Appendix D

Application of uncertainty analysis methods – knowledge from other fields

D.1 INTRODUCTION

The overall objective of this chapter is to incorporate knowledge from other fields on applications of uncertainty analysis methods. The fields selected were chemical and hydrogeological (groundwater) engineering, as they share similarities with wastewater treatment (WWT). The scope and objectives of the work are as follows:

- Identify the key attributes of the chosen fields and how they compare to wastewater treatment;
- Determine how uncertainty is typically accounted for in model-based studies in the chosen fields;
- Determine the main uncertainty methods used and whether there are any novel methods not used in wastewater treatment that are transferable to the wastewater treatment field.

The research was based on a targeted literature search and review of the uncertainty analysis methods in the selected fields. Based on the experience of the team members, key areas of research were selected for review. Each team member selected an area of focus and performed an initial screening of the available research papers, followed by a detailed review of a selected set of key papers. The initial screening focused on identifying key researchers and research groups in uncertainty analysis in the selected fields. The work of these researchers formed the basis of the detailed review. A review of the different uncertainty frameworks uncovered is provided followed by the literature review.

D.2 REVIEW OF UNCERTAINTY ANALYSIS METHODS IN CHEMICAL ENGINEERING

D.2.1 Comparison of chemical engineering with wastewater treatment

D.2.1.1 Background

In general, chemical engineering deals with the production, transportation and separation of chemical products. The focus is typically on using chemical reactions to create a compound and then using

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vapour/liquid and solid/liquid separation processes to purify the product. The reactants and products are often fluids (liquids, gases, or solid slurries).

In a classic sense, chemical engineering does not involve living matter but because research in classic areas has matured (e.g., refinery operation, catalysis, batch process optimization), recent developments in society (e.g., biofuels) have pushed the boundaries of the field towards a broader set of applications. As such, chemical engineering researchers, consultants and industries are increasingly venturing into newer, unexplored areas. This includes biochemical engineering and engineering of particulate processes (e.g., powder formulations of pharmaceuticals). This also means that in these particular areas, less knowledge is available and, as a result, more uncertainty exists for such applications. However, uncertainty has not been explored to a great extent in these emerging areas.

D.2.1.2 Similarities

Wastewater treatment plants (WWTPs) share similarities with chemical plants in that they often use a series of interconnected processes to purify influent water streams using a combination of biologically mediated reactions and solid/liquid separation processes. The basic mechanistic modelling and simulation principles remain essentially the same between the two fields, with plant models being based on mass and energy balances and consisting of algebraic and/or ordinary and partial differential equations (ODE and PDE) that are solved using numerical methods. In both fields, the fluid is often assumed to be incompressible and reactors are often assumed to be well-mixed. This means that the continuity equation for fluid motion can be described by a simple volume continuity equation. When more complex analysis of fluid motion is required, both fields employ computational fluid dynamics (CFD) analysis, although this is a more recent phenomenon in WWT. CFD analysis uses numerical methods to solve the conservation equations for linear momentum, known as the Navier–Stokes equations.

Process models are used in both fields for planning, process synthesis and design, control design, comparison of alternatives, 'what-if studies', and trouble-shooting. To date, the chemical engineering field has placed more emphasis on model-based control and optimization of its plants. This has led to the use of advanced control methods such as model-predictive control (MPC) and model-based optimization of plant design and operation using techniques such as linear programming (LP), non-linear programming (NLP), mixed-integer non-linear programming (MINLP), dynamic optimization, and optimization under uncertainty.

Both industries make use of empirical models, but the chemical process industries have made greater use of data-driven models such as Box–Jenkins time-series models, neural network models, and latent variable models (i.e., principal components analysis (PCA) and partial least squares (PLS)).

D.2.1.3 Differences

The major differences between the chemical engineering field and WWT, which are of importance when considering model-based analysis, are as follows:

- Process inputs and operational variables are more certain in the chemical process industries.
- Sensors are more widely used, and the process variables are often easier to measure.
- Process inputs in the chemical process industries have less variability.
- Raw material inputs into a chemical process system are tightly controlled and buffered. Wastewater streams have a high degree of variability in flow and composition and are subject to regular daily, weekly and annual variations as well as unexpected storms and industrial discharges.
- Process inputs in the chemical process industries are often not as strongly correlated with each other.

- The raw materials are usually independently controlled in a chemical process whereas influent pollutant variables are correlated in a WWT process.
- The underlying processes operate on much faster time-scales in chemical process systems and therefore can be more easily controlled. There is more interaction between control loops in chemical process systems due to similar time-scales, which is less of a problem in WWTPs.

D.2.1.4 Comparison in the context of model-based projects

A summary of how the chemical engineering field compares with the WWT field in terms of modelling, simulation, and uncertainty issues is given in Table D.1.

It is natural for evolving scientific fields to borrow modelling, analysis, control, and optimization techniques from other fields that are further advanced. Chemical engineering and process systems engineering (PSE) have borrowed heavily from the electrical engineering, operations research, and aeronautics fields. In turn, the WWT field has drawn heavily from chemical engineering. This technology transfer has flowed from industries where the phenomena are known with greater certainty and operate on faster time-scales to industries where the phenomena are known with less certainty and operate on slower time-scales. It follows that chemical engineering is an important field to consider when looking for novel uncertainty analysis techniques, but the techniques must be tailored to the WWT field.

D.2.2 Uncertainty methods used in chemical engineering

D.2.2.1 Methods overview

Uncertainty analysis has not received as much attention in the chemical engineering literature, as compared to fields such as WWT and hydrology. This is largely because uncertainty is perceived to be a less of an issue. The perception is that process inputs and outputs are more tightly controlled and precisely known, and first principle models are generally considered to be good representations of the processes. This perception is changing, and plants are being designed for flexibility. Uncertainty in chemical engineering appears more in the context of raw material availability and pricing, changes in weather, availability of power, and product demand. For example, one source of uncertainty could be that a company may decide to change product lines in a plant depending on market demand or may decide to start producing a product that the plant was not designed for.

In chemical engineering, the largest fraction of the literature deals with finding a best model, where best is usually stated as expectation, maximum likelihood or maximum posteriori likelihood (e.g., Maria, 2004). There are also papers dealing with parameter estimation, either using a specific data set or with continually updated online data. In these studies, uncertainty is not a concern, but approximate confidence intervals or regions do follow from the Kalman filter theory or non-linear regression theory. See Vachhani *et al.* (2001), Jang *et al.* (1986), and Ramamurthi *et al.* (1993) for examples where parameters are estimated online by means of inclusion as states in the applied model or by means of recursive estimation schemes.

There are several potential reasons for the lack of attention to uncertainty analysis in chemical engineering as compared to WWT:

- Models have largely been used in the context of operation and design of potentially unsafe systems, for which constraint satisfaction (e.g., physical constraints, safety constraints) has been considered a more important problem to solve.

Table D.1 Comparison of wastewater treatment and chemical engineering fields in terms of uncertainty analysis.

Characteristic	Wastewater Treatment Field	Chemical Process Industries/Process Systems Engineering
Types of models used	Mainly continuous models Steady-state and dynamic Linear and non-linear algebraic equations Ordinary differential equations, partial differential equations, and differential/algebraic equations Some data-driven models such as latent variable models (PCA/PLS) and neural networks	Both continuous and discrete models Steady-state and dynamic Linear, non-linear, mixed-integer linear, mixed-integer non-linear algebraic equations Ordinary differential equations, PDEs, and differential/algebraic equations Data-driven models such as latent variable models (PCA/PLS) and neural networks Stochastic differential-difference equations for chemical reaction networks
Level of detail in the models	Usually lumped parameter models (spatial variation of variables and parameters ignored) so ODEs used instead of PDEs Distributed parameter models used for biofilm modelling CFD modelling becoming more prevalent Usually, model surrogate organisms not individual bacteria	Usually, lumped parameter models Distributed parameter models also used CFD modelling commonly used Stochastic simulation approach models processes at the molecular level
Sources of uncertainty	Unexpected equipment failures and operational disturbances Influent conditions (flow rate, concentrations) Variability found in influent due to diurnal, weekly, and annual patterns Variability may be well characterized but can have storm events and industrial discharges that are unexpected and unknown in advance Population growth patterns and changing water-use and climate patterns that are uncertain Future regulations	Unexpected equipment failures and operational disturbances Unexpected changes in inlet and operational conditions Changes in economic value of product Changes in availability or quality of raw materials

(*Continued*)

Table D.1 Comparison of wastewater treatment and chemical engineering fields in terms of uncertainty analysis (*Continued*).

Characteristic	Wastewater Treatment Field	Chemical Process Industries/Process Systems Engineering
Numerical methods used	Nonlinear algebraic solvers Differential equation solvers including stiff solvers	Linear and nonlinear algebraic solvers Differential equation solvers including stiff solvers Linear programming Nonlinear programming algorithms Mixed integer, non-linear programming methods
Data typically available	Depends on region of world Can be very limited Additional sampling campaigns typically required when doing modelling studies	Large amount of highly correlated data Data often collected with on-line instrumentation
Are models calibrated/fitted to field data? Methods used?	Yes, depends on how model used Typically use manual calibration with visual inspection	Yes, depends on how model used Typically use formal parameter estimation techniques
What are models used for?	Most common: Planning, design, control design, comparison of alternatives, and what-if studies Less common: Model-based control, process monitoring, soft sensors, plant operational advice, trouble-shooting, and optimization	Planning, scheduling, comparison of alternatives, 'what-if' studies, plant design, product design, process monitoring, soft sensors, optimization, control design and model-based control, trouble-shooting
How is uncertainty addressed within the field?	Monte Carlo analysis and error propagation analysis	Most common: Optimization under bounded uncertainty, explicit modelling of input and output disturbances, and error propagation analysis Less common: Monte Carlo analysis, polynomial chaos
What is the tolerance for uncertainty in the field?	Historically high as plants designed with large safety factors to handle the expected uncertainty in loading conditions Effluent limits are often based on averages calculated over long time periods	Low as products must meet tight quality standards and plants subject to more safety concerns due to possibility of explosions, release of toxic compounds to the atmosphere, etc.

- First principles knowledge (chemistry, thermodynamics) and extensive laboratory scale testing means that more precise identification of kinetic models for many applications can be made before full-scale modelling is attempted.
- Inputs to chemical process systems are often of a constant or well-characterized nature and process control is aimed mostly at steady-state operation in a single, well-known condition, leading to limited uncertainty and effective use of linearized models around the operating point.
- The available measurements are often easier to interpret. For example, in a refinery, temperatures, pressures, and flow rates have an explicit and unambiguous meaning. In contrast, many variables (e.g., TSS) in WWT are reflective of the process but are not easily linked with the underlying variables of interest.

Despite this, researchers in the field have developed and/or used fundamental methods to deal with uncertainty. The literature review uncovered the following methods used to account for uncertainty in a chemical engineering context:

- **Error propagation analysis**: To determine how uncertainties are propagated through an equation or a model. The main drawbacks are that its results are approximate and specific to the local solution to the parameter estimation problem.
- **Explicit modelling of input and output disturbances**: To deal with uncertainty by modelling input and output disturbances explicitly, using state estimators, like Kalman filters (Brown & Hwang, 1996; Harvey, 1989). It is often assumed that the modelling of input disturbances effectively deals with uncertainty in the parameters, so that the input disturbances are regarded as a lumped source of uncertainty, which includes parameter uncertainty.
- **Sampling methods (i.e., Monte Carlo methods) and stochastic simulation**: To eventually approximate the true distribution of uncertainties in the model inputs and parameters. One issue that is explored is whether research exists on accounting for model input correlations when using sampling techniques as part of stochastic simulation. In wastewater influents, the pollutant concentrations are correlated with each other and with other plant operational indicators (e.g., SVI) but this is often not accounted for in Monte Carlo simulation studies.
- **Bounded uncertainty**: To solve problems in production planning and scheduling, location, transportation, finance, and engineering design, using robust control algorithms and model-based decision-making. Uncertainties and disturbances are assumed to occur in a limited region. In the case of robust control, which finds control actions for the worst of possible disturbance sequences within bounds, the bounds which describe the disturbance intervals are usually used as a tuning parameter (Skogestad *et al.*, 1988; Skogestad & Postlethwaite, 1996).
- **Polynomial chaos**: To determine uncertainty propagation in predictive models. Such methods often offer a computational advantage over stochastic sampling methods (e.g., Monte Carlo), though the computational load can be still be substantial. Note that the uncertainties in the model inputs and parameters are required to be quantified ahead of time. For detailed explanations of the technique and examples of its use in chemical engineering, see Androulakis *et al.* (2006), Balakrishnan *et al.* (2002), Damian *et al.* (2002), Lovett *et al.* (2006), Mathelin *et al.* (2005), Phenix *et al.* (1998), Reagan *et al.* (2003), Reagan *et al.* (2004), Reagan *et al.* (2005), and Xiu and Karniadakis (2002).

A more thorough review of sampling methods, stochastic simulation and bounded uncertainty is provided below.

D.2.2.2 Error propagation analysis

This approach has been well documented and is widely used for calculating confidence regions for model outputs and model parameters. A typical example is in nonlinear least-squares parameter estimation, where parameter and model response uncertainty are typically assessed through the calculation of approximate joint confidence regions for the parameters and approximate confidence limits on individual model responses and parameters. The inference regions and limits are often estimated by extending linear regression theory. The model residuals are linearized using a Taylor-series expansion and analogous formulas as those used for linear regression inference regions and bands are developed.

D.2.2.3 Explicit modelling of input and output disturbances

State estimators, like Kalman filters (Brown & Hwang, 1996; Harvey, 1989), deal with uncertainty by modelling input and output disturbances explicitly. In most cases, the parameters are fixed following first principles modelling and/or model calibration. It is often assumed that the modelling of input disturbances effectively deals with uncertainty in the parameters, that is, the input disturbances are regarded as a lumped source of uncertainty which includes parameter uncertainty.

The Kalman filter is popularly interpreted as a Bayesian method for state estimation, see for example, Roweiss & Ghahramani (1999). Special challenges occur when the modelled system behaves non-linearly (nonlinear differential equations) or when the measurements are nonlinear in the state variables (nonlinear observer equations). Historically, this has been handled with the extended Kalman filter (EKF) (Becerra *et al.*, 2001; Brown & Hwang, 1996; Fotopoulos *et al.*, 1998; Harvey, 1989), which linearizes the model around the last state estimate at each time step. However, the EKF has been shown to be unstable in certain cases. In addition, the EKF cannot handle (equality and inequality) constraints very well (e.g., non-negativity of concentrations; thermodynamic balances). Particle filters (Arulampalam *et al.*, 2002; Doucet *et al.*, 2001), also called sequential Monte Carlo methods, are better suited for systems with non-linear dynamics, discrete states and non-Gaussian disturbances. Such filters are based on stochastic sampling methods, akin to Monte Carlo sampling in Bayesian integration. The downside of this approach is the computational load which comes with all stochastic sampling methods. This can be prohibitive for on-line applications. In such cases, the unscented Kalman filter (UKF) has been proposed as the better method compared to the EKF (Wan & Van der Merwe, 2000). The UKF achieves second-order accuracy (e.g., it estimates means and variances correctly) with a limited number of deterministic samples (in particle filtering the samples are numerous and chosen randomly). The UKF has been used and adapted to handle nonlinear dynamics, nonlinear observer equations, equality and inequality constraints (e.g., Mandela *et al.*, 2010; Romanenko *et al.*, 2004; Teixeira *et al.*, 2010). Note that it does not handle non-Gaussian distribution of disturbances. As a last method, the moving horizon estimation (MHE) is mentioned (Rao & Rawlings, 2002; Rao *et al.*, 2003). The MHE estimates process states at a time in the past given current and past observations. As such it is smoother, rather than a filter. Smoothers are less sensitive to disturbances because additional information is available (the observations after the considered time instant). In contrast to classic smoothers based on the Kalman filter (Kalman smoother, extended Kalman smoother), it delivers the maximum likelihood trajectory of states over a time window instead of the expected trajectory.

D.2.2.4 Sampling-based methods

Sampling methods, also known as Monte Carlo methods, use statistical sampling techniques to obtain a probabilistic approximation to the solution of a mathematical model or problem. Monte Carlo methods are discussed in the chemical engineering and PSE literature, although their use for uncertainty analysis

appears to not be as prevalent as in water and wastewater engineering. Many applications of the method are not in the context of uncertainty analysis but involve the solution of mathematical problems that are difficult or impossible to solve with other numerical methods.

Gazi *et al.* (1996), Lee *et al.* (1996), Sin *et al.* (2010), Tørvi and Hertzberg (1998), Vásquez and Whiting (2000), and Vásquez *et al.* (2010) report the use of Monte Carlo methods to estimate the uncertainty in models used in the chemical process industries. Tørvi and Hertzberg studied different sampling methods including basic Monte Carlo, median Latin hypercube sampling, a Halton sequence, and a method based on Gaussian quadrature. Gaussian quadrature was found to be very accurate but not well suited to larger problems.

Gazi *et al.* (1996) use dynamic simulation for controller verification in the presence of uncertainties and employ Monte Carlo simulation to quantify the uncertainties. Qualitative reasoning techniques such as QSIM (Kuipers, 1986) are used to translate the Monte Carlo results into qualitative descriptions of the possible behaviour of the system. The qualitative descriptions are summarized in a tree structure which can be checked for interesting behaviours using computation tree logic. The approach is reported to provide the answers to qualitative questions about a system concerning its safety, reliability, and operability.

Lee *et al.* (1996) use Monte Carlo simulation in the context of dynamic chemical process simulation. Monte Carlo simulations are used to assess the uncertainty in the dynamic modelling results given the uncertainties in model inputs and parameters. The handling of discrete events such as start-up or shut-down of equipment is incorporated into their modelling approach. Statistical analysis is then used to interpret the results of the Monte Carlo analysis such scatterplots and regression analysis of the input and output samples.

Vásquez *et al.* (2010) used Monte Carlo analysis to obtain confidence limits on the output variables of a chemical process simulation models. To account for systematic errors, they used values from either the uniform distribution or another appropriate distribution when a priori information was available. Gaussian probability distributions were used to characterize random variables. The presence of systematic errors can lead to heavy tails in the probability distributions of the output variables, and Vásquez *et al.* (2010) developed a technique for estimation of the confidence intervals in these situations.

The research group led by Gintaras V. Reklaitis at Purdue has studied supply chain management and have used Monte Carlo simulation to evaluate schedule robustness under planning uncertainty (see Honkomp *et al.*, 1999; Mignon *et al.*, 1995). They have also incorporated Monte Carlo simulation into deterministic supply chain planning and scheduling models (Jung *et al.*, 2004).

The inputs to a simulation model may be correlated in some way and this can be accounted for when running Monte Carlo simulations. Wu and Tsang (2004) demonstrate the use of four different methods for generating correlated random numbers in the context of ecological modelling: Iman-Conover, standard normal transformation, normal copula, and maximum-entropy copula. The Iman and Conover (1982) method is the most well-known method and is used in software such as Crystal Ball and @Risk. The basis of the method is that independent random numbers can be transformed into correlated ones using an orthogonal transformation. The correlation matrix between the input variables is decomposed using the Cholesky decomposition. The resulting lower triangular matrix is then multiplied by the matrix of independent random numbers ($N \times k$ matrix; N sets of k independent random numbers) to produce a matrix of correlated random variables which serves as an input into the Monte Carlo simulations. In this manner, the Monte Carlo analysis is not biased by unreasonable combinations of variable values.

Sin *et al.* (2010) used Monte Carlo simulations to determine the model output uncertainty in cellulose hydrolysis models used in biofuel process design. They considered both input variable and model parameter uncertainty and considered correlation between the input parameters using the method of Iman and Conover (1982).

Vásquez and Whiting (2000) used equal probability sampling (EPS) to analyse uncertainty in thermodynamic models. They report that EPS provides more realistic results than other sampling techniques, such as Latin hypercube sampling or shifted Hammersley sampling when the model parameters are highly correlated. The EPS method involves stratifying the parameter space of the parameter estimation objective function. This is done by stratifying the probability distribution of the objective function into a number of intervals of equal probability. The inverse images of these intervals form shells of equal probability in the parameter space. A resampling scheme for each of the shells is used to ensure uniform coverage of the parameter space.

D.2.2.5 Stochastic simulation algorithm (SSA)

A variation on the Monte Carlo simulation approach, described in the physical chemistry literature, is the stochastic simulation algorithm (SSA) first discussed by Gillespie (1977). The SSA regards the time evolution of a chemical reaction system as random-walk process governed by a single differential-difference equation instead of a set of coupled ODEs. This differential-difference equation is often mathematically intractable and does not lend itself well to numerical solution (Gillespie, 1977). Instead, the stochastic simulation problem can be solved using Monte Carlo methods. The difference between the SSA and traditional Monte Carlo simulation is that in the SSA, random numbers are generated at each time step and used to determine when the next reaction will occur (how far along the next time step occurs) and what kind of reaction occurs.

The stochastic simulation approach has a firmer theoretical basis than the deterministic one as chemical reaction systems are actually discrete, stochastic processes. Molecular population levels can only change by discrete integer amounts and chemical reactions require molecular collisions which are essentially random processes when the molecules are at thermal equilibrium.

For many problems that can be represented as linear or nonlinear ODEs or PDEs, the stochastic simulation algorithm (SSA) gives results that are comparable to the numerical solution of the deterministic differential equations. The SSA produces results that have the appearance of 'noisy' solutions of the differential equations (Erban *et al.*, 2007). There are certain problems where the SSA gives results that cannot be obtained by solving the deterministic model. Examples include chemical reaction systems that have two or more stable steady states, where the SSA can predict random switching between steady states due to fluctuations in the number of molecules, or systems with self-induced stochastic resonance, where the SSA predicts oscillatory solutions.

The SSA has been applied to biological reaction−diffusion systems involving cell growth. Testing of the technique in the context of activated sludge modelling would be required to determine if the SSA has practical applications in the field of WWT. The SSA would not be used to evaluate the impact of model input or parameter uncertainty on simulation results, but instead to assess the potential for uncertain stochastic processes to impact the outcome of processes over time.

D.2.2.6 Bounded uncertainty

The concept of bounded uncertainty is used to solve chemical engineering problems where decisions are made in the presence of uncertainty, such as production planning and scheduling, transportation and location problems, finance, and engineering design. In these problems, uncertainty is considered to impact the weather, the prices of fuels, the availability of power, and the demand for resources (Sahinidis, 2004).

The study of optimization under uncertainty began with the works of Beale (1955), Bellman (1957), Charnes and Cooper (1959), Dantzig (1955), and Tintner (1955). The main approaches to optimization

under uncertainty are: stochastic programming, fuzzy programming, and stochastic dynamic programming (Sahinidis, 2004).

Grossman and Sargent (1978) and Halemane and Grossman (1983) published some of the earlier studies of deterministic flexible programming approach in the field of chemical engineering. Their objective was to determine optimal process designs under uncertainty. As in stochastic programming, a two-stage strategy is used that takes advantage of the fact that control variables can be adjusted during operation to satisfy the design specifications of the plant, and that only the design of the plant remains fixed in the second stage. The strategy is intended to avoid overdesign, which can lead to non-optimal or even infeasible operation. The model used is a combination of equations and inequalities. The model variables include stage 1 design variables (plant structure and equipment sizes), stage 2 control variables that can be adjusted during operation (e.g., flow rates), state variables that describe the process, and uncertain parameters. For a given design (determined in stage 1), the next step is to solve the so-called feasibility problem to determine if the design is feasible for a realization of the uncertain parameters (stage 2). The more general problem of quantifying flexibility involves finding the maximum deviation that a given design can tolerate such that every point in the uncertain parameter space is feasible.

Dynamic programming involves the solution of multi-stage decision processes such as discrete-time systems. The problems often suffer from the curse of dimensionality as the number of state and control variables increases. See Sahinidis (2004) for a discussion of dynamic programming.

The literature review found the following areas of research and associated research papers in the field of optimization under uncertainty in chemical engineering:

(1) Optimal design of chemical plants under uncertainty:
   (a) Flexible programming with bounded uncertainties: Grossman and Sargent (1978), Halemane and Grossman (1983), Ostrovsky *et al.* (2003), Rooney and Biegler (2003), Song *et al.* (2002).
   (b) Use of a sensitivity analysis and parametric programming approach for linear process engineering problems under uncertainty: Acevedo and Pistikopoulos (1997).
   (c) Flexible programming with probability distribution functions for the uncertainties: Acevedo and Pistikopoulos (1998), Ierapetritou *et al.* (1996).
   (d) Flexible programming for dynamic systems: Mohideen *et al.* (1996)
(2) Reviews of optimization under uncertainty: Biegler and Grossmann (2004), Pistikopoulos (1995), Sahinidis (2004).
(3) Process scheduling under uncertainty: Li and Ierapetritou (2007).
(4) Supply chain design and planning under demand uncertainty: You *et al.* (2009), You and Grossmann (2010).
(5) Pharmaceutical waste management under uncertainty: Linninger and Chakraborty (2001).

D.2.2.7 Polynomial chaos expansion

Polynomial chaos is another available technique for uncertainty propagation in predictive models. The theory is based on the fact that a stochastic process can be described as an infinite combination of linear processes (spectral decomposition). Therefore, the distribution in the next time interval can be approximated based on the distributions in the current one.

The main requirement is that the uncertainties in the parameters or system inputs are quantified and are available in the form of probability density functions (PDF). Polynomial chaos techniques then proceed by expanding the available density function into an expanded basis function. Each original parameter is then converted into a set of parameters which describe its density function. Usually, a polynomial basis is

used for this purpose (e.g., Hermite polynomials, Legendre polynomials). This parametric description of the density function is then propagated through a predictive model. Following this propagation, one can then recover the density function at each successive time interval. Such methods often offer a computational advantage over stochastic sampling methods (e.g., Monte Carlo), though the computational load can still be substantial. Note that the uncertainties in the model inputs and parameters are required to be quantified ahead of time. The technique is often used as part of a stochastic response surface methodology.

For detailed explanations of the technique and examples of its use in chemical engineering, see Androulakis *et al.* (2006), Balakrishnan *et al.* (2002), Damian *et al.* (2002), Lovett *et al.* (2006), Mathelin *et al.* (2005), Phenix *et al.* (1998), Reagan *et al.* (2003), Reagan *et al.* (2004), Reagan *et al.* (2005), and Xiu and Karniadakis (2002).

D.2.3 Applicability to WWT

There are some uncertainty analysis techniques used in the chemical engineering field that could be adapted for use in WWT. Optimization uncertainty appears to be a technique that could provide benefits in the area of plant design and operation. Research is needed to determine how the techniques could be best applied and whether they provide significant benefits over traditional methods. Problems based on linear programming are typically easier to solve, and may provide the most benefits with the least computational burden. The interesting aspect is that optimization under uncertainty has the potential to assist in developing plant designs that not only focus on robustness, but also flexibility and operability.

Monte Carlo methods are used in chemical engineering as in WWT, but there are some unique techniques used that warrant further study. The SSA of Gillespie (1977) may be of interest to those studying biological transformations at the cellular level. Its applicability to whole plant uncertainty analysis is likely limited. The techniques for incorporating correlation among input parameters should be tested for applicability in WWT.

Inclusion of explicit disturbances as part of state estimation or process modelling in general is a topic of interest. The concept has been applied in WWT modelling, but there may be some ideas (e.g., the disturbance models) that could be taken from chemical engineering that could improve the methodology. Running long-term dynamic simulations with realistic input disturbances is a method of uncertainty analysis and has the benefits of simplicity.

Polynomial chaos is an interesting concept and has been used by a number of researchers in chemical engineering. Further study is required to determine if whether its potential to reduce the computational load would provide benefits over existing Monte Carlo-based methods.

D.3 REVIEW OF UNCERTAINTY ANALYSIS METHODS IN HYDROGEOLOGICAL (GROUNDWATER) ENGINEERING

D.3.1 Comparison of hydrogeological engineering with WWT

D.3.1.1 Background

The modelling of hydrogeological processes shares a similar focus as WWTP modelling in that it deals with the prediction of liquid component concentrations, has dynamically varying inputs, and is concerned with the spatial/temporal variability of parameters.

Hydrogeological (groundwater) modelling focuses on the following:

- Modelling of the flow of liquids (of various densities) in a partially or fully saturated porous heterogeneous media;

- Transport of contaminants in porous or fractured heterogeneous media via advective, diffusive or dispersive processes; and
- Transformative processes during transport (e.g., biodegradation, sorption to media surfaces, volatilization, dissolution of dense phase liquids).

D.3.1.2 Comparison in the context of model-based projects

Despite some of the similarities between hydrogeological processes and WWTPs, the associated uncertainty is often fundamentally different than WWTP uncertainty. The major sources of uncertainty in hydrogeological modelling are in the characteristics of the systems (i.e., aquifers) being modelled. Aquifers can be difficult to model for the following reasons:

- They are buried underground out of plain sight, and often not easily observable/measurable,
- Are spatially heterogeneous,
- Have boundaries (in three dimensions) that are often unknown,
- Can hydraulically connect to other aquifers,
- Can be difficult and expensive to sample, and
- Conceptual structural models are often assumed to be 'correct' if they can be calibrated, and subsequently can be difficult to disprove once accepted.

A summary of the differences between groundwater and WWTP models is provided in Table D.2.

Table D.2 Comparison of groundwater and WWTP models.

Groundwater Models	WWTP Models
System size, boundaries, composition often unknown/unmeasurable	Well-defined, measurable tanks, with known hydraulic connectivity
Significant spatial heterogeneity (e.g., porosity, conductivity)	Effective tank volumes often well known.
Potentially significant discontinuities from depositional origins (e.g., discrete boundaries between clay and silt layers) not easily identified	Biofilm structure not as well known. Aerated/non-aerated zones are often defined by design, and often well-known and/or measurable
Underlying model structure definition (e.g., aquifer thickness) unlikely to change temporally, even if not well known.	Some system definition can change temporally (e.g., tank volumes in SBRs) but more likely to be known/measurable.

As in our review of the chemical engineering field, the focus of this report is on methods for accounting for uncertainty in model-based projects. Common uncertainty analysis methods used in this field include:

- Calculation of approximate confidence regions and limits around parameters and model outputs as part of parameter estimation.
- Stochastic simulation in classic and Bayesian frameworks.

Due to the nature of the systems modelled, application of the above techniques can be computationally intensive. In addition, aquifer systems can be very non-linear and discontinuous, limiting the use of approximate confidence regions and intervals.

D.3.2 Uncertainty methods used in hydrogeological engineering

D.3.2.1 Model structure uncertainty

It is a widespread challenge in science to develop and use models without any explicit fundamental philosophy. The lack of interdisciplinary knowledge, particularly in mathematics, is often the reason for a scientist, working for instance in the field of hydrology, to develop solutions that are numerically incorrect.

Other limitations can be the constraints of current knowledge, computing capabilities and observational technologies. In the Bayesian approach to inverse problems, prior estimates of model parameter distributions are adjusted on the basis of a likelihood measure that can demonstrate how well a model predicts the available set of observations to calculate a posterior distribution of parameters. In this approach, likelihood functions can be used to approximate parameter values. With increased availability of experimental data, the use of these likelihood functions can potentially lead to reduced uncertainty in parameter values.

This probabilistic framework is considered as one of the only potential approaches to address model uncertainty. However, one cannot treat the entire range of sources of uncertainty in an aggregate form because, for instance, model structure uncertainties are nonlinear, non-stationary and non-additive (Beven, 2006). Thus, they cannot be accounted for by the likelihood-based approach.

Bayes methods have a number of advantages, one of them being that different model structures can be compared and combined. For many hydrological models, and presumably for WWTP models, the definition of a formal likelihood measure can lead to misleading results if the assumptions on which it is based upon are not valid. That is, it is questionable whether the various sources of uncertainty can be represented adequately by a formal uncertainty structure, which defines the appropriate likelihood function. For most of the hydrological models, being subject to uncertainty derived from input, boundary conditions and model structure uncertainty, it is generally only possible to approximately represent the complexity of the uncertainties. As a result, the likelihood function will only be an approximate, and the resulting parameter estimates may well be biased.

From a statistical viewpoint, one can argue that model structure uncertainty can be represented by means of a model discrepancy function. O'Hagan and Oakley (2004) suggest that the complexity of observed uncertainty series in most of the hydrogeological problems does not directly imply that one should not use a formal likelihood approach, but that finding an appropriate likelihood function may require some more detailed assessment of various tools. Then, it is noteworthy that the problem is that the more complex the model of the uncertainty used, the more the number of statistical parameters that must be estimated. In some hydrogeological cases with complex uncertainty structures, the method can still be applied using a transformation of the modelling uncertainty so that the assumptions of a simple formal likelihood measure are more closely approximated. Other less formal methods are also used in the area, in cases where the choice of a formal likelihood would be incoherent.

D.3.2.2 Model identifiability (equifinality)

When using statistical methods for model calibration (Pareto optimal set approach), there is an underlying presumption that the experimental data are adequate to identify an optimal model structure (or Pareto optimal set of models). This should be the case for Bayesian methods that aim to identify the complete multi-parameter posterior distribution. Beven and Young (2003) argue that oversimplification of likelihood functions often leads to this result in hydrogeological simulations. In general, there is no such thing as the correct model structure, and one can only find true model parameters for a given model structure.

An acceptance of model equifinality is, in part, the recognition of possible model structure and input data uncertainties. It means that the formal model of equations that are used to represent the hydrogeological systems may be, at times, a poor approximation of the relevant processes. It also accounts for the possibility that, even if there was a correct model structure, it may be difficult to specify accurately all the boundary conditions (e.g., shape and size of an aquifer) required to run the correct model. There is, however, not much one can do about model structure uncertainty in most hydrogeological modelling cases since, if there were obvious improvements to be made, then there would be no reason why this should not be done (limit: computational feasibility).

D.3.2.3 Conceptual model uncertainty

There are many studies in the hydrogeological literature that report on the difficulties of finding a single 'true' model to represent a process. It seems that model structure uncertainty is something that is endemic to most of the models in the field. Beven and Freer (2001), and Rojas *et al.* (2010), both illustrate the tendency for practitioners to assume that well calibrated models can be accepted as 'true' interpretations of a system structure.

Refsgaard (2006) demonstrate an example of how model structure can introduce considerable variance in model results. Results from a hydrogeologic modelling exercise in the County of Copenhagen, Denmark, are used to illustrate the effects of different model structures on final model results. Five different consulting companies were asked to develop models of groundwater contamination risk in a 175 km^2 area west of Copenhagen. Each of the consultants was well-respected in the industry, with considerable experience in modelling contaminant flow. Each of the consultants took a different approach to the model structure, with some using a criteria-based method for risk assessment, while others used hydrological models of varying levels of complexity. In each case, the consultant assumed the underlying model structure was suitably correct, based upon past experience. The results from the five consultants differed substantially, even though all five were using the same raw data (and therefore the same data uncertainty) indicating the major source of uncertainty in model predictions was due to differences in model structure.

D.3.2.4 Model conditioning

Alternative approaches to model calibration are required to account for the effects of model structure and data uncertainty – again, despite the fact that some of these uncertainties cannot be represented explicitly. One alternative option in the field of hydrology is to identify a set of equations that derive acceptable uncertainty in the range of the available data – a process called as model conditioning. In hydrogeology, such approaches have generally been based on some form of Monte Carlo sampling from the population of feasible models. Based on the simulation results obtained with each model in the selected population, a qualitative or quantitative assessment is undertaken as to whether a particular model is accepted/rejected as behavioural. This is the basis for the generalized likelihood uncertainty estimation (GLUE) methodology, which was used, for the first time, by Beven and Binley (1992) in an application to a hydrological model.

The GLUE methodology, used with a formal uncertainty model and likelihood, infers essentially identical results to that obtained using a formal Bayesian likelihood approach. It has been noted that, for forward simulations, a set of behavioural models can be used to provide a prediction range of model variables as conditioned on the process of model evaluation. The fuzzy or probabilistic weights associated with each model can be used to weigh the model simulation to reflect how well that particular model has performed in the past.

Traditional use of the GLUE methodology in groundwater modelling supplements the forward propagation of parametric uncertainty (and/or spatial variability of parameters) through the model with posterior information on the level of correspondence between model predictions and field observations. The posterior analysis assists in the development of uncertainty bounds for each input parameter. Because these measurements of uncertainty use measured field observations in the analysis of input parameter uncertainty, the analysis is restricted to only those systems for which suitable data can be observed. This diminishes the usefulness of traditional GLUE analyses to only model evaluation, and not situations where predictive modelling is carried out (Hassan *et al.*, 2008).

To address this issue, several alternative variations on the GLUE methodology have been proposed. Rojas *et al.* (2008) combine GLUE methodology with Bayesian model averaging (BMA) to account for the uncertainty associated with the choice of model structure. In addition to propagating parametric uncertainty, the variability associated with models of different structures is incorporated into the analysis by modelling the system with a group of plausible models. A hypothetical example of the prediction of groundwater flow and head distribution within an aquifer is used to illustrate that while some predictions varied considerably among the three models used, a comparison of predictions to the observed data was unable to distinguish between models. When considering a combined prediction using BMA, the combined prediction was more conservative than individual predictions from each model. Most importantly, 30% of the total uncertainty was associated with the choice of model structure.

Rojas *et al.* (2010) applied the above multi-model approach to a real aquifer system in the Walenbos Nature Reserve area in Belgium. Using a combination of GLUE and BMA, the authors modelled the flow through the aquifer with three different models (of different levels of geological knowledge), with associated input parameter distributions. Some parameters were common amongst the three models, while others were unique. The concept of equifinality, as defined above, states that the combination of many alternative models and parameter sets can produce equally good results when compared to limited observations (Beven & Freer, 2001). In this study, GLUE analysis provided weights for each conceptual model, and the results were combined via BMA. This approach, which no longer relies on a single parameter set or conceptual model, was applied to the hydrogeologically complex aquifer system to model the hydraulic budget under various recharge scenarios.

A key conclusion of the study illustrates that typically limited observational data (in this case, observations of head in various locations in the aquifer) often cannot discriminate between conceptual models, as shown by small differences in posterior model probabilities. An additional important conclusion is that despite these small differences, the *predictive* distributions were different in shape and spread among the alternative conceptual models and scenarios analysed. The authors emphasize the point that relying on a single conceptual model driven by a particular simulation scenario will likely produce 'biased and under-dispersive estimations of predictive uncertainty'.

D.3.3 Applicability to wastewater treatment

For parameter uncertainty analysis, simple Bayesian approaches used in the hydrogeological sciences are applicable to WWT modelling, even though wastewater systems are generally more well defined than groundwater aquifers. The lack of easily observable information on the completeness of mixing in biological reactors is an example of a source of uncertainty that is analogous to the lack of information on aquifer heterogeneity in the field. Approaches to assessing this unknown and quantifying the predictive uncertainty in the hydrogeological field would be transferrable to WWT modelling.

In particular, the GLUE and BMA methods would be useful to assist in quantifying the uncertainty associated with model structure. While model structure uncertainty is generally limited to describing the

physical characteristics of the aquifer systems in groundwater modelling (which is analogous to the mixing issue in wastewater modelling), there is an opportunity in the wastewater field to extend the multi-model approach to the biological model structure as well.

In groundwater modelling, the active physical processes (advection, sorption/desorption, volatilization, etc.) are well understood and well described by mathematical relationships. The major source of uncertainty comes from the spatial heterogeneity of the physical properties of the aquifer. By contrast, the active biological processes in an activated sludge tank are more complex and less well described mathematically (e.g., hydrolysis, biomass growth, etc.) than the physical characteristics of the system (e.g., hydraulic connectivity, effective tank volume, etc.). The opportunity exists to apply the multi-model approach to account for conceptual model uncertainty in the biological model specifically. With a set of activated sludge models already established in the industry (ASM1, ASM2d, ASM3, commercial simulator default models), a WWT system could be easily modelled with several biological models to provide an evaluation of the uncertainty associated with the conceptual model structure.

REFERENCES

References for uncertainty analysis in chemical engineering

Acevedo J. and Pistikopoulos E. N. (1997). A multiparametric programming approach for linear process engineering problems under uncertainty. *Industrial & Engineering Chemistry Research*, **36**, 717–728.

Acevedo J. and Pistikopoulos E. N. (1998). Stochastic optimization-based algorithms for process synthesis under uncertainty. *Computers & Chemical Engineering*, **22**(4/5), 647–671.

Androulakis I. P., Grenda M. G., Barckholtz T. A. and Bozzelli J. W. (2006). Propagation of uncertainty in chemically activated systems. *AICHE Journal*, **52**(9), 3246–3256.

Arulampalam S., Maskell S., Gordon N. and Clapp T. (2002). A tutorial on particle filters for online nonlinear/non-Gaussian Bayesian tracking. *IEEE Transactions Signal Processing*, **50**, 174–188.

Balakrishnan S., Georgopoulos P., Banerjee I. and Ierapetritou M. (2002). Uncertainty considerations for describing complex reaction systems. *AIChE Journal*, **48**(12), 2875–2889.

Beale E. M. L. (1955). On minimizing a convex function subject to linear inequalities. *Journal of the Royal Statistical Society*, **17B**, 173–184.

Becerra V. M., Roberts P. D. and Griffiths G. W. (2001). Applying the extended Kalman filter to systems described by nonlinear differential-algebraic equations. *Control Engineering Practice*, **9**, 267–281.

Bellman R. E. (1957). Dynamic Programming. Princeton University Press, Princeton, PA.

Biegler L. T. and Grossmann I. E. (2004). Retrospective on optimization. *Computers & Chemical Engineering*, **28**, 1169–1192.

Brown R. G. and Hwang P. Y. C. (1996). Introduction to Random Signals and Applied Kalman Filtering with Matlab Exercises and Solutions, 4th edn, published by Wiley, USA.

Charnes A. and Cooper W. W. (1959). Chance-constrained programming. *Management Science*, **6**, 73–79.

Damian V., Sandu A., Damian M., Potra F. and Carmichael G. R. (2002). The kinetic PreProcessor KPP − a software environment for solving chemical kinetics. *Computers and Chemical Engineering*, **26**, 1567–1579.

Dantzig G. B. (1955). Linear programming under uncertainty. *Management Science*, **1**, 197–206.

Doucet A., De Freitas N. and Gordon N. J. (2001). Sequential Monte Carlo Methods in Practice. Springer, New York, NY. https://doi.org/10.1007/978-1-4757-3437-9 Springer.

Erban R., Chapman J. and Maini P. (2007). A practical guide to stochastic simulations of reaction-diffusion processes. *arXiv*, **0704**, 1908 [q-bio.SC].

Fotopoulos J., Georgakis C. and Stenger Jr., H. G. (1998). Use of tendency models and their uncertainty in the design of state estimators for batch reactors. *Chemical Engineering and Processing*, **37**, 545–558.

Gazi E., Ungar L. H., Seider W. D. and Kuipers B. J. (1996). Automatic analysis of Monte-Carlo simulations of dynamic chemical plants. *Computers & Chemical Engineering*, **20**(Suppl.), S987–S992.

Gillespie D. T. (1977). Exact stochastic simulation of coupled chemical reactions. *Journal of Physical Chemistry*, **81**(25), 2340–2360.

Grossman I. E. and Sargent R. W. H. (1978). Optimum design of chemical plants with uncertain parameters. *AIChE Journal*, **24**(6), 1021–1028.

Halemane K. P. and Grossmann I. E. (1983). Optimal process design under uncertainty. *AIChE Journal*, **29**(3), 425–433.

Harvey A. C. (1989). Forecasting, Structural Time Series Models and the Kalman Filter. Cambridge University Press, UK.

Honkomp S. J., Mockus L. and Reklaitis G. V. (1999). A framework for schedule evaluation with processing uncertainty. *Computers & Chemical Engineering*, **23**, 595–609.

Ierapetritou M. G., Acevedo J. and Pistikopoulos E. N. (1996). An optimization approach for process engineering problems under uncertainty. *Computers & Chemical Engineering*, **20**(6/7), 703–709.

Iman R. L. and Conover W. J. (1982). A distribution-free approach to inducing rank order correlation among input variables. *Communications in Statistics – Simulation and Computation*, **11**, 311–334.

Jang S., Joseph B. and Mukal H. (1986). Comparison of two approaches to on-line parameter and state estimation of nonlinear systems. *Industrial & Engineering Chemistry Process Design and Development*, **25**, 809–814.

Jung J. Y., Blau G., Pekny J. F., Reklaitis G. V. and Eversdyk D. (2004). A simulation based optimization approach to supply chain management under design uncertainty. *Computers & Chemical Engineering*, **28**, 2087–2106.

Kuipers B. J. (1986). Qualitative simulation. *Artificial Intelligence*, **29**, 289–338.

Lee K. W., Kang J. L., Choi S. H. and Yoon E. S. (1996). Stochastic dynamic simulation of chemical processes with changing uncertainties. *Computers & Chemical Engineering*, **20**, Suppl., S557–S562.

Li Z. and Ierapetritou M. G. (2007). Process scheduling under uncertainty using multiparametric programming. *AIChE Journal*, **53**(12), 3183–3203.

Linninger A. A. and Chakraborty A. (2001). Pharmaceutical waste management under uncertainty. *Computers and Chemical Engineering*, **25**, 675–681.

Lovett T. E., Ponci F. and Monti A. (2006). A polynomial chaos approach to measurement uncertainty. *IEEE Transactions on Instrumentation and Measurement*, **55**(3), 729–736.

Mandela R. K., Rengaswamy R., Narasimhan S. and Sridhar L. N. (2010). Recursive state estimation techniques for nonlinear differential algebraic systems. *Chemical Engineering Science*, **65**(16), pp. 4548–4556.

Maria G. (2004) A review of algorithms and trends in kinetic model identification for chemical and biochemical systems, *Chemical and Biochemical Engineering Quarterly*, **18**(3), 195–222.

Mathelin L., Hussaini M. Y. and Zang T. A. (2005). Stochastic approaches to uncertainty quantification in CFD simulations. *Numerical Algorithms*, **38**(1), 209–236.

Mignon D. J., Honkomp S. J. and Reklaitis G. V. (1995). A framework for investigating schedule robustness under uncertainty. *Computers & Chemical Engineering*, **19**, Suppl., S557–S562.

Mohideen M. J., Perkins J. D. and Pistikopoulos E. N. (1996). Optimal design of dynamic systems under uncertainty. *AIChE Journal*, **42**(8), 2251–2271.

Ostrovsky G. M., Datskov I. V., Achenie L. E. K. and Volin Y. M. (2003). Process uncertainty: case of insufficient process data at the operation stage. *AIChE Journal*, **49**(5), 1216–1232.

Phenix B. D., Dinaro J. L., Tatang M. A., Tester J. W., Howard J. B. and McRae G. J. (1998) Incorporation of parametric uncertainty into complex kinetic mechanisms: application to hydrogen oxidation in supercritical water. *Combustion and Flame*, **112**, 132–146.

Pistikopoulos E. N. (1995). Uncertainty in process design and operations. *Computers & Chemical Engineering*, **19**, S553–S563.

Ramamurthi Y., Sistu P. and Bequette B. (1993). Control relevant dynamic data reconciliation and parameter estimation. *Computers & Chemical Engineering*, **17**, 41–59.

Reagan M. T., Najm H. N., Ghanem R. G. and Knio O. M. (2003). Uncertainty quantification in reacting flow simulations through non-intrusive spectral projection. *Combustion and Flame*, **132**, 45–55.

Reagan M. T., Najm H. N., Debusschere B. J., Le Maître O. P., Knio O. M. and Ghanem R. G. (2004). Spectral stochastic uncertainty quantification in chemical systems. *Combustion Theory and Modeling*, **8**, 607–632.

Reagan M. T., Najm H. N., Pébay P. P., Knio O. M. and Ghanem R. G. (2005). Quantifying uncertainty in chemical systems modeling. *International Journal of Chemical Kinetics*, **37**(6), 368–382.

Romanenko A., Santos L. O. and Afonso P. A. F. N. A. (2004). Unscented Kalman filtering of a simulated pH system. *Industrial & Engineering Chemistry Research*, **43**(23), 7531–7538.

Rooney W. C. and Biegler L. T. (2003). Optimal process design with model parameter uncertainty and process variability. *AIChE Journal*, **49**(2), 438–448.

Roweiss S and Ghahramani Z. (1999). A unifying review of linear Gaussian models. *Neural Computation*, **11**, 305–345.

Sahinidis N. V. (2004). Optimization under uncertainty: state-of-the-art and opportunities. *Computers and Chemical Engineering*, **28**, 971–983.

Sin G., Meyer A and Gernaey K. V. (2010). Assessing reliability of cellulose hydrolysis models to support biofuel process design – identifiability and uncertainty analysis. *Computers and Chemical Engineering*, **34**, 1385–1392.

Skogestad S. and Postlethwaite I. (1996). Multivariate Feedback Control. John Wiley & Sons, NJ, USA.

Skogestad S., Morari M. and Doyle J. C. (1988) Robust control of ill-conditioned plants: high-purity distillation. *IEEE Transactions on Automatic Control*, **33**, 1092–1105.

Song J., Stephanopoulos G. and Green W. H. (2002). Valid parameter range analyses for chemical reaction kinetic models. *Chemical Engineering Science*, **57**, 4475–4491.

Teixeira B. O. S., Torres L. A. B., Aguirre L. A. and Bernstein D. S. (2010). On unscented Kalman filtering with state interval constraints. *Journal of Process Control*, **20**, pp. 45–57.

Tintner G. (1955). Stochastic linear programming with applications to agricultural economics. In: Proceedings of the Second Symposium in Linear Programming, H. A. Antosiewicz (ed.), National Bureau of Standards, Washington, DC, pp. 197–228.

Vachhani P., Rengaswamy R. and Venkatasubramanian V. (2001). A framework for integrating diagnostic knowledge with nonlinear optimization for data reconciliation and parameter estimation in dynamic systems. *Chemical Engineering. Science*, **56**, 2133–2148.

Vásquez V. R. and Whiting W. B. (2000). Uncertainty and sensitivity analysis of thermodynamic models using equal probability sampling (EPS). *Computers & Chemical Engineering*, **23**, 1825–1838.

Vásquez V. R., Whiting W. B. and Meerschaert M. M. (2010). Confidence interval estimation under the presence of non-Gaussian random errors: applications to uncertainty analysis of chemical processes and simulation. *Computers & Chemical Engineering*, **34**, 298–305.

Wan E. A. and Van der Merwe R. (2000). The unscented Kalman filter for nonlinear estimation. *Proceedings Symposium. Adaptive Systems Signal Processing Communications and Control*. Lake Louise, AB, Canada, October 2000.

Wu F. and Tsang Y. (2004). Second-order Monte Carlo uncertainty/variability analysis using correlated model parameters: application to salmonid embryo survival risk assessment. *Ecological Modelling*, **177**, 393–414.

Xiu D. and Karniadakis G. E. (2002). The Wiener–Askey polynomial chaos for stochastic differential equations. *SIAM Journal on Scientific Computing*, **24**(2), 619–644.

You F. and Grossmann I. E. (2010). Integrated multi-echelon supply chain design with inventories under uncertainty: MINLP models, computational strategies. *AIChE Journal*, **56**(2), 419–439.

You F., Wassick J. M. and Grossmann I. E. (2009). Risk management for a global supply chain planning under uncertainty: models and algorithms. *AIChE Journal*, **55**(4), 931–945.

References for uncertainty analysis in hydrogeological engineering

Beven K. J. (2006). A manifesto for the equifinality thesis. *Journal of Hydrology*, **320**, 18–36.

Beven K. and Binley A. (1992). The future of distributed models – model calibration and uncertainty prediction. *Hydrological Processes*, **6**(3), 279–298.

Beven K. and Freer J. (2001). Equifinality, data assimilation, and uncertainty estimation in mechanistic modelling of complex environmental systems using the GLUE methodology. *Journal of Hydrology*, **249**, 11–29.

Beven K. and Young P. (2003). Comment on 'Bayesian recursive parameter estimation for hydrologic models' by M. Thiemann, M. Trosset, H. Gupta and S. Sorooshian, *Water Resources Research*, **39**(5), Article Number: 1116, Com 1-4.

Hassan A., Bekhit H. and Chapman J. (2008). Uncertainty assessment of a stochastic groundwater flow model using GLUE analysis. *Journal of Hydrology*, **362**, 89–109.

O'Hagan A. and Oakley J. E. (2004). Probability is perfect, but we can't elicit it perfectly. *Reliability Engineering and System Safety*, **85**(1–3), 239–248.

Rao C. V. and Rawlings J. B. (2002). Constrained process monitoring: Moving-Horizon approach. *AIChE Journal*, **48** (1), 97–109. DOI: 10.1002/aic.690480111.

Rao C. V., Rawlings J. B. and Mayne D. Q. (2003). Constrained State Estimation for Nonlinear Discrete-Time Systems: Stability and Moving Horizon Approximations. *IEEE Trans. on Auto. Cont*, **48**(2), 246–257.

Refsgaard J. (2006). A framework for dealing with uncertainty due to model structure error. *Advances in Water Resources*, **29**, 1586–1597.

Rojas R., Feyen L. and Dassargues A. (2008). Conceptual model uncertainty in groundwater modelling: Combining generalised likelihood uncertainty estimation and Bayesian model averaging. *Water Resources Research*, **44** (12), 16, Article W12418.

Rojas R., Samalie K., Peeters L., Batelaan O., Feyen L. and Dassargues A. (2010). Application of a multimodel approach to account for conceptual model and scenario uncertainty in groundwater modelling. *Journal of Hydrology*, **394**, 416–435.

Tørvi H. and Hertzberg T. (1998). Methods for evaluating uncertainties in dynamic simulation – A comparison of performance. *Computers & Chemical Engineering*, **22**, Supplement 1, 15, S985–S988.