Next, the assessment framework is employed for each operational policy by following the modular procedure, in terms of settings 1 to 5, each one resulting in 1000 ensembles of output variables, namely profits, energy production, and reliability indices. The model results are grouped in this respect, as shown in Figure 7.14. Combining the three aforementioned graphs, a reasonable choice for the best-compromise operational policy will be the median one. Specifically, in terms of profits, the energy-centric and the median are similar, while from a reliability perspective, the uncertainty range of this policy is wider, thus making it unacceptable for some scenarios. In this respect, the uncertainty-aware optimization framework is next implemented for the median operational policy and the last setting (holistic approach, accounting for all investigated sources of uncertainty).

Table 16: Optimal reservoir levels and performance metrics for the three operational policies of the power plant, driven by historical data (conventional approach).

Level/metric	Conservative	Median	Energy-centric
z_{energy} (m)	776.7	778.2	778.2
z_{irrig} (m)	777.1	782.1	791.3
Profits (M€)	17.05	19.64	19.69
Water supply reliability	1.000	1.000	0.997
Irrigation reliability	1.000	0.856	0.783

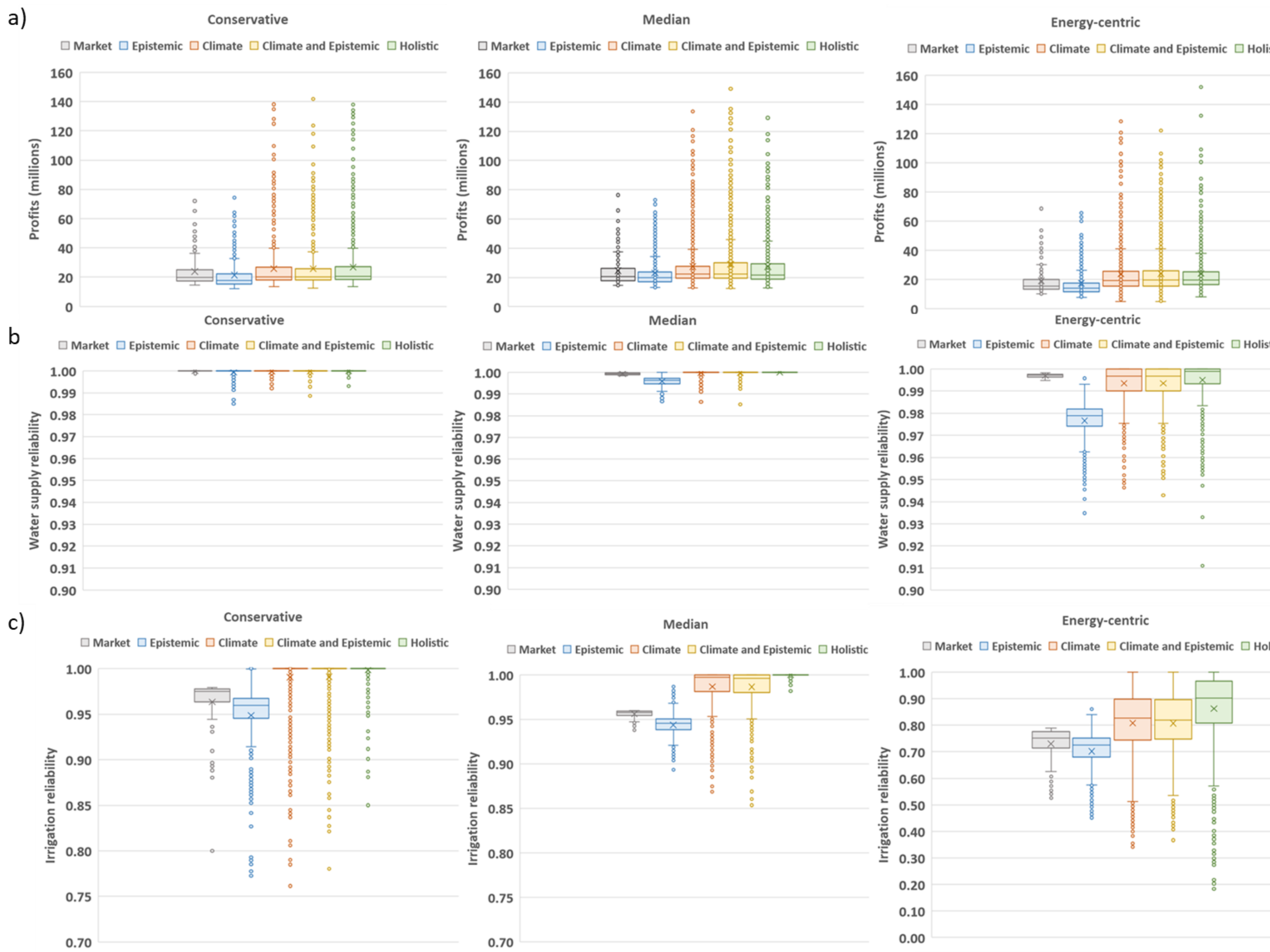


Figure 7.14: Box plots of (a) profits, (b) water supply reliability, and (c) irrigation reliability resulting from the uncertainty-aware assessment analysis.

7.3.7 Uncertainty-aware optimization

6.3.7.1 Rationale

The proper representation of uncertainty and its incorporation within a strategic management policy of water-energy systems has a significant operational interest. The assessment study so far revealed the necessity for more sophisticated approaches with respect to optimizing this policy by single-using historical data, thus ignoring aleatory and epistemic uncertainties.

In this respect, the uncertainty-aware optimization is developed in order to assist stakeholders via intuitive management tools. Specifically, taking advantage of the holistic approach (setting 5, embedding climatic, epistemic, energy market, and social uncertainty), we seek a globally optimized parameter set, z^*_{irrig} and z^*_{energy} by running each one of the 1000 ensembles and maximizing the average profit. The resulting optimized variables are $z^*_{irrig} = 776.7$ and $z^*_{energy} = 777.1$.

The advantages of optimizing the operational policy under uncertainty instead of employing conventional, i.e., deterministic, practices are highlighted by introducing, for each scenario, the so-called unit benefit of the system, e^*, expressed as the ratio of the mean annual profit to the mean annual energy production (€/MWh). This can be contrasted to the corresponding mean electricity price, while their difference denotes the additional unit benefit from the multipurpose character of the reservoir, i.e., passing water through the turbines to produce electricity and next fulfilling two other consumptive uses. This unit benefit e^* is increased under the uncertainty-aware optimization procedure, thus revealing the necessity of incorporating all facets of uncertainty within the real-world operation of the system (Figure 7.15).

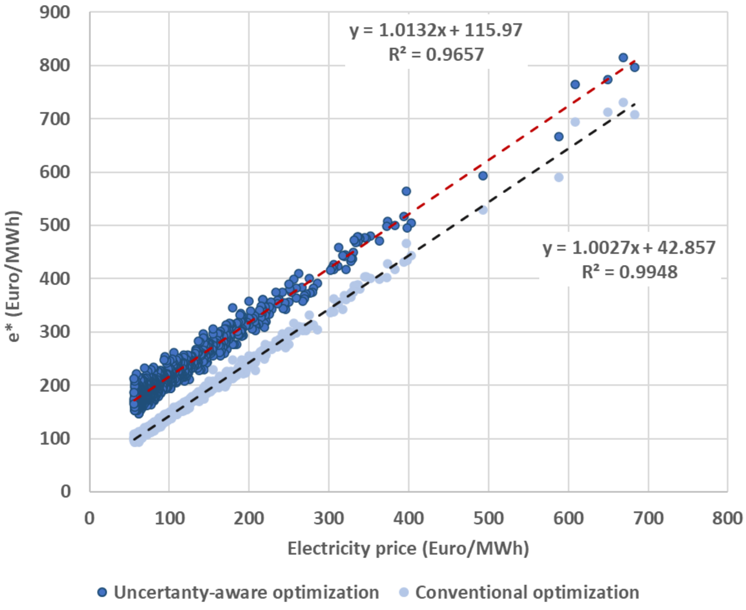


Figure 7.15: Comparison of the two optimization procedures regarding the additional benefit e^* gained with uncertainty-aware approach with respect to the conventional one.

7.4 Clarifying uncertainty for stakeholders

We argue that such sophisticated approaches are hardly to be employed by the stakeholders. In this respect, a challenge is hidden to "unwrap" the driver's uncertainty to provide simple decision-making and insights tools. Considering that the primary uncertain factors originate from the climate and the energy market, the focus is given to the correlation patterns of the expected profits with respect to the electricity price and precipitation, respectively (Figure 7.16). The first tool is a simple regression model for estimating the expected annual profits, as functions of annual precipitation, p, and mean daily electricity price, e. By analysing the optimized outcomes of the 1000 stochastic scenarios, two areas of interest are distinguished according to an electricity price threshold, $e_0 = 80$ €/MWh, as follows:

$$Profit = \begin{cases} 129.2\, p^{0.57}\ e^{0.55}, e \leq 80 \text{ €/MWh} \\ 3.41\, p^{0.87}\ e^{0.66}, e > 80 \text{ €/MWh} \end{cases} \quad (1)$$

By using this empirical formula, the operator of the system can predict with good accuracy the expected annual profits (M€) for different conditions of its external environment by means of climate and energy market, i.e., under combinations of wet/dry years with high/low electricity prices.

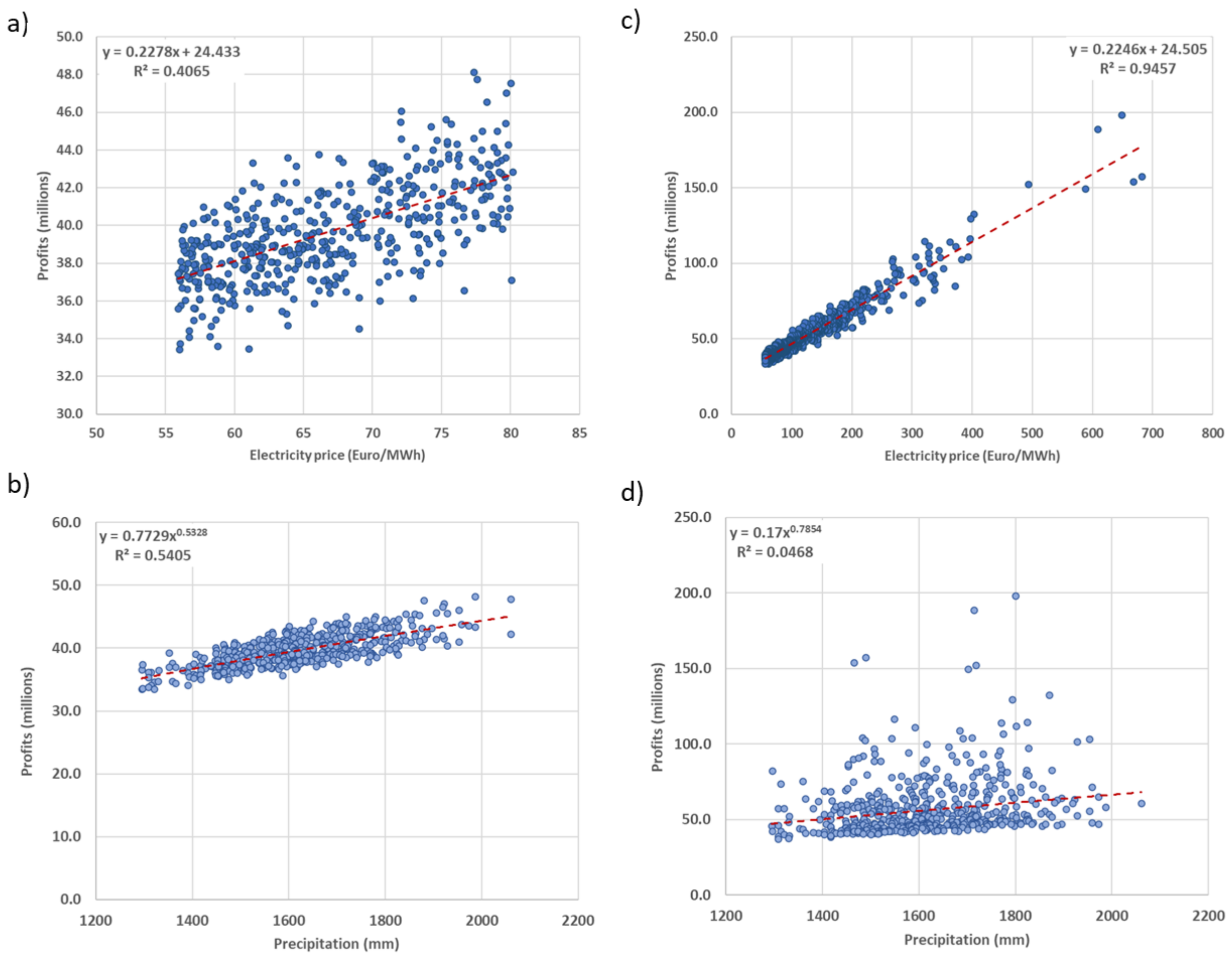


Figure 7.16: Estimation of profits correlated with electricity price and precipitation for the two areas of electricity price. a) and b) refer to the area below threshold e_0 , while c) and d) to the area above e_0.

Under changing conditions, this feature can be further improved by accounting for elasticity metrics. The concept of elasticity is widely explored in finance (Loderer et al., 1991), engineering (Westergaard, 1952), and hydrology (Andréassian et al., 2016), as well. To all these applications, this metric describes the sensitivity of the changes in a variable related to changes in its driver. In this respect, the system is studied under the elasticity metric of profits, i.e., the rate of change of profits through the partial derivatives of precipitation and electricity price. Thus, a second decision support tool is introduced. Specifically, for the two areas of electricity prices, i.e., below and above e_0, the rate of change of profits due to the uncertain precipitation and electricity price is calculated. Thus, a manager can estimate the expected change in profits and the associated risk due to climate or market-oriented shifts using the copula-based tools in Figure 7.17. Specifically, copulas (a) and (c) depict the partial derivatives of precipitation, while (b) and (d) are the partial derivatives of electricity prices for the two areas of interest. An interesting outcome of this stochastic analysis is that under high electricity prices, a change in the average precipitation is not crucial for the associated profits, while small changes in the electricity price dramatically affect the expected outcomes. This denotes that the expected profits are highly uncertain and unstable in the high electricity price era. In contrast, as shown in Figures a) and c), under relatively low electricity prices, the joint distribution of the two variables follows Gaussian copulas, thus underlying a "normal" response of the system with respect to changes in its external drivers.

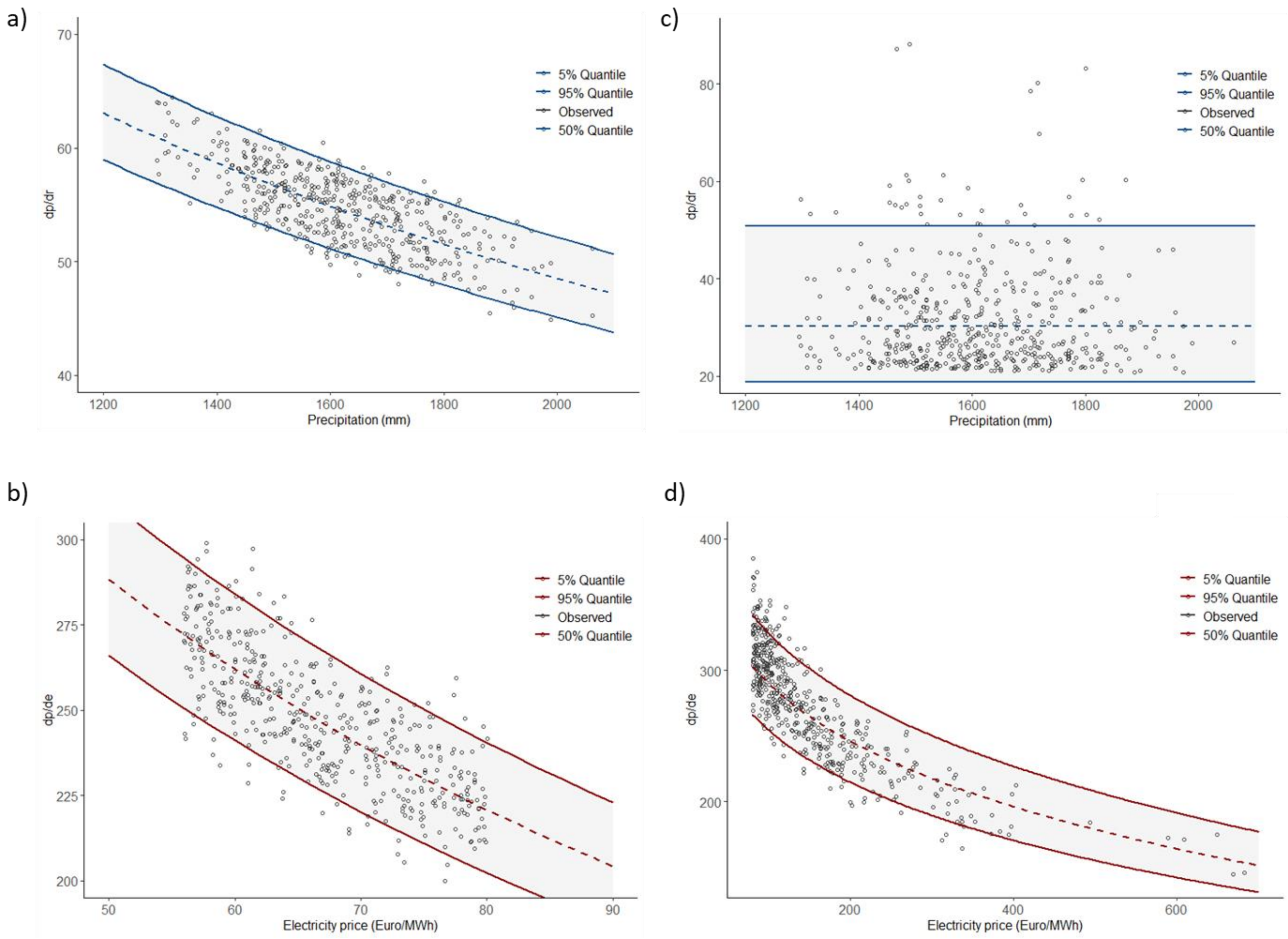


Figure 7.17: Copula-based tools for the estimation of the rate of change of profits by changing the precipitation and the electricity price for the two areas of electricity price. a) and b) refer to the area below threshold e_0 , while c) and d) to the area above e_0.

7.5 Conclusions

The objective of this chapter is the assessment and optimization of the operation policy of hydropower plants under multiple facets of uncertainty. In this respect, the proposed framework has been adapted for supporting stakeholders and operators in managing multipurpose hydropower reservoirs in a changing world. Its aim is to represent and incorporate both aleatory and epistemic uncertainty into a robust and generic modelling framework, which comprises six highly interconnected models. These are rainfall and electricity price generators, rainfall-runoff model, irrigation demand generator, hydropower policy and water-energy system operation model. All aforementioned models are flexible to account for all uncertain factors. In the context of the case study, the aleatory uncertainty refers to climatic, social and energy-market processes, while the epistemic uncertainty to the calibration parameters of the rainfall-runoff model.

First, the principles and modelling specifications are set of handling the uncertainty across multipurpose reservoirs. Regarding the representation of climatic and energy-market uncertainty, we consider their underlying processes as random variables, and use stochastic models for the generation of synthetic rainfall and electricity price data. Next, for the description of the human-induced procedures, these are discriminated into direct and indirect, corresponding to the water demands and the operation policy, respectively. For the direct component, i.e., the social response, a statistical analysis is employed to express the water demands as dependent random variables against rainfall and the reservoir state. For the indirect one, involving the operation policy of the hydropower plant, a copula-based tool is developed that estimates the desirable energy target according to day-ahead electricity prices and the operator's willingness. At the end, three quantiles of interest are denoted that correspond to conservative, median, and energy-centric management policies of the system.

The proposed framework is applied to Plastiras reservoir in Central Greece, which represents 5% of hydropower production of the country and is subject to multiple and increasing conflicts and trade-offs between stakeholders and the operator, as well. To reveal the benefits of the proposed methodology over more conventional, deterministic approaches, a modular scheme is demonstrated to disentangle the key sources of uncertainty, aleatory and epistemic. Our results indicate that a better understanding of uncertainty can lead to more efficient operation policies (as shown in the optimization problem). For instance, in terms of profits, the energy-centric and median scenarios may be similar, while from a reliability perspective, their uncertainty range is quite different and for some scenarios unacceptable.

Supporting real-world applications of the proposed methodology is a key aim of the overall research. To this effect, we offer a toolbox that unwraps the driver's uncertainty, facilitating decision-making and providing valuable insights, including the estimation of expected profits and their elasticity. Using the toolbox, an operator can predict with good accuracy the expected annual profits for a wide ensemble of future conditions, considering both climatic and energy market changes. They can also estimate the expected change in the overall system performance and the associated level of risk.

In conclusion, this case study not only demonstrates a novel, integrated approach to hydropower reservoir management under uncertainty but also provides a practical, adaptable toolbox, paving the way for more resilient and efficient hydropower systems in an era of significant environmental and market variability.

8 Conclusions and Discussion

8.1 Summary of thesis key research novelties

This thesis, entitled 'Uncertainty-aware simulation-optimization framework for water-energy systems", addresses key facets of uncertainty within the water-energy nexus across different scales of interest. These spans from the design and the operation of standalone works to the long-term management and operation of complex water-energy systems, offering a wide range of valuable tools for policy-making.

In particular, the general key novelties are:

- We combined three probabilistic theories, by introducing the so-called triptych of: (a) statistics, (b) stochastics and (c) copulas. Each theory is formalized to serve several modelling approaches, i.e., statistics for accounting for the marginal properties of independent variables, stochastics also for accounting for dependencies across scales, and copulas for describing correlations among variables and also quantifying the joint uncertainty of simulated outcomes.
- We explored and described all key drivers, internal processes and their feedbacks across the water-energy nexus, originated from the climate, the technical system, the society and the energy market, in an uncertainty-wise way. This contributes towards the necessitated paradigm shift in the design, long-term management and assessment of water-energy systems, since our research provides the methodological architecture of handling hydroclimatic, social, technical and energy market components under an uncertainty context.
- By integrating these multidimensional factors, varying from climate to the socioeconomic environment, our research sets the specifications and provides a robust modelling framework capable of accounting for the multifaceted uncertainties within the water-energy nexus. Thus, we introduce a generic uncertainty-aware simulation-optimization framework for the water-energy nexus that, eventually, offers valuable tools for policymakers, planners, and stakeholders to make informed decisions and formulate robust strategies for managing water and energy resources in an uncertain future.
- Taking advantage of real-world case studies, our framework is tailored for stakeholders to unwrap the driver's uncertainty, providing valuable insights, including the estimation of expected profits and their elasticity. Specifically, by using all proposed decision-support tools the system's operator is well-informed to predict with good accuracy the expected annual profits and the level of risk for a wide ensemble of future conditions, considering climatic, social and energy market changes.

In addition, the specific key innovations are:

- We introduced a generic formula to describe the fuel-energy conversions under uncertainty. This comprises six parameters, the first four refers to the technical characteristics of the power plant, while the last two denote as random variables and define the shape of the efficiency curve.
- We formulated a generic procedure for simulating the renewable energy sources, expressing its key components as random variables. In this respect, all related engineering problems, i.e., design, long-term performance assessment, scheduling are effortlessly expressed in probabilistic terms.

- Focusing on the social uncertainty, we substitute the oversimplified and static concept of the entire urban area as a “node” by a dynamic social sub-system, which interacts with the technical one, and reflects the behavioral rules of society. On top of that, we embedded the indirect incorporation of the energy market (and its uncertainty, within a water supply system, by considering the energy price as a stochastic component, thus leading to a stochastic water price.
- Focusing on the energy market uncertainty, we provided a stochastic modelling framework for reproducing the electricity price in stochastic terms and offered a copula-based tool for predicting the electricity price across different temporal scales of interest.

In Table 17, we provide a “checkbox” that includes the water-energy case studies, starting from a standalone case (i.e., energy market, renewable project) ending with a water-energy-society nexus (i.e., hydropower reservoir), as explored in this research, with the associated uncertainties.

Table 17: Overview of water-energy cases (chapter titles) and investigated uncertainties.

Case	Climatic	Social	Energy market	Epistemic
From long-run simulation to forecasting of EU electricity market			X	
Uncertainty-wise design and assessment of renewable projects	X		X	X
Water supply systems under the concept of water-energy society-nexus	X	X	X	
Dealing with the conflicts of the water-energy nexus: the case of multipurpose reservoirs	X	X	X	X

8.2 Future research questions

The future research paths follow a question-based pyramid. In particular, these are:

What if we expand this framework to incorporate additional facets of uncertainty?

The proposed framework is easily adjustable to incorporate more facets of uncertainty, since its architecture follows a “lego” technic, by building each source of uncertainty block by block within the simulation-optimization. By considering an even wider range of uncertainties, we can create a more robust and adaptable system that reflects the complexities of real-world scenarios. This could involve accounting for facets of uncertainty derived by technological progress, operational disruptions, geopolitical risks, and more socio-economic factors (i.e., operator’s decisions etc.). In particular, this framework can be easily adjusted in order to consider technological improvement of the equipment, and/or disruption due to maintenance within the lifecycle of the project. In addition, we can incorporate harmful events for the project under study, e.g., cyber-physical attacks. Overall, the expansion of this framework to incorporate more facets of uncertainty could enhance its effectiveness and applicability.

How can we couple large-scale water-energy systems, such as those at the country level, and describe them in terms of the proposed framework?

The embedding of large-scale systems within the proposed framework requires to consider several key aspects. Firstly, we must account for the interconnectedness and conflicts between water and energy systems, recognizing that changes in one can significantly impact the other at the large-scale. This involves understanding the complex dynamics of water availability, energy production, and consumption patterns within the context of broader environmental and socioeconomic factors. In this respect, the framework should be expand to allow for the modeling of large-scale feedback loops and dependencies across the water-energy nexus. For instance, at the basin scale the hydropower reservoirs serve as water sources and flood regulators, while at the national grid scale these are the major power sources to offer the desirable stability. However, extreme events, i.e., an extended drought, affects both the country's hydropower generation (national scale) and the water supply (basin scale). In addition, we remark the need of the integration of various sources of uncertainty that affect both water and energy systems. This could include factors such as large-scale hydroclimatic variability, under a multivariate stochastic context, anthropogeography estimations, technological advancements, policy changes, and geopolitical tensions. Overall, integrating large-scale water-energy systems into the proposed framework requires a comprehensive understanding of their complexities and uncertainties. By capturing them, we can better understand the potential cascading effects of disruptions within the system and identify strategies to enhance resilience.

What if we develop a decision-support system that incorporates the proposed framework?

Building on the suggested architecture, a decision-support system (DSS) could greatly improve our capacity to make well-informed choices for large-scale water-energy systems. In particular, by leveraging data analytics, modeling techniques, and scenario analyses within the framework, the decision-support system may offer valuable perspectives on the possible effects of various approaches and interventions on the water-energy nexus being examined. Moreover, a decision-support system could facilitate stakeholder engagement and collaboration by providing a platform for sharing information, conducting simulations, and exploring alternative scenarios. This cooperative strategy can strengthen agreement, improve decision-making processes, and enhance the resilience of water-energy systems to future uncertainties and shocks. In addition, this would enable involved parties to evaluate trade-offs, prioritize actions, and develop robust plans that account for uncertainties and complexities inherent in these systems.

How can we provide more tools to policy makers, that incorporate simultaneously long-term and operational information?

Policy-makers need to be ensured against long-term objectives and immediate operational strategies. In this respect, an enhancement of the proposed framework that dynamically evaluate policies and interventions over time within two horizons, short and long-term is needed. Specifically, this should involve monitoring the effectiveness of policies, adjusting strategies as needed, and incorporating new information to ensure alignment with long-term goals while addressing short-term challenges. Undoubtedly, this is in line with the decision support system, that incorporates all uncertainty-aware scenarios and interventions.

9 References

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10 Appendix

10.1 Supplementary material for chapter 4

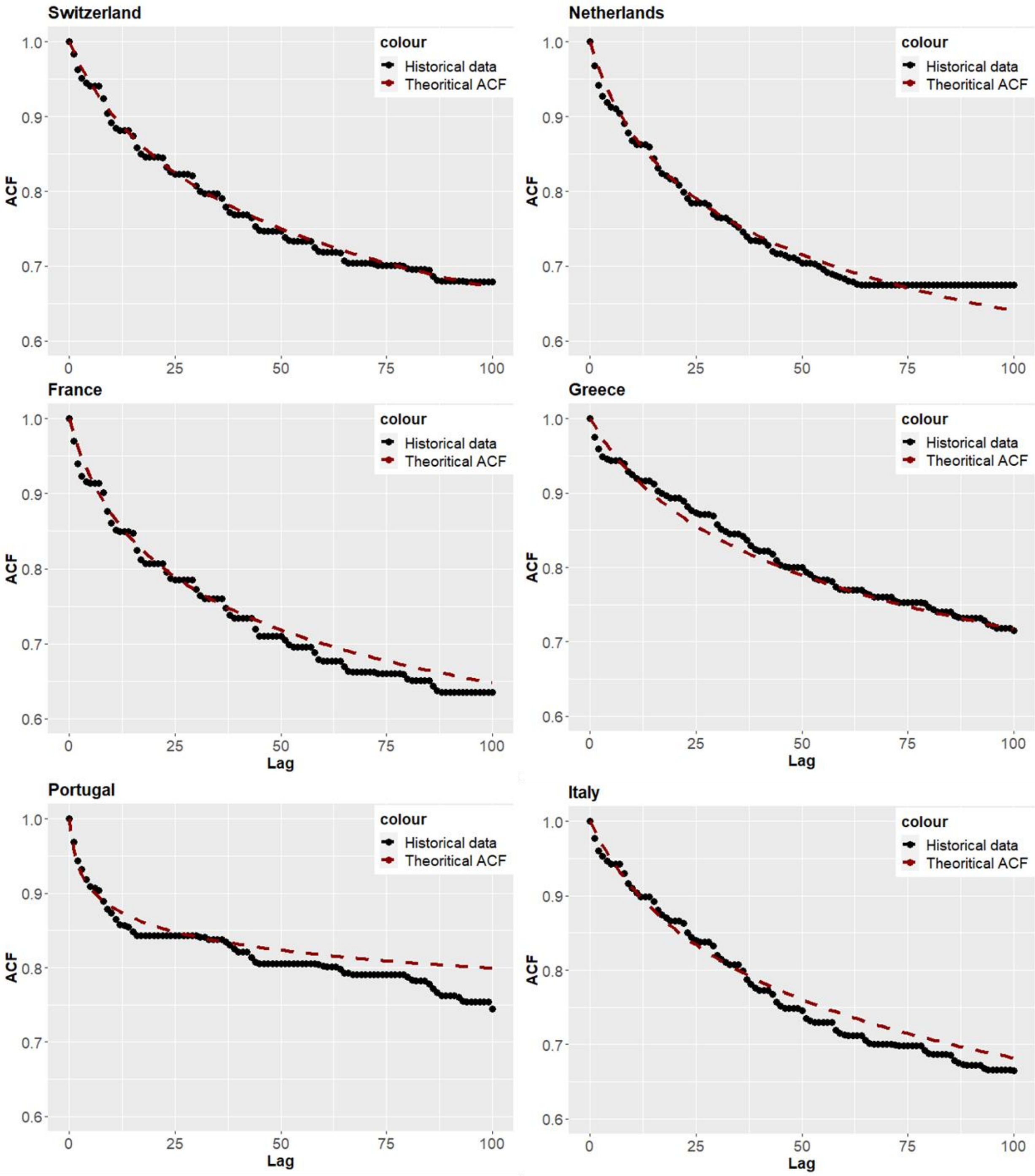

Figure 10.1: Fitting of the theoretical autocorrelation function to the historical electricity prices for Switzerland, Netherlands, France, Greece, Portugal, Italy.

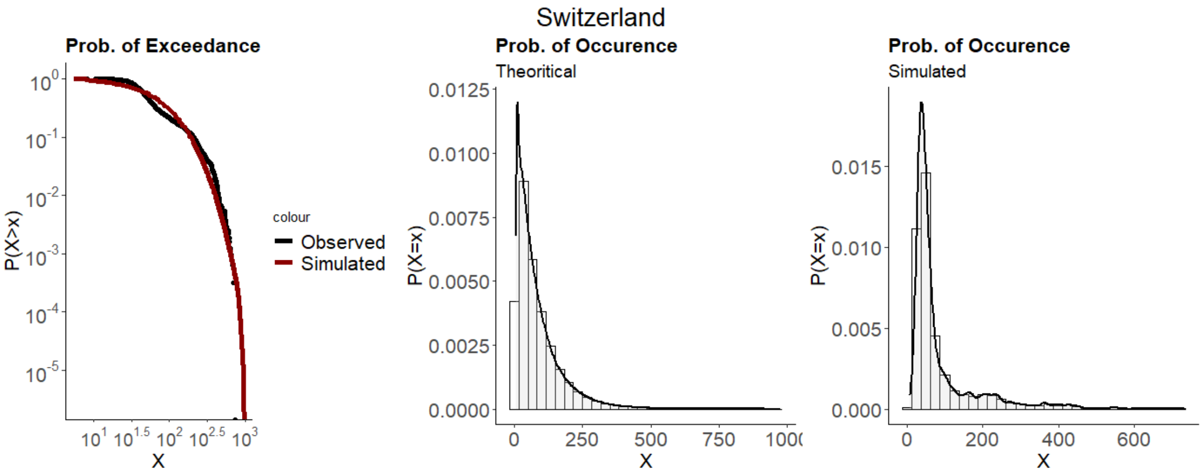

Figure 10.2: Fitting of three-parameter Gamma distribution function to the historical and simulated electricity price data of Switzerland.

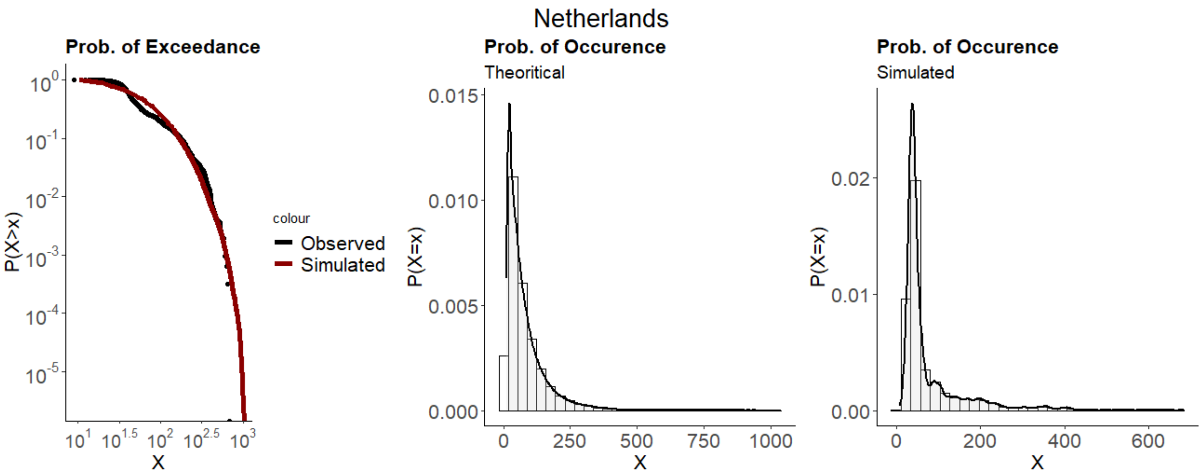

Figure 10.3: Fitting of three-parameter Gamma distribution function to the historical and simulated electricity price data of Netherlands.

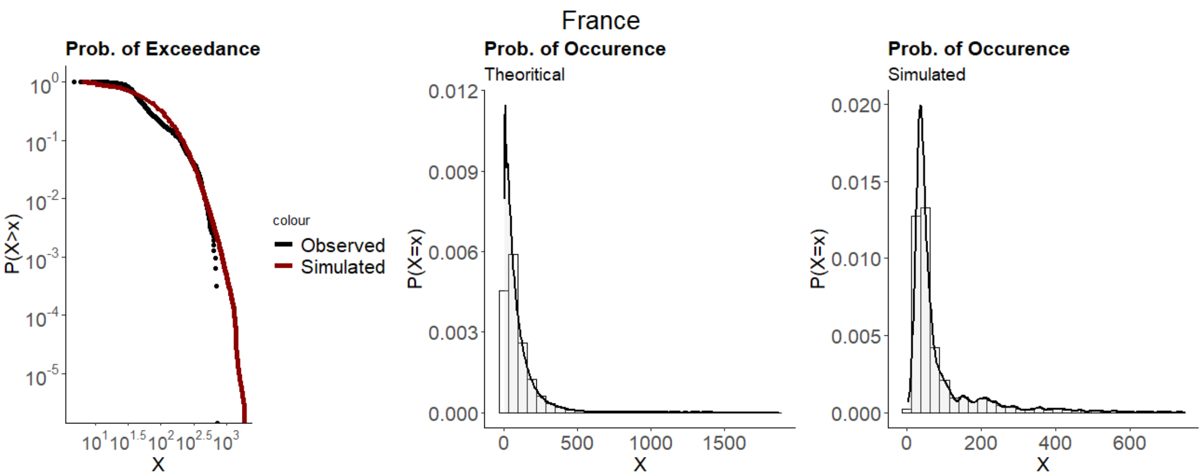

Figure 10.4: Fitting of three-parameter Gamma distribution function to the historical and simulated electricity price data of France.

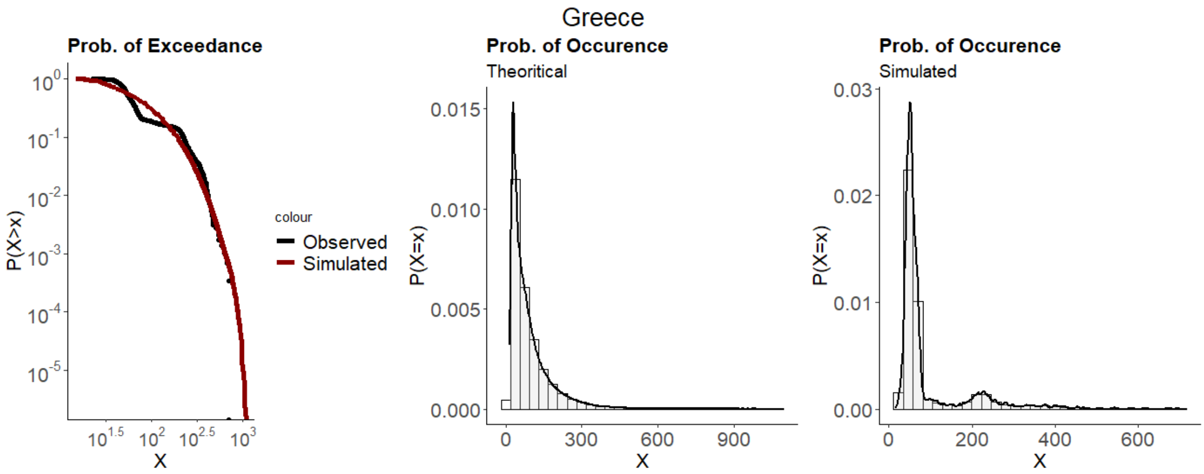

Figure 10.5: Fitting of three-parameter Gamma distribution function to the historical and simulated electricity price data of Greece.

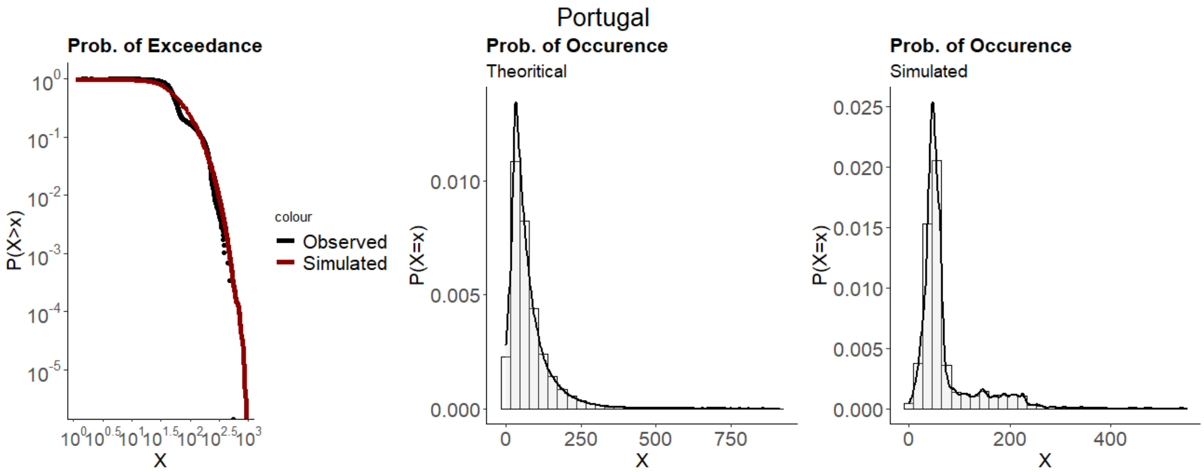

Figure 10.6: Fitting of three-parameter Gamma distribution function to the historical and simulated electricity price data of Portugal.

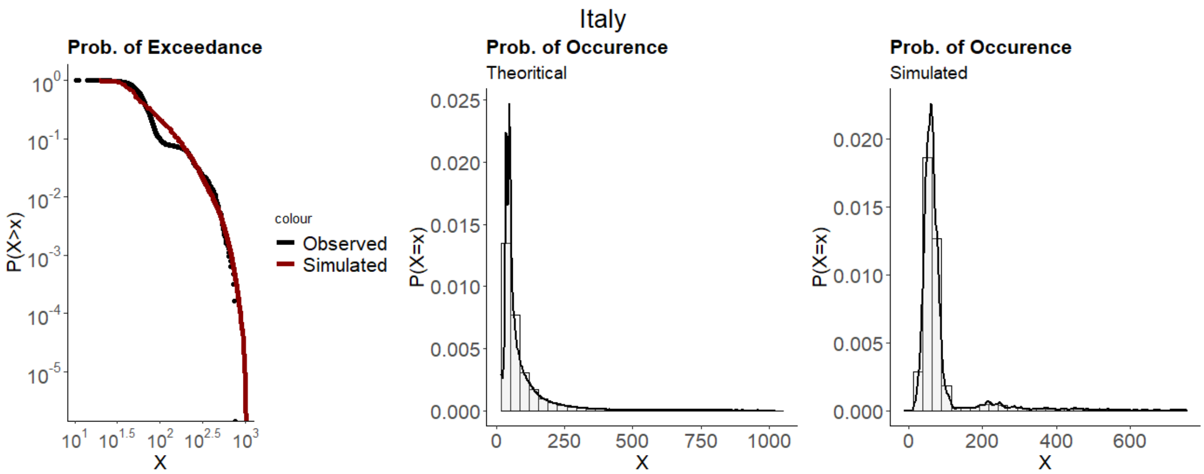

Figure 10.7: Fitting of three-parameter Gamma distribution function to the historical and simulated electricity price data of Italy.

Table 18: Monthly-based comparison of historical and synthetic mean values for the daily electricity price (Switzerland, France, Greece, Netherlands, Portugal, Italy).

		Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sept	Oct	Nov	Dec
Switz.	**Hist**	82.9	74.3	81.3	67.3	59.6	66.7	87.1	97.0	98.5	89.1	90.5	106.9
	Sim	82.1	76.1	86.2	68.5	60.6	67.0	90.3	99.5	100.5	87.6	89.2	108.2
France	**Hist**	76.2	68.4	76.6	66.8	58.0	66.4	89.6	97.3	97.0	82.5	85.0	100.9
	Sim	83.9	76.8	91.5	77.6	65.9	77.0	108.5	120.8	114.1	88.9	92.1	116.4
Greece	**Hist**	81.9	72.3	77.9	72.1	72.4	76.8	94.5	107.4	108.3	95.5	96.9	108.5
	Sim	81.4	72.5	77.4	71.8	72.5	76.5	93.4	107.4	108.7	95.6	96.1	107.9
Neth.	**Hist**	68.8	63.6	71.2	61.4	58.1	65.2	78.1	92.7	92.3	75.2	76.0	91.6
	Sim	71.4	66.0	75.6	63.1	60.6	66.5	83.1	105.8	99.4	77.7	78.4	100.9
Port.	**Hist**	72.0	60.2	70.3	59.4	61.7	66.4	66.8	68.5	74.3	79.8	75.9	82.2
	Sim	75.9	62.5	79.8	63.2	65.3	69.0	68.9	71.3	77.2	83.5	78.7	86.9
Italy	**Hist**	77.0	70.4	78.6	69.2	62.7	71.2	98.2	106.7	106.1	88.9	84.1	96.3
	Sim	77.5	73.2	77.5	70.0	65.7	70.9	89.6	93.6	95.8	84.8	88.1	99.8

Table 19: Monthly-based comparison of historical and synthetic standard deviation values for the daily electricity price (Switzerland, France, Greece, Netherlands, Portugal, Italy).

		Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sept	Oct	Nov	Dec
Switz.	**Hist**	61.5	56.2	90.3	67.7	55.5	72.1	111.0	142.1	120.0	67.4	71.1	111.2
	Sim	57.8	55.6	86.9	64.8	53.7	68.9	102.6	121.6	106.0	62.4	66.4	104.4
France	**Hist**	60.9	52.7	87.3	70.9	55.7	70.9	119.7	145.1	118.4	63.7	66.1	113.8
	Sim	68.3	58.9	98.9	81.1	64.5	79.9	134.3	154.7	128.0	68.2	70.2	124.5
Greece	**Hist**	58.8	51.4	76.5	67.2	58.8	63.8	97.1	126.9	124.8	77.4	75.2	93.4
	Sim	56.2	50.3	74.8	65.8	56.4	60.5	92.2	119.0	119.5	77.5	72.0	89.3
Neth.	**Hist**	53.9	47.1	76.7	55.7	50.6	58.1	87.3	131.1	102.6	58.5	60.0	102.6
	Sim	52.8	47.3	74.5	53.3	50.1	56.2	83.1	123.0	97.1	55.3	58.2	98.2
Port.	**Hist**	52.1	52.2	87.1	55.3	50.3	43.5	34.3	39.4	45.6	55.8	49.5	71.9
	Sim	58.2	57.6	97.5	61.2	58.0	49.9	38.7	44.0	51.8	62.6	54.8	80.2
Italy	**Hist**	59.7	54.9	89.8	71.7	59.5	75.2	127.3	155.2	126.5	71.2	64.3	102.6
	Sim	46.9	39.2	69.4	52.8	46.1	57.1	96.8	118.4	97.3	64.0	65.2	93.9

Table 20: Monthly-based comparison of historical and synthetic skewness values for the daily electricity price (Switzerland, France, Greece, Netherlands, Portugal, Italy).

		Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sept	Oct	Nov	Dec
Switz.	**Hist**	1.620	1.638	2.560	2.139	1.856	2.483	2.399	2.717	2.572	1.621	1.593	1.820
	Sim	1.640	1.831	1.917	1.891	1.772	2.162	2.198	2.040	2.083	1.932	1.841	1.769
France	**Hist**	1.779	1.578	2.461	2.803	1.919	2.521	2.585	2.736	2.599	1.866	1.700	1.869
	Sim	2.098	1.845	2.207	2.741	2.458	2.342	2.879	2.519	2.225	2.054	2.019	2.275
Greece	**Hist**	2.290	2.364	2.515	2.321	2.152	2.436	2.332	2.490	2.371	1.651	1.391	1.558
	Sim	2.066	2.142	2.305	2.054	1.768	1.799	1.945	2.091	2.034	2.211	2.040	2.074
Neth.	**Hist**	1.901	1.697	2.567	2.112	2.139	2.330	2.499	2.841	2.437	1.866	1.802	1.964
	Sim	1.966	2.162	2.044	1.906	2.102	2.304	2.189	2.195	2.223	1.841	2.024	2.107
Port.	**Hist**	2.085	2.254	2.835	2.351	1.865	2.069	1.453	1.482	1.307	1.669	1.806	2.246
	Sim	1.912	2.187	2.101	2.021	2.298	2.209	2.039	2.082	2.349	2.024	1.900	1.848
Italy	**Hist**	1.970	1.814	2.633	2.510	2.044	2.454	2.471	2.572	2.364	1.732	1.834	2.070
	Sim	2.880	2.708	2.837	2.962	3.079	3.036	3.108	2.873	2.906	3.125	2.863	2.865

10.2 Supplementary material for section 5.3.4

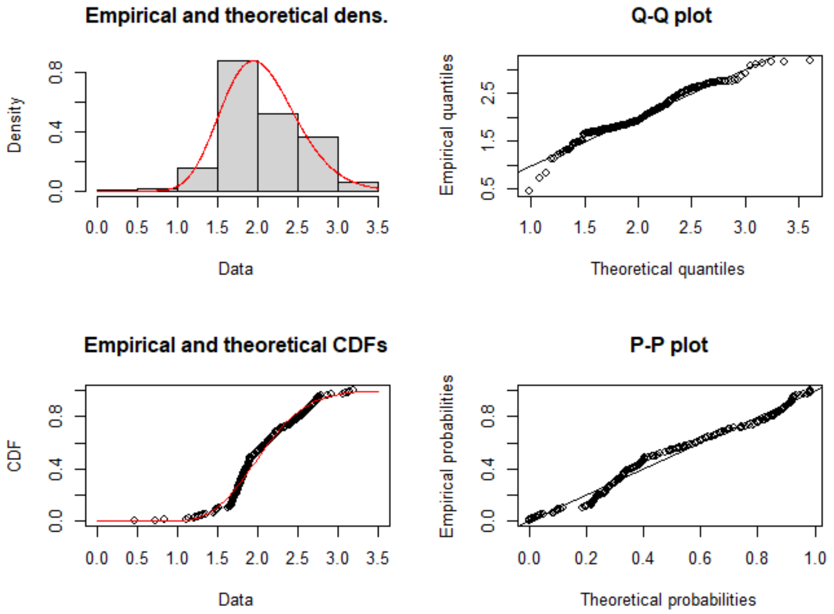

Figure 10.8: Fitting of marginal distribution of the monthly-based error processes, w'_s, regarding the January's data.

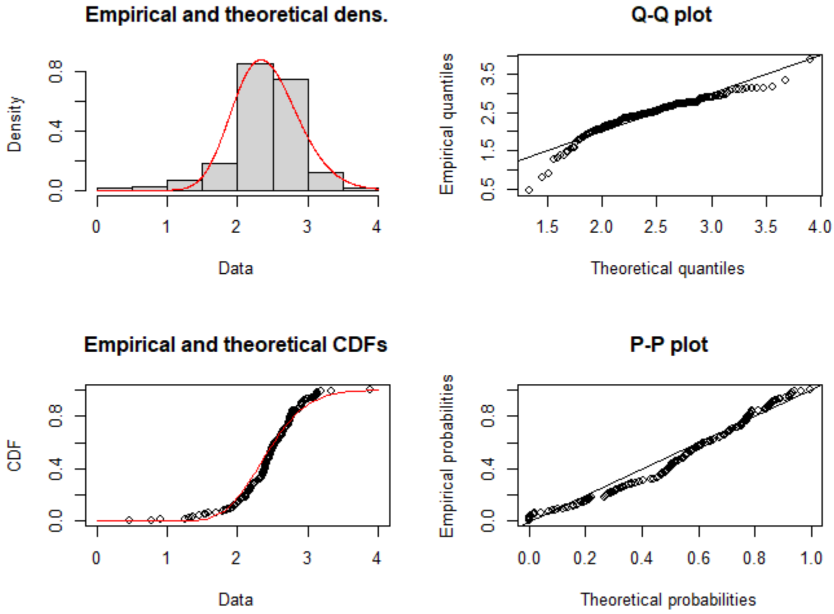

Figure 10.9: Fitting of marginal distribution of the monthly-based error processes, w'_s, regarding the February's data.

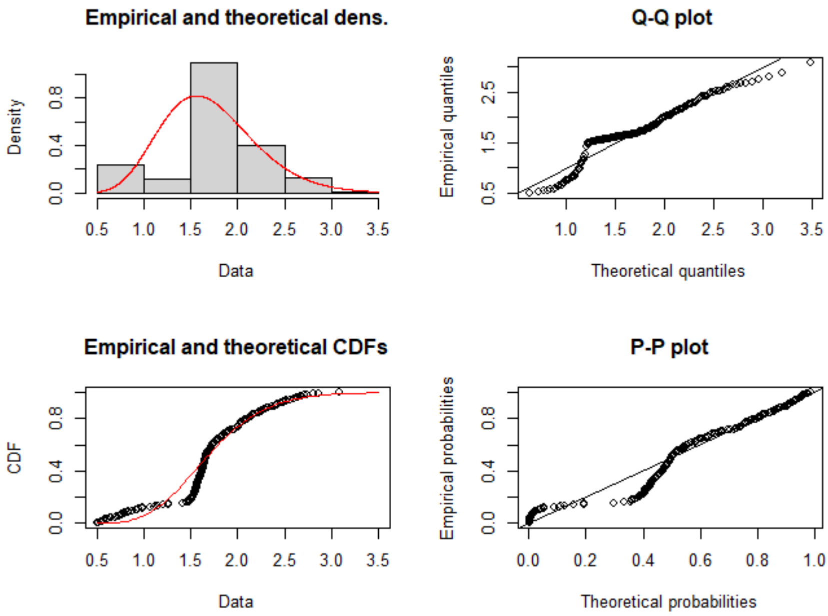

Figure 10.10: Fitting of marginal distribution of the monthly-based error processes, w'_s, regarding the March data.

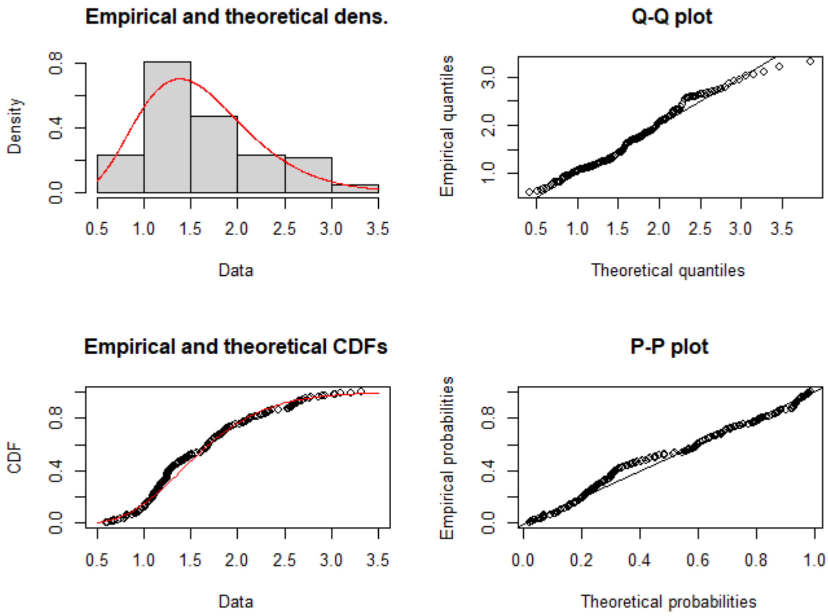

Figure 10.11: Fitting of marginal distribution of the monthly-based error processes, w'_s, regarding the April data.

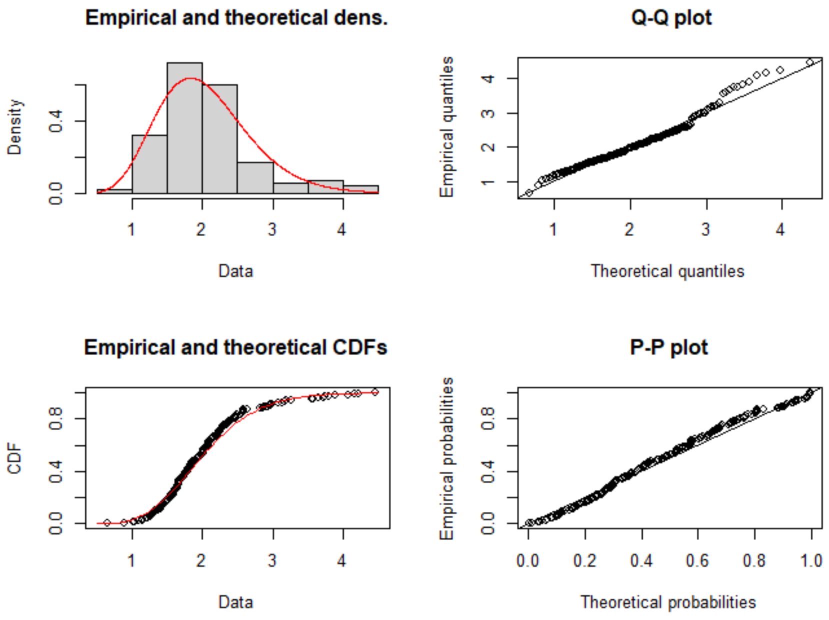

Figure 10.12: Fitting of marginal distribution of the monthly-based error processes, w'_s, regarding the June data.

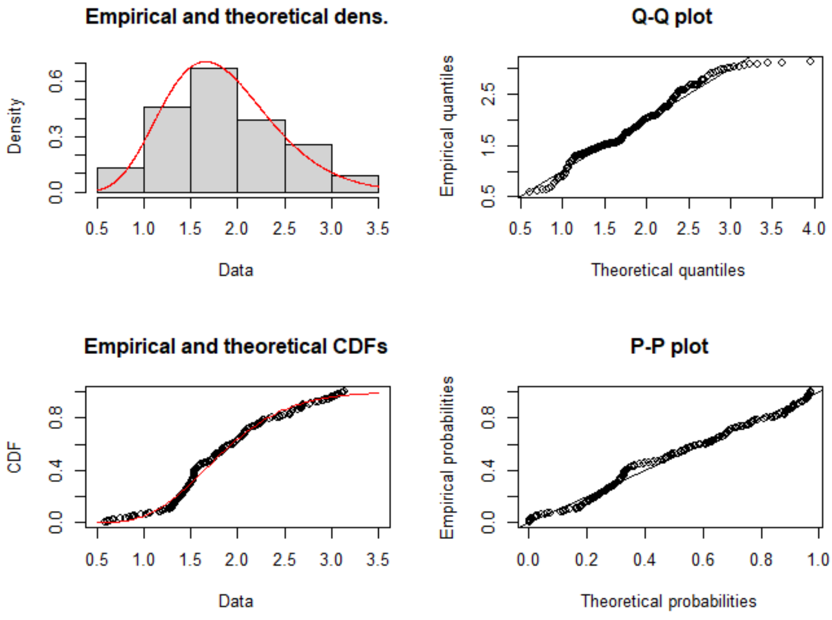

Figure 10.13: Fitting of marginal distribution of the monthly-based error processes, w'_s, regarding the July data.

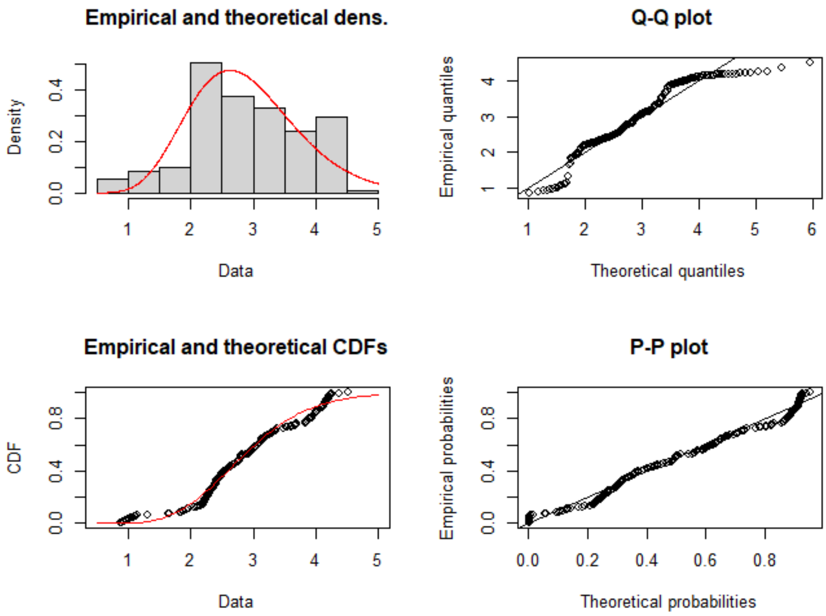

Figure 10.14: Fitting of marginal distribution of the monthly-based error processes, w'_s, regarding the August data.

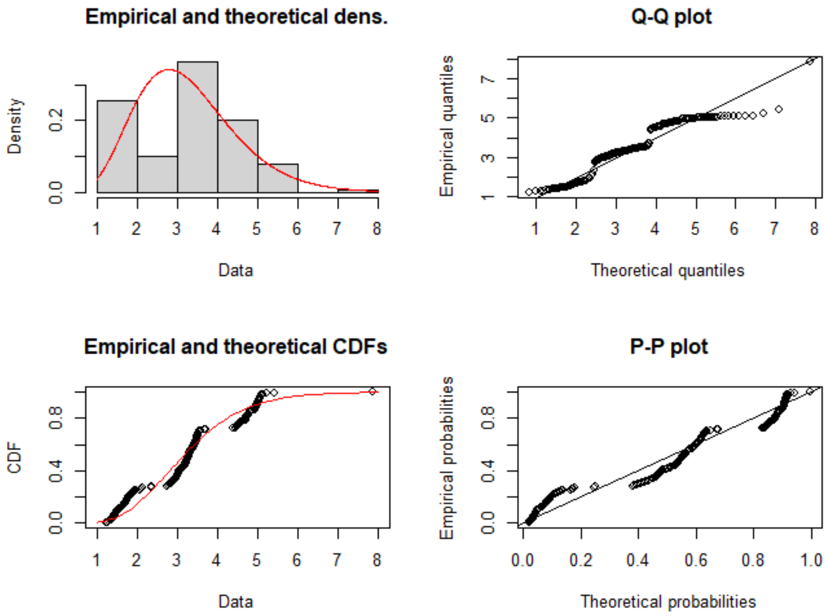

Figure 10.15: Fitting of marginal distribution of the monthly-based error processes, w'_s, regarding the September data.

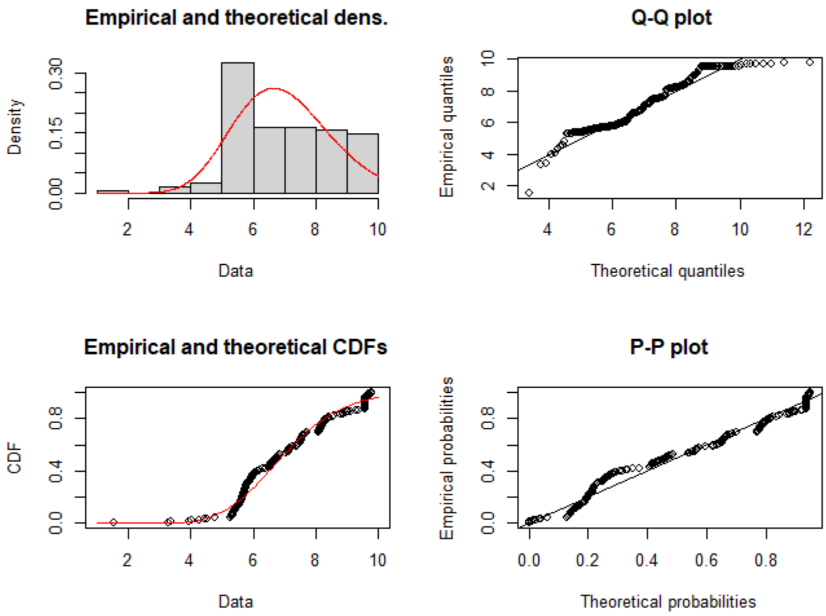

Figure 10.16: Fitting of marginal distribution of the monthly-based error processes, w'_s, regarding the October data.

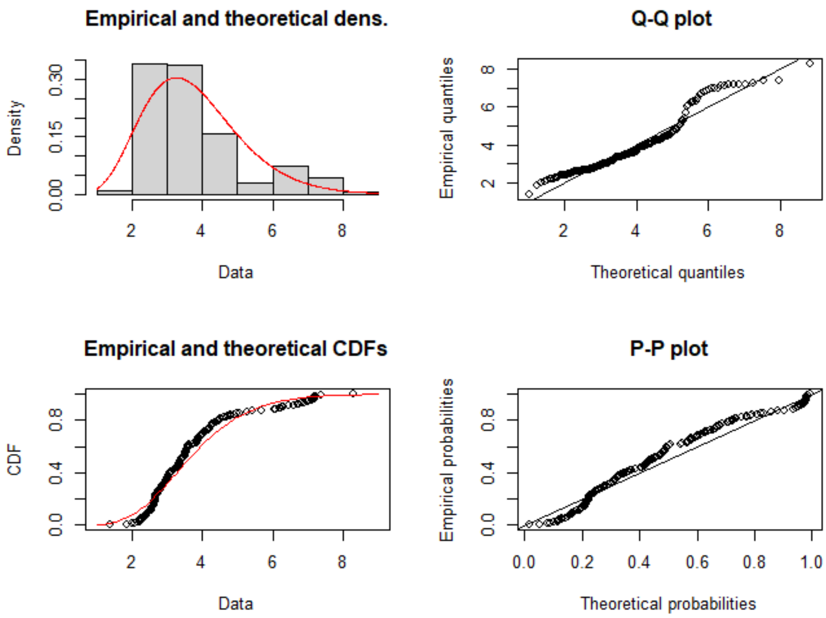

Figure 10.17: Fitting of marginal distribution of the monthly-based error processes, w'_s, regarding the November data.

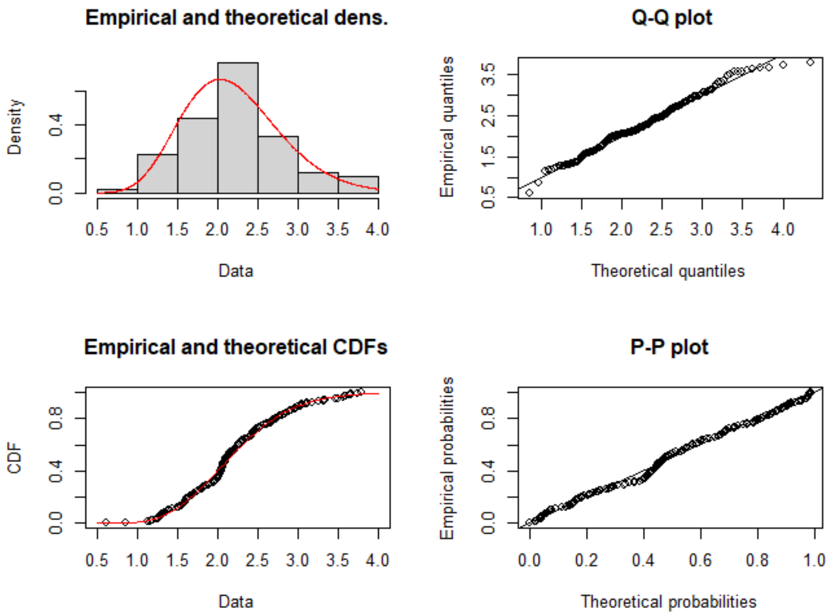

Figure 10.18: Fitting of marginal distribution of the monthly-based error processes, w'_s , regarding the December data.