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Conversion of Deterministic Models into Stochastic Models

Approach and three worked out examples as guidance for application of data assimilation

Report

December, 2005
Conversion of Deterministic Models into Stochastic Models

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1 Introduction

1.1 Data assimilation

In the present document, the concept of data assimilation is used in the sense of structured combination of values from a numerical model simulation and observations. This integration of model and data is realised by mathematical techniques in such a way, that the quality of the desired result is enhanced. Examples of data assimilation are model calibration to improve the model representation, or forms of filtering to improve operational forecast information.

Rijkswaterstaat is realizing a problem solving environment in which data assimilation tools can be combined with process models through generic and flexible interfaces in the COSTA project within Technical University of Delft.

Delft Hydraulics is developing a generic data assimilation toolbox DATools, which can be used in combination with all major Delft Hydraulics’ process models, through OpenMI coupling or through the so-called Published Interface within FEWS. Rijkswaterstaat and Delft Hydraulics have decided to work closely together on these developments. The anticipated advantages are improved design of both developments, opportunities to exchange and test each others modules and overall increased efficiency during the development cycle. The present document is one of the spin-offs of the cooperation.

1.2 Stochastic modelling and uncertainties

Flow models, models for transport and spreading, models for wave propagation and rainfall runoff models are well known numerical models of geophysical processes. By their nature, models provide schematic representations of the real world. They focus on and represent those phenomena of the real world that are of specific practical interest, characterised by associated temporal and spatial scales of interest. These models therefore by nature contain approximations, which are often formulated as “errors” or “uncertainties”. These occur in the model concept as such, in the various model parameters, the driving forces, and in the modelling result. A model uncertainty of general nature is associated with the representativity of model results for observed entities. Equally, field measurements or observations also suffer from errors or uncertainties. These may be the result of equipment (in)accuracy, instrument drift, equipment fouling or malfunctioning, sampling frequency, data processing and interpretation, and other.

The application of structured data assimilation techniques essentially makes use of the statistical characteristics of the errors or uncertainties in the model and in the data. By prescribing known (or assumed) uncertainties, their propagation through the model in time is calculated. The better the uncertainty characteristics of the various parameters, data series, etc. are known, the more accurate and effective the data assimilation technique can be in estimating the desired result and optimising the errors and/or uncertainty in that estimate.
By introducing uncertainties on the deterministic equations for the model the model is converted into a so-called stochastic model. The data assimilation procedures use these new stochastic equations in order to derive the desired optimal result by suitable combination.

1.3 Objective of the present document

The objective of the present document is to provide the users of COSTA with the necessary background understanding on the approach how to convert deterministic models into stochastic ones. It is intended as a guidance for modellers using COSTA and DATools. This methodology will be illustrated on two simple cases and a more complex one, each describing a different field of process modelling. In Chapter 2, the various concepts will be introduced and the approach will be illustrated on a one-dimensional advection diffusion equation. This chapter is the most extensive one, going into much detail on the considerations, physical meanings and other relevant points regarding uncertainties and stochastic modelling. Much of this is generic and relevant for the other cases as well. In Chapter 3, an example will be shown for a rainfall-runoff model. For this, the HBV-96 model is chosen, which is widely used among hydrologists in Europe. Finally, in Chapter 4 the case of a real life Sobek flow application is illustrated. Given the extensive generic treatment of the first case, the other two cases focus more on the details of their particular cases.

For each example it is shown how the model needs to be adapted in order to anticipate on uncertainties and to enable a combination of model and observations by means of (sequential) data assimilation procedures.

Important issues for all are the identification or selection of uncertain parameters and their stochastic representation by prescription of suitable noise for these uncertainties. Each case is worked out including the mathematical formulae.

The uncertainty aspects that are generic for all applications and examples are presented in a rigorous mathematical treatment in an Appendix.

1.4 Status of the present document

The present document presents a guidance for users of data assimilation tools on the aspects that are associated with uncertainties and the transformation of a deterministic model into a stochastic model. Besides a rigorous mathematical treatment of uncertainty issues, the document presents three relatively simple examples, each describing a different process model and relevant application field.

The document is intended as a living document – an extended or improved version should be made to incorporate growing insight based on further experience with practical applications of the data assimilation software environment and tools.
2 One dimensional-advection dispersion models

2.1 Physical problem description

Transport of dissolved or suspended matter is an important issue in the modelling of water systems such as ground water basins, and surface waters as for example rivers, lakes, estuaries, and seas. As typical examples of transports in water systems the dispersion of salt, suspended sediment and all kind of other contaminants or pollutants can be mentioned. Apart from these ‘material’ quantities, the transport can also refer to ‘substances’ such as heat or temperature, or turbulent kinetic energy.

As important and well known examples of such 1D model systems SOBEK or ZWENDL can be mentioned. ZWENDL (Zout- en Waterbeweging Eén-Dimensionaal) is a former 1D model system of Rijkswaterstaat, which in the past was frequently applied for the prediction of flows and salt intrusion in the Rhine-Meuse Estuary.

Transports refer to the temporal evolution of a spatial distribution of matter. In physical terms this distribution is usually represented by a concentration expressing the amount of mass per unit volume (i.e. in $kg/m^3$). The temporal evolution of a concentration distribution (and more specifically the total mass in a system) can be affected by several factors, both internally, and externally. These factors consist of the flow induced displacement and spread of a substance as well as chemical reactions, physical decay or bio-degradation, external loads, etc, that affect the total mass.

A quantitative analysis, description, or mathematical modelling of transports is often based on so called advection-dispersion equations (ADE). These have the form of partial differential equations. The terms in these relations reflect the transport mechanisms that are involved as e.g. displacement of substance induced by the (mean) flow, and diffusive (dispersive) transport due to spatial concentration gradients. By means of one or more other terms (source-sink terms) other mechanisms can be included that affect the mass balance in a non-conservative way.

In this chapter we will restrict the analysis to ADE in one dimension (1D, with regard to the spatial coordinate) and in later sections of this chapter the mathematical formulation will be presented. Comments will be formulated with regard to the physical meaning and interpretation of (the terms in) such a 1D ADE, as well as its applicability in practice. This applicability is highly related to the underlying assumptions and uncertainties in the model. Below, these uncertainties will be considered in further detail, and an important topic will be how to deal with these in practical applications, especially when applying (sequential) data assimilation techniques.
2.2 The deterministic model

2.2.1 The conceptual model and model parameters

We restrict ourselves to advection-dispersion equations (ADE) as often implemented in one dimensional model systems for flows and transports in water systems.

In continuous temporal and spatial coordinates, \( t \) and \( x \), the mathematical formulation of a 1D ADE reads:

\[
\frac{\partial (A \cdot c)}{\partial t} + \frac{\partial (Q \cdot c)}{\partial x} = \frac{\partial}{\partial x} \left( E \cdot A \cdot \frac{\partial c}{\partial x} \right) + S \tag{2.1}
\]

In the remainder this mathematical formulation of a 1D ADE will also be referred to as the conceptual model for 1D transport processes.

In equation 2.1 the term \( \frac{\partial (A \cdot c)}{\partial t} \) is associated to the storage of mass, and \( \frac{\partial (Q \cdot c)}{\partial x} \) is an advection term. The term \( \frac{\partial}{\partial x} \left( E \cdot A \cdot \frac{\partial c}{\partial x} \right) \) represents the dispersion of the substance. While the storage and advection determine the displacement of the peak of a “patch”, the dispersion governs the temporal increase of its size (see Section 2.2.4 where this is illustrated by means of an analytical solution of the ADE).

\( S(\cdot) \) represents the effect of all processes that affect the total mass in the system. It consists of one or more source or sink terms, and/or other external system inputs or forcing.

The physical meaning and SI-units of the several symbols in equation 2.1 are as follows. \( c(\cdot) \) is the concentration of a substance in \( \text{kg} / \text{m}^3 \), \( A(\cdot) \) denotes the cross-section area in \( \text{m}^2 \), \( Q(\cdot) \) is the flow discharge in \( \text{m}^3 / \text{s} \), and \( E(\cdot) \) represents the dispersion coefficient in \( \text{m}^2 / \text{s} \). In general all these quantities are neither constant (in time) nor uniform (in the spatial direction), and can depend on both \( t \) and \( x \). For a further illustration of source (or sink) terms \( S(\cdot) \) three examples are mentioned:

1. \[ S(x,t) = -\gamma(x,t) \cdot A(x,t) \cdot c(x,t) \] (2.2)
   This represents the case of an exponential decay of dissolved matter, where the disappearance of the substance (caused by chemical reactions, biodegradation or consumption) occurs at a rate that is proportional to the concentration.

2. \[ S(x,t) = q_0(x,t) \cdot c_0(x,t) \] (2.3)
   This formulation of \( S(\cdot) \) represents an external load to the system, here in the form of a lateral discharge \( q_0(\cdot) \) with a concentration \( c_0(\cdot) \) (in \( \text{m}^3 / \text{s} \)) of the substance. Note that the \( q_0(\cdot) \) (\( q_0(\cdot) \geq 0 \), and in \( \text{m}^2 / \text{s} \)) is actually a discharge per unit length, and thus represents a discharge density. In this case of an external ‘forcing’ the source term \( S(\cdot) \) does not depend on the system’s concentration distribution.
3. \[ S(x,t) = -q_0(x,t) \cdot c(x,t) \quad (2.4) \]

This formulation deals with the case that discharges are extracted from the system (with a discharge density \( q_0(t) \geq 0 \), in \( m^2/s \)) and through this extraction of water mass of the substance is also lost.

In practical applications of ADE-models the cross section area \( A(\cdot) \) and discharge \( Q(\cdot) \) are usually provided by a numerical flow model (or must be available or prescribed in another way). When the density of the substance does not affect the flow the ADE can be solved ‘stand alone’. In the other case the ADE and the flow equations (momentum and continuity equations) are coupled and should be solved simultaneously. It must then be realised that the initialisation of the other coefficients in the ADE (\( E(\cdot) \) and \( S(\cdot) \)) may affect the flow. Via the flow quantities \( A(\cdot) \) and \( Q(\cdot) \) this may again induce ‘secondary’ effects on the transport as computed by the ADE.

In practice one dimensional flow and transport models are sometimes applied to water systems that geometrically have the form of a network of 1D river branches. The Rhine-Meuse estuary can be mentioned as a characteristic example, see Figure 1 for an illustration of this delta region with the most important river branches. For such networks the model of equation 2.1 is then applied for each branch, and at the junction points of two or more branches appropriate ‘internal boundary or “coupling” conditions’ must be prescribed.

In the next sections some other practical issues about the modelling, applications, and interpretation of ADE will be formulated. In the remainder we will restrict to only one substance, and source and sink terms will also no longer be considered.

Figure 1 Rhine-Meuse delta, a water system that is often modelled as a network of 1D river branches

Figure 2.1 Rhine-Meuse delta region
2.2.2 Boundary conditions and model forcing

Appropriate initial and boundary conditions must be provided to obtain a solution of the ADE on some spatial domain \([X_1, X_2]\) and time interval \([T_0, T]\), respectively.

As a matter of the mathematical properties of an ADE (a parabolic partial differential equation) two boundary conditions must be prescribed. Boundary conditions describe how the concentration in the model connects to that just outside the modelled area, e.g. the interaction between the concentration in the non-modelled area and the modelled area. Usually this is done by assigning one of these to the boundary at \(X_1\) and the other at \(X_2\). The \(X_1\) and \(X_2\) may e.g. represent the downstream and upstream boundary of an estuary. When dealing with salt intrusion the boundary condition at \(X_2\) can be prescribed by means of a time series \(c(X_2, \cdot)\). In case \(X_2\) is sufficiently far away from the sea-river interface this \(c(X_2, \cdot)\) may be constant (and equal to the salinity background level) or even zero. For the downstream boundary \(X_1\), which may be situated at the mouth of the river, a boundary condition in the form of a time series \(c(X_1, \cdot)\) may also be possible when dealing with a historic period and an observed/measured salinity series \(\tilde{c}(\cdot)|_{X_2}\) is available. Otherwise other forms of boundary conditions must be constructed, and often so called weak forms of boundary conditions are prescribed. In mathematical terms these are formulated as \(\frac{\partial c}{\partial X_{1\to X_2}} = 0\) (no dispersive transport over the boundary at \(X_1\)) or \(\frac{\partial^2 c}{\partial X^2}|_{X_2} = 0\) (linear extrapolation of a spatial concentration profile over the boundary). In other cases combinations of strong and weak boundary conditions may even be applied. The so called Thatcher-Harleman formulation serves as an important example commonly used for salt intrusion. See Paragraph 2.2.3.4 below for further details.

For the initial condition a concentration profile \(c(X_1, t_0)|_{X_1 \leq x \leq X_2}\) must be prescribed. In practice such an initial system state is often not available, however. In that case use can be made of the property that the initial state in an ADE is transient and after some time the distribution of the concentration is completely determined by the boundary conditions. This suggests a start of the computation at a time \(t_0\) that is sufficiently long before the time interval of interest, allowing for “a spin up” of the model to dynamic equilibrium.

Finally it must be remarked that a model forcing must also be supplied in case of external system inputs. See for example the case of an external load by means of a lateral discharge as formulated in equation 2.3.

2.2.3 Examples of parameterisations/formulations in ADE

For practical applications of the ADE proper formulations must be available for the dispersion coefficient, initial and boundary conditions, and the model’s forcing. Often these formulations are based on parameterisations of these coefficients. In this section this is illustrated by means of a few examples.
2.2.3.1 Constant/uniform dispersion coefficient

The dispersion coefficient $E(\cdot)$ is sometimes assumed to be independent of time and uniform over the spatial domain. In a formula:

$$E(x,t|\Theta) = \Theta \quad (2.5)$$

The $\Theta$ is a univariate constant parameter that must be non-negative. This parameterisation will make sense for isotropic and stationary dispersion processes only.

2.2.3.2 Spatially varying dispersion coefficients

The dispersion coefficient is assumed to be independent of time, but may vary as function of the spatial coordinate. This spatial dependency is modelled with a one or more parameters $\Theta$. A typical example is the case where the flow and ADE-model are defined on a branched 1D network, and where the dispersion coefficient is set uniform and constant per branch. For different branches this constant may be different. In a formula: $\Theta = (\Theta_1, \Theta_2, \ldots, \Theta_L)$ and $E(x,t|\Theta) = \Theta_\ell$ for all (nodes) $x$ on the $\ell$-th branch of the network. The parameterisation may be further generalised or refined by defining a linear or polynomial profile for $E(\cdot)$ along a branch. Alternatively the number of parameters can be reduced by restricting the parameterisation to parts of the network only.

2.2.3.3 Thatcher-Harleman based formulations of the dispersion coefficient

Here some examples of dispersion coefficients are given that in the past have been proposed within the (numerical) modelling of unsteady salinity intrusion in estuaries. In this case the parameterisation $E(\cdot|\Theta)$ includes geometric properties of the estuary as well as features of the tidal flow. As a “basic” formulation the one of Thatcher and Harleman (1972) can be mentioned:

$$E(x,t|\Theta) = \Theta_1 \cdot u^*_0 \cdot L_0 \cdot E^{-\frac{1}{2}} \cdot \frac{\partial s^*}{\partial x} + \Theta_2 \quad (2.6)$$

The scaled salinity concentration $s^*$ and scaled spatial coordinate $x^*$ are defined by $s^* := s/s_0$ (with $s_0$ the salinity concentration at the sea boundary) and $x^* := x/L_0$ (with $L_0$ the characteristic length of the estuary). $u^*_0$ is a characteristic flood velocity at the mouth of the estuary, while $E$ is the estuary number.

The parameter $\Theta_1$ is a scale parameter with regard to the effect of concentration gradient on the dispersion rate, while $\Theta_2$ represent a Taylor type dispersion coefficient that is important in the parts of the estuary where concentration gradients are absent or less prominent.

In the former 1D salt intrusion model ZWENDL of Rijkswaterstaat several alternatives and extensions of equation 2.6 have been implemented and verified. One of these is mentioned as an illustration:
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\[ E(x,t|\Theta) = \Theta_1 \cdot \frac{u_0^* \cdot L_0^2}{c_0} \cdot \left[ T \cdot g \cdot h_0 \cdot \varepsilon \right]^{\frac{1}{2}} \cdot \left[ \frac{Q_f}{P_1 \cdot u_0^*} \right]^{\frac{1}{2}} \cdot \frac{\partial c}{\partial t} + \frac{\partial^2 c}{\partial x^2} + \Theta_2 \cdot h_1 \cdot \frac{\sqrt{g}}{C} \cdot |u_1| + \Theta_3 \]  

(2.7)

The individual terms and symbols in this formula represent several flow and concentration characteristics as well as geophysical properties of the estuary. Important flow parameters are for example the \( u_0^* \) and \( u_0 \) (the characteristic and maximum flood velocity at the mouth of the estuary), \( u \) (the local velocity at position \( x \) and time \( t \)), \( h_0 \) and \( h_1 \) (water depth at the mouth of the estuary, and the local water depth), \( P_f \) (flood volume) and \( Q_f \) (the river’s fresh water discharge). \( c_0 \) and \( c_x \) are the concentration at the sea boundary and its local value, respectively. The symbol “\( \varepsilon \)” denotes a temporal averaging of these quantities over two preceding tidal cycles. The \( \varepsilon \) is the relative difference of the water density at sea and at the river (in ZWENDL and for the Rhine Meuse estuary \( \varepsilon = 0.023 \)). We note that this \( \varepsilon \) is also related to the concentration distribution. \( L_0 \) (characteristic estuary length) and \( T \) (tidal period, which can be seen as a characteristic time scale in estuarine processes) are typical examples of geophysical parameters representing the dominant length and time scales in the physical process. The Chézy bed roughness coefficient \( C \) can also be seen as a geophysical characteristic of the estuary.

Clearly the first term in the right hand side of equation 2.7 (i.e. the part scaled by a calibration parameter \( \Theta_1 \)) is highly relevant near the sea-river interface where the highest concentration and concentration gradients will be present. The second term (scaled by a calibration parameter \( \Theta_2 \)) is fully flow dominated, and independent of the actual concentration distribution. The third term can be seen as a background dispersion level, which in combination with the second term determines the amount of dispersion in the upstream, fresh water region of the estuary or river. As a result of all these terms the total dispersion coefficient will decrease in magnitude in the upstream direction. For an impression of these magnitudes in practice the following can be mentioned for salt intrusion in the Rhine Meuse estuary. On the basis of concentration measurements dispersion coefficient values of about 1000-2000 \( m^2/s \) were reported in (Rijkswaterstaat, 1985a) for the Nieuwe Waterweg (i.e. near the downstream boundary of the estuary). Upstream, in the fresh river area, the magnitude is about 50 \( m^2/s \). It must be noted, however, that this value for the fresh region is based on calibration experiments with the 1D model ZWENDL, rather than ‘directly’ derived from observations (Rijkswaterstaat, 1985b).

For further details and motivation of the dispersion coefficient of equation 2.7 one is referred to (Rijkswaterstaat, 1985b). We merely want to emphasize that physically based formulations can be highly complex, and may contain several (uncertain or calibration) parameters. Moreover, such formulations can lead to dispersion coefficients that depend on time and on the spatial coordinate.
2.2.3.4 Example of a parameterisation of a downstream boundary in salt intrusion

When applying 1D ADE-models for salt intrusion in estuaries, the downstream boundary condition is often uncertain. The main source of uncertainty is the salinity of the water that was discharged before during ebb, and which now re-enters during flood tide. Immediately after low water slack (LWSK) the salinity concentration of this water may then be significantly smaller than the (maximum flood) concentration at sea. Within the modelling the salinity concentration of this ‘external’ water re-entering the estuary (at the model’s boundary) is not known, and a proper formulation must be constructed. To obtain a temporally continuous boundary condition around LWSK a Thatcher-Harleman condition is often applied (Thatcher and Harleman, 1972). In this formulation a return time (or time scale) \( T_0 \) is introduced, for which the model remembers the outflow concentration at LWSK. With \( c_{LWSK} \) the (computed) salinity concentration at \( t_{LWSK} \), and \( c_{Max} \) a maximum flood concentration that is assumed to be ‘recovered’ at \( t_{LWSK} + T_0 \), the salinity is prescribed by a half-cosine profile according to:

\[
c(t) = c_{LWSK} + (c_{Max} - c_{LWSK}) \cdot \frac{1}{2} \left(1 + \cos \left( \pi \cdot \left(1 + \frac{t - t_{LWSK}}{T_0}\right) \right) \right) \quad \text{for} \quad t_{LWSK} \leq t \leq t_{LWSK} + T_0
\]  

(2.8)

Next, i.e. for \( t > t_{LWSK} + T_0 \), the concentration is assumed to remain maximal, \( c_{Max} \), until the time \( t_{HWSK} \) of the next high water slack:

\[
c(t) = c_{Max} \quad \text{for} \quad t_{LWSK} + T_0 < t \leq t_{HWSK},
\]  

(2.9)

Finally a weak form of boundary condition is prescribed during outflow (the ebb phase) which actually is in a form of no dispersive salinity transport across the boundary:

\[
\frac{\partial^2 c}{\partial x^2} = 0 \quad \text{for} \quad t_{LWSK} \leq t \leq t_{LWSK} + T_0
\]  

(2.10)

Clearly this formulation of the boundary condition contains uncertain parameters as for example the return time \( T_0 \) and the maximum concentration \( c_{Max} \). In fact, while for \( T_0 \) it may be reasonable to assume that it is a (unknown) system constant, the \( c_{Max} \) can be highly variable as it will depend on dynamic conditions such as tide, meteorological forcing, and the river’s fresh water discharge. These conditions may contain several non-stationarities, for example seasonal or other quasi-periodic behaviour, or even long term trends.

2.2.4 Notes on the physical interpretation of the model

To obtain a fair idea of the (physical) effect of the coefficients in the ADE of equation 2.1 on the temporal evolution of the spatial distribution of a dissolved substance a special case is considered that provides an analytical solution for \( c(\cdot) \). Such an analytical solution is available when the flow and dispersion coefficients \( A(\cdot), Q(\cdot) \) and \( E(\cdot) \) are constant
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\((A_0, Q_0, E_0, \text{say})\), and an unbounded medium is considered (i.e. \(-\infty < x < \infty\), and \(c(\cdot) = 0\) at the boundaries). At time \(t = 0\) an instantaneous point emission of a total mass \(M_0\) takes place at location \(x = x_0\). In absence of external forcing the (analytical) solution of the ADE then reads:

\[
c(x,t) = \frac{M_0}{\sqrt{4\pi \cdot E_0 \cdot t}} \cdot \exp\left(\frac{-(x-x_0-u_0 \cdot t)^2}{4 \cdot E_0 \cdot t}\right), \quad t > 0
\]  

(2.11)

The \(u_0\) in this expression is defined by \(u_0 = \frac{Q_0}{A_0}\) and physically this quantity represents a constant flow velocity.

From equation 2.11 it can then easily be verified that at time \(t\) the concentration is maximal at \(x = x_0 + u_0 \cdot t\), while the spread of the concentration profile (after normalising it to a probability density distribution) is given by \(\sigma(t) = \sqrt{2 \cdot E \cdot t}\). Although ‘merely’ representing a very special case, these expressions provide a clear physical interpretation of the (effects of) the several components of an ADE. In fact, while the storage and advection determine the displacement of the peak of a “patch”, the dispersion governs the temporal increase of its size.

Returning to the general case, a few notes must still be formulated for a proper interpretation of the meaning of dispersion coefficients when dealing with 1D ADE models. It must be realised that dispersion coefficients \(E(\cdot)\) in ADE-models account for the mixing in the medium, which in particular can be induced by the flow. Turbulence processes are then often a main source of mixing. Turbulence is essentially a 3D process. When dealing with 1D ADE models their effect on the dispersion of a substance can merely be included in an approximate form, rather than in a physically and mathematically fully consistent, complete, and correct way. Therefore the dispersion coefficient in a 1D ADE is often not much better than a lumped or aggregate formulation of turbulence induced mixing.

Another issue in 1D modelling of transports (though somehow related to the preceding) is that formally the flow is assumed to be uniform over the vertical (“\(z\)”) and transversal (“\(y\)”) spatial directions (\(x\) represents the longitudinal spatial coordinate). In water systems, as e.g. estuaries with large stratification, a significant vertical shear may be present in the longitudinal velocity, however. In that case the displacement of a patch depends on the vertical position. Formally this dispersion can not be included appropriately in a 1D model. In an informal way this spread in the longitudinal direction induced by a vertical shear is nevertheless often included in the 1D model and usually this is done by means of an increased dispersion coefficient \(E(\cdot)\). This \(E(\cdot)\) must then again be understood as a lumped or aggregated coefficient.

For these reasons the parameterisation of the dispersion coefficient in 1D models is highly determined by (non-resolved) flow properties and molecular diffusion is hardly or not relevant. Clearly a dispersion coefficient will not be uniform, neither constant, and may depend in a complicated way on the flow properties. Because many 3D-effects may be absorbed in a 1D formulation it is evident that dispersion coefficients are one of the most prominent sources of uncertainty in ADE models.
2.3 Uncertainties in Advection Dispersion Equations

ADE are based on mass balances. To derive an ADE a control volume may be considered and for some time interval, \([t, t + \Delta t] \), the effects of inflows and outflows on the storage in the control volume are evaluated. The inflows and outflows are the actual transport and can be due to advection and dispersion (a transport induced by spatial gradients of the concentration). In this way ADE models have a sound physical basis. Nevertheless several uncertainties remain, and these are discussed below in further detail.

2.3.1 Main sources of uncertainty in ADE

2.3.1.1 “External”: the flow coefficients \(A(\cdot)\) and \(Q(\cdot)\)

The cross section area and discharge are often computed by a numerical 1D flow model as for example SOBEK. In case of density effects, where the concentration of the substance explicitly affects the flow, the equations for the flow and concentration are coupled and should be solved simultaneously. In any case, errors in the flow computation are “imported” in the ADE and thus it’s evaluation of the dispersion of a substance. These errors may degrade significantly the accuracy of the advective part of the transport. Unfortunately, within the actual ADE, little or nothing can be done to reduce these advective errors.

2.3.1.2 The dispersion coefficient \(E(\cdot)\)

The dispersion of a substance often depends on dynamic flow properties (turbulence, stratification, vertical shear of currents, etc.) and the dispersion coefficient \(E(\cdot)\) will not be uniform and neither constant. In practice many formulations have been proposed for flow dependent dispersion coefficients (e.g. salt intrusion, ZWENDL). Even with rather complex expressions for \(E(\cdot)\), the accuracy of the ADE model may still be limited. For this reason the dispersion coefficient can be a large source of uncertainty in ADE. It must be realised, however, that a main reason for this uncertainty may be the fact that a 1D model is applied to conditions where the flow properties are essentially 2D or even 3D.

2.3.1.3 Boundary conditions

Boundary conditions may also be an important source of uncertainty in modelling and predicting the spread of a substance using an ADE. As a typical example salt intrusion in an estuary can be mentioned. For the ADE’s boundary conditions must be prescribed downstream, at the mouth of the estuary, and at the upstream boundary nodes. Especially the downstream boundary conditions (i.e. at the sea-river interface) are difficult to deal with in salt intrusion models. One of the main problems is that at the beginning of a flood period the inflow from the sea partially consists of fresh water that was released by the river within the previous ebb-period. The concentration of this partly fresh water is formally unknown and must be modelled appropriately. This can be done by a so called Thatcher-Harleman formulation, see Paragraph 2.2.3.4. In such a formulation uncertainties remain, however, as will be the case in many other formulations.
2.3.2 Parameterisation of uncertainties

The coefficients listed above can depend on both the spatial and temporal coordinate. The same holds, of course, for the uncertainties in these coefficients. A mathematical description of these uncertainties may thus involve a large number of degrees of freedom. In practice a large number of uncertainties may not be meaningful since the amount of observations is usually too limited to identify all these. By means of parameterisations the amount of uncertainty can be reduced to a limited number of unknown model parameters $\Theta$. In Section 2.2.3 some examples were shown of parameterisations of the dispersion coefficient and boundary conditions. By considering these parameters as random variables rather than fixed constants, a model for the uncertainties in the coefficient or boundary condition is obtained automatically. Estimates of (parameterised) uncertainties can be obtained by means of model-calibration. Otherwise physical expert knowledge will be necessary to find a proper guess. In both cases uncertainties will remain, however.

Effectively, the preceding suggests that the parameters $\Theta$ can be seen as the uncertainties in the deterministic model. It will hardly ever be the case, however, that apart from these uncertain parameters the model is perfect. In fact, many assumptions that were made in the derivation of the conceptual model will not fully be satisfied in practical applications. These errors in the conceptual model (and/or additional errors induced by its discretisation to obtain a numerical model) are distributed over all model components (as e.g. the storage, advection and dispersion terms) and cannot easily be identified, let alone be described by separate parameterisations. Therefore such distributed errors can much more conveniently be represented by stochastic models. This will lead to an extension of the deterministic model to a stochastic model. This will be the issue of Section 2.4.

2.4 Stochastic modelling of uncertainties in ADE

In this section some notes and comments are formulated about the stochastic modelling of uncertainties in a one dimensional ADE. For the generic aspects of this, applicable to any process model, we refer to Appendix A. The general guidelines in Appendix A for the extension of deterministic (conceptual/numerical) models with stochastic processes to account for model uncertainties will be closely followed below. We recall that in this framework three levels are considered for model uncertainties. At the most elementary level uncertainties are assigned to ‘single’ parameters $\Theta$, which are treated as constants in the deterministic model. See Section 2.4.1. Secondly, in Section 2.4.2 uncertainties for distributed parameters will be considered. Such distributed parameters must be understood as model coefficients that can depend on time and the spatial coordinate. Thirdly, Section 2.4.3, uncertainties are assigned to the actual model, i.e. the state variables that are computed at some discrete time $t$, or the model’s equations that the state variables must satisfy.

As uncertain entities in the 1D ADE-model dispersion coefficients the coefficient $E(\cdot)$ and the model’s boundary condition $B(\cdot)$ will again be considered. In preparing to apply a sequential data assimilation procedure these coefficients will often be parameterised already so that we will formally write $E(\cdot | \Theta)$ and $B(\cdot | \Theta)$. 
A real life example (formulae and discussion) will be presented in Section 2.4.4 dealing with the modelling of uncertainties in the dispersion coefficient of an ADE-model for salt intrusion.

### 2.4.1 Stochastic modelling of uncertain model parameters

The idea behind a stochastic modelling of the parameters \( \Theta \) in a deterministic formulation of \( E(\cdot) \) and/or \( B(\cdot) \) is to extend (one or more of) these constants with a random function in time. See Section A.1 in Appendix A for the mathematical formulations. In this way we can account for temporal variability not resolved in the deterministic model.

For the dispersion these temporal variations may e.g. refer to sub-grid short term fluctuations originating from turbulence, density currents, entrainment, or other flow or wave induced mixing. Alternatively (quasi)periodic and or longer term non-stationary effects induced by tide or seasonal variability may be possible sources that require a (mild) temporal variation of the originally constant parameters \( \Theta \).

Errors or uncertainty in the deterministic prescription of a boundary condition may necessitate an extension of this quantity with random fluctuations. As an example the Thatcher-Harleman formulation can again be mentioned with \( \Theta \) the parameter \( c_{M} \) denoting the maximum salinity concentration at sea. This often not accurately known parameter need not be a constant and can depend on the recent history of freshwater outflows, and/or a non-uniform salinity distribution at sea, with in particular pronounced patches.

In adapting constant parameters \( \Theta \) there is an important difference for the dispersion coefficient and a boundary condition. While changes of a dispersion coefficient do not change the total mass in the system, mass can be lost or ‘imported’ when parameters are changed within the formulation of a boundary condition. This can readily be verified from the mathematical formulation of the conceptual model.

It must be noted that the present randomisation of uncertain parameters does not essentially affect the generic form of a dispersion coefficient or boundary condition. For example a Thatcher-Harleman parameterisation \( E(\cdot | \Theta) \) or \( B(\cdot | \Theta) \) is “conserved” (albeit with of time dependent random parameters) and the \( E(\cdot) \) or \( B(\cdot) \) cannot vary arbitrarily. In this way physical properties in these coefficients are more or less respected.

### 2.4.2 Stochastic modelling of uncertain model coefficients

For the stochastic modelling of uncertain coefficients in ADE the same issues and consequences can be mentioned as before when restricting to merely a few model parameters. There are a few other aspects that must also be considered with care, however. For dispersion coefficients a random noise may be added to the dispersion coefficient at any grid point of the numerical model. Formally these random processes may be independent (or at least different) for every grid point. This may lead to large gradients, and consequently to (too) large dispersive transports. Therefore, spatial correlation in the noises of different spatial positions is an important issue (see Section A.2 in Appendix A). Moreover, even when large spatial correlations are enforced the perturbations \( \delta E(\cdot) \) can exhibit a wide variety of spatial and temporal variations. A so adapted dispersion coefficient need not to be consistent anymore with an originally derived parameterisation \( E(\cdot | \Theta) \). In this way, physically based
deterministic formulations, as e.g. the one based on Thatcher Harleman, may not be respected anymore within the extended stochastic model. From a more global viewpoint, the stochastic model is not affected and is still of type ADE, however.

Similar issues hold for (random) uncertainties in a boundary condition. For example, the conditions \( \frac{\partial c}{\partial x} \bigg|_{x=X_1} = 0 \) or \( \frac{\partial^2 c}{\partial x^2} \bigg|_{x=X_1} = 0 \), used in a deterministic Thatcher Harleman formulation during outflow, will not be satisfied anymore when the uncertainty in the boundary condition \( c(\cdot) \bigg|_{x=X_1} \) is modelled by a random noise. The total mass in the system will neither be preserved.

### 2.4.3 Stochastic modelling of the state variables

In this case random noises are assigned to the concentrations predicted by the numerical model or, alternatively, to the state equations that these state variables must satisfy. Rather than localised in a few model parameters or coefficients, these noises now represent a lumped or aggregated representation of the model’s uncertainties. Clearly the concentrations are a distributed “parameter” and the stochastic models for the uncertainties in the state variables are very similar to those designed for model coefficients. See Section A.3 in Appendix A for further (mathematical) details and notes about the physical background.

Random noises are assigned to the concentration (or the model’s equation) at every spatial grid point. These noises can then be seen as a distributed external system load or force and the mass balance will be affected. By means of appropriate constraints to the noises (effectively: spatial correlations) a zero net mass change can be realised. This can be achieved, for example, by adding the uncertainties to the total mass flux in the ADE (i.e. the term \( Q \cdot c + E \cdot A \cdot \frac{\partial c}{\partial x} \) in the conceptual model). In case uncertainties are explicitly assigned to the state variables (i.e. the concentrations \( c(\cdot) \)) the algorithm for a mass conserving ensemble of noises will be less easy, however. Spatial correlation will also be required in case smoothness is required. This constraint tends to be much more important when the noise is assigned to a newly computed concentration distribution than when assigned to the model equations. The reason is that in the first case spatial derivatives (in the evaluation of both the advection and dispersion term) of the perturbed concentration are computed when on the basis of the model the concentration distribution is propagated forward in time. These derivatives may magnify the perturbations. Fortunately, as a result of the diffusive properties of an ADE these perturbations will gradually be smoothed. Although less strict, similar arguments can be formulated that reflect the smoothness of the random noises as function of time.

In case random uncertainties are assigned to both the state variables (or state equations) and a boundary condition, care must taken that these are defined in a consistent way.

### 2.4.4 Example of a stochastic model for the uncertainty in a dispersion coefficient

In this section the issues of Sections 2.4.1-2.4.3 are reconsidered but now more explicitly in the form of an example how a stochastic model for the uncertainty in a dispersion coefficient can be constructed in practice. This example is again inspired by salt intrusion in an estuary. We consider a 1D trajectory along the estuary that starts at the downstream boundary and via one or more branches ends at an upstream boundary. Taking the Rhine-Meuse estuary as an illustrative example from practice such a trajectory could be from Hoek van Holland to Tiel, following the path formed by the water ways Nieuwe Waterweg, Scheur, Nieuwe Maas,
Noord, Beneden Merwede, Waal. The spatial positions of the numerical grid (on which the
discretised ADE is solved) that are on this trajectory are denoted by \( x_i, x_2, x_3, \ldots, x_n, \ldots, x_N \)
(in ascending order, and with for example \( x_i \equiv \) Hoek van Holland, and \( x_N \equiv \) Tiel).

2.4.4.1 Stochastic model for the uncertainties in \( E(\cdot) \)

In the numerical ADE model the dispersion coefficient \( E(\cdot) \) can be written as a (discrete)
time dependent \( N \)-dimensional vector \( \tilde{E}_i \) with its \( n \)-th component representing \( E(x_n, t) \).
Following the generic approaches outlined in Appendix A, a stochastic model for the
uncertainty in the dispersion coefficient \( \tilde{E}_i \) may then be of the following form:

\[
\begin{align*}
\tilde{E}_i &= \tilde{E}_{i-1} + \tilde{Z}_i \\
\tilde{Z}_i &= A \cdot \tilde{Z}_{i-1} + \tilde{W}_i
\end{align*}
\]  

(2.12)

In order to obtain “convenient” (i.e. compact, explicit, and fully analytical) expressions for
the statistical properties of the uncertainty \( \tilde{Z}_i \) in \( \tilde{E}_i \, , \) and thus facilitate their interpretation
and directions how to set up the stochastic model of equation 2.12, a few (but non-essential)
additional assumptions are made:

1. \( \tilde{W}_i \) is a zero mean stationary white random noise (with regard to its temporal evolution)
meaning that \( E[\tilde{W}_i] = 0 \, , \) and \( E[\tilde{W}_i \cdot \tilde{W}_i^T] = 0 \) for times \( s \) and \( t \) when \( s \neq t \).
2. \( A \) is a diagonal matrix of the form \( A = a \cdot \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 \end{pmatrix} \) \) with \( |a| < 1 \).

On this basis the \( \tilde{Z}_i \) will be a stationary noise with zero mean as well, and its spatial and
temporal properties are now evaluated. When the covariance matrix of \( \tilde{W}_i \) is denoted by the
\( N \times N \) matrix \( \Gamma_0^{(W)} := E[\tilde{W}_i \cdot \tilde{W}_i^T] \) it can be shown that the covariance matrix
\( \Gamma_0^{(Z)} := E[\tilde{Z}_i \cdot \tilde{Z}_i^T] \) of the uncertainty \( \tilde{Z}_i \) of \( \tilde{E}_i \) satisfies:

\[
\Gamma_0^{(Z)} = \frac{1}{1-a^2} \cdot \Gamma_0^{(W)} \quad \iff \quad \Gamma_0^{(W)} = (1-a^2) \cdot \Gamma_0^{(Z)}
\]  

(2.13)

This \( N \times N \) covariance matrix \( \Gamma_0^{(Z)} \) represents the spatial properties of the uncertainty in the
dispersion coefficient. In fact, the diagonal entries of \( \Gamma_0^{(Z)} \) provide the variance of the noise
assigned to the dispersion coefficient (thus dealing with the “size”, or “magnitude”, or
“energy” of the uncertainty). In particular, the \( n \)-th diagonal entry corresponds to the variance
at spatial position \( x_n \) in the estuary. Similarly, the off-diagonal entries of covariance matrix
\( \Gamma_0^{(Z)} \) represent the mutual dependency of the noises for different spatial positions.
While covariance matrix $\Gamma_{0}^{(Z)}$ deals with the spatial distribution of the uncertainty in $\tilde{E}$, the temporal properties are characterised by the auto-covariance function $\Gamma_{\tau}^{(Z)}$ of $\tilde{Z}$, defined by $\Gamma_{\tau}^{(Z)} = E[\tilde{Z}_{t} \cdot \tilde{Z}_{t+\tau}^{T}]$. This $\Gamma_{\tau}^{(Z)}$ is again an $N \times N$ matrix, and for the present model it can be shown that it satisfies the following equation when expressed in the model parameters $a$ and $\Gamma_{0}^{(Z)}$:

$$
\Gamma_{\tau}^{(Z)} = \Gamma_{0}^{(Z)} \cdot a^{\tau} = \frac{1}{1-a^{2}} \cdot \Gamma_{0}^{(W)} \cdot a^{\tau} = \frac{1}{1-a^{2}} \cdot \Gamma_{0}^{(W)} \cdot \exp\left(\tau \cdot \ell n(a)\right)
$$

(2.14)

The $\tau$ is an integer time shift in units $\Delta t$ ($\Delta t$ is the time step in the discretised model). Equation 2.14 reveals that the $\tilde{Z}$ is not a white random noise and evolves in time with a memory. A measure for this temporal memory is the auto-correlation time $T_{AC}^{(Z)}$ which is the lag for which the auto-correlation is a fraction $\frac{1}{2}$ of its maximum at lag zero. In ‘physical’ time units this temporal memory is then:

$$
T_{AC}^{(Z)} = \frac{\Delta t}{\ell n(a)} \iff a = \exp\left(-\frac{\Delta t}{T_{AC}^{(Z)}}\right) \tag{2.15}
$$

When accepting this model for the uncertainty a proper choice must be made for the temporal memory (i.e. $T_{AC}^{(Z)}$) and spatial properties (i.e. $\Gamma_{0}^{(Z)}$). This will be the issue of the remainder of this section. At the moment that suitable (and consistent) estimates are indeed available for $T_{AC}^{(Z)}$ and $\Gamma_{0}^{(Z)}$, the right hand sides of equations 2.13 and 2.15 can be used to obtain the associated parameters $a$ and $\Gamma_{0}^{(W)}$ in the stochastic model of equation 2.12.

### 2.4.4.2 Estimate for $T_{AC}^{(Z)}$

When dealing with salt intrusion in an estuary the period $T_{Tide}$ of the (main component of the) tidal cycle represents a characteristic time scale and as long as other information is absent it will be reasonable to assume that the temporal memory in the uncertainties of the dispersion coefficient is of the same order. This suggests to choose $T_{AC}^{(Z)} = \varepsilon \cdot T_{Tide}$ with $\varepsilon$ in the range of 0.5 to 2.

### 2.4.4.3 Estimate for $\Gamma_{0}^{(Z)}$

For reasons of physical interpretation it is most convenient to follow a two step approach for the quantification of the spatial properties of the uncertainty. In the first step one may decide about the size of the uncertainty, and in the second step consider its spatial length scale. In more detail these two steps are worked out below.
Step 1. The first step involves a proper choice for the spread of the noise as function of the spatial coordinate. Actually this means that for every gridpoint \( x_n \) a (positive) spread \( \sigma_n \) must be defined. These spreads (or estimates for these) are preferably based on physical or expert knowledge. A reasonable way to do this is to relate these spreads to the characteristics of the (local) flow and concentration distribution, just as is commonly done in a Thatcher-Harleman based formulation of the dispersion coefficient when dealing with salt intrusion. For example, near the mouth of the estuary the largest dispersion will be found due to intensive sea-river interactions leading to non-uniform flows in both the horizontal and the vertical directions, large stratification effects, gravitation circulation, entrainment effects, etc. Due to all these complex processes significant errors may be expected in the (1D) model and particularly the formulation of the dispersion coefficient. Therefore the uncertainties will be much larger there than near the upstream boundary. This would suggest a spread \( \sigma_n \) that decreases in the upstream direction as function of the spatial coordinate \( x_n \). As an example, a recipe for \( \sigma_n \) could then be,

\[
\sigma_n = \sigma_{\text{Min}} + (\sigma_{\text{Max}} - \sigma_{\text{Min}}) \cdot \exp \left( -\frac{x_n}{\lambda_S} \right)
\]  

with the \( \sigma_{\text{Min}} \) a minimum spread for within the fresh water region, and \( \sigma_{\text{Max}} \) a maximum spread at the sea-river boundary. The \( \lambda_S \) represents a length scale and will be related to estuary’s salt intrusion length. As a practical example, for the Rhine-Meuse estuary the \( \sigma \) dispersion coefficient is in the order of 1000-2000 \( m^2/s \) at the mouth, and about 50 \( m^2/s \) in the fresh river parts. A fair estimate for \( \sigma_{\text{Max}} \) and \( \sigma_{\text{Max}} \) could then be 100 and 10 \( m^2/s \). The salt intrusion length \( \lambda_S \) may e.g. be taken as the distance of the downstream boundary to the upstream position where the maximum (or root mean square) concentration is about \( \frac{1}{e} \) of its (maximum) value at the mouth. For the Rhine-Meuse estuary a \( \lambda_S \) of 10 à 20 km could be realistic.

Finally, for later use an \( N \times N \) matrix \( S \) is defined that has the \( N \) spreads \( \sigma_n \) on its diagonal, while all the off diagonal entries are zero. In formula

\[
S := \begin{pmatrix}
\sigma_1 & 0 & \cdots & 0 \\
0 & \sigma_2 & \cdots & \vdots \\
\vdots & \ddots & \ddots & 0 \\
0 & \cdots & 0 & \sigma_N
\end{pmatrix}
\]

The diagonal entries \( \sigma_n \) can originate from the example of equation 2.16 but can also be the result of another choice of a spatially dependent spread.

Step 2. In the second step spatial length scales will be involved as well, but now with regard to the mutual dependency of the noises at different spatial positions \( x_n \) and \( x_m \). From the viewpoint of physical interpretation it will be most convenient to prescribe the dependency of
the noise components $W_i(x_n)$ and $W_j(x_m)$ by means of a correlation coefficient $\rho_{n,m}$ (with $-1 \leq \rho_{n,m} \leq 1$). All these correlation coefficients form an $N \times N$ matrix $R$ defined by:

$$R := 
\begin{pmatrix}
\rho_{1,1} & \rho_{1,2} & \cdots & \rho_{1,N} \\
\rho_{2,1} & \rho_{2,2} & \ddots & \vdots \\
\vdots & \ddots & \ddots & \rho_{N-1,N} \\
\rho_{N,1} & \cdots & \rho_{N,N-1} & \rho_{N,N}
\end{pmatrix}
$$

(2.18)

In practice the correlation coefficients $\rho_{n,m}$ are often modelled as a function of the distance $d_{n,m}$ of $x_n$ and $x_m$. This distance must be evaluated along the river’s trajectory, however, rather than in the standard geometrical way. With such a distance definition $d_{n,m} (= d_{m,n})$ a feasible parameterisation of the correlation coefficient can be

$$\rho_{n,m} = \exp \left( - \left( \frac{d_{n,m}}{\lambda_C} \right)^\nu \right)$$

(2.19a)

As an alternative example with a longer support of the spatial correlation the following prescription be mentioned:

$$\rho_{n,m} = \frac{1}{1 + \left( \frac{d_{n,m}}{\lambda_C} \right)^\nu}$$

(2.19b)

In order that these or alternative formulations define a well defined spatial correlation structure the $N \times N$ matrix $R$ must satisfy that all its diagonal entries $\left\{ \rho_{n,n} \right\}_{n=1}^N$ are equal to 1, and that $R$ is a symmetric positive definite matrix (meaning that all its eigenvalues are positive or at least non-negative). For this reason the shape parameter $\nu$ in equation 2.19 must be at least 1. Similar as the $\lambda_S$ above, the $\lambda_C$ in equation 2.18 can again be seen as a spatial length scale parameter. While the $\lambda_S$ is a length scale for the magnitude of the errors in the dispersion coefficient, the $\lambda_C$ represents a correlation length (“spatial memory”) of these errors. In many cases a $\lambda_C$ will be chosen that is equal to, or of the same order as, the salt intrusion length so that usually these two length scales will be not be significantly different after all.

On the basis of the so modelled spatial properties of the uncertainty, leading to the matrices $S$ (spreads) and $R$ (spatial correlation matrix) as defined in equations 2.17 and 2.19 the following result is than obtained for the desired covariance matrix $\Gamma_0^{(Z)}$

$$\Gamma_0^{(Z)} = S \cdot R \cdot S$$

(2.20)

The $(n,m)$-th entry of this $\Gamma_0^{(Z)}$ then reads:
2.4.5 Verification of the stochastic model

From the preceding it will be clear that several choices and/or assumptions must be made in the definition of the model for the uncertainties. Moreover, a high sensitivity may be present for the actual model area (different estuaries have different geometry, flow, and salt intrusion characteristics) and the associated system conditions (low or high river discharges, low or strong meteorological forcing), and the substance that is considered (salt, heat, suspended sediment, pollutants, etc.). Apart from this the quality of the deterministic model may have an effect in the sense that the higher this quality, the smaller the spreads and variances in the uncertainty model need to be.

For all these reasons it is recommended that in applications a proper verification of the stochastic model is carried out. Prior to data assimilation experiments this can be done by generating an ensemble of realisations of the dispersion coefficient, and an ensemble of the concentration distributions that follow according to the deterministic model. From these ensembles the statistics can be inspected, the amount of variation, extremes, correlation of the several quantities, etc., and the sensitivity of the concentration distributions for variations of the dispersion coefficient. On this basis a reasonable initial guess for the (range of the) several parameters (of the stochastic model, such as the temporal memory $T_{AC}$, and spatial properties induced by the covariance matrix $\Gamma_{0}^{(Z)}$) can be established already. If measurements are available the statistics of residuals (i.e. the difference of observed concentrations and their predictions by the deterministic model) can be used for a further improvement of the initial guesses.

Apart from these “theoretical” aspects it is worthwhile to verify critically the numerical aspects as well. These aspects are for example stability, accuracy and smoothness issues. Such a verification and/or sensitivity analysis must be done as well within subsequent data assimilation experiments. In such experiments the assimilated dispersion coefficient and/or concentration distributions can be analysed, as well as the hind cast estimates of the uncertainties in the model. It must then be assessed whether or not the statistical properties of these estimates for the uncertainties are in reasonable agreement with the stochastic model that was assumed. In case of significant differences the initial guesses should be corrected to obtain a better consistency. This step must possibly be repeated a few times. Actually this iterative procedure represents a calibration of the stochastic model.

2.5 Practical user aspects for ADE

Below a few issues are mentioned that must be considered with care in practical applications of ADE. These comments deal with the actual deterministic model, the parameterisation of model-coefficients, and the stochastic modelling of uncertainties. Both comments and warnings are included. The order of these comments is more or less arbitrary.

1. **Number of model parameters.** The larger the number of parameters $\Theta$ in the formulation $E(\cdot|\Theta)$ of a dispersion (or other uncertain) coefficient the better the spatial and temporal dependencies can be represented. On the other hand, however, sufficient observed data must be available to obtain well defined estimates for these parameters (both for a model calibration, and when applying sequential data assimilation procedures). For meaningful estimates the number of parameters should be small compared to the
amount of observations. Otherwise the estimates of the \( \Theta \) may be very sensitive for noise in the observations, or even inconsistent when the large number of degrees of freedom is ‘merely’ used for the modelling of systematic errors (i.e. spatial and/or temporal variations in the data that are not resolved in the actual model).

2. **Non-negative concentrations.** ADE are applied to predict concentrations. These must be positive or at least non-negative. While for the deterministic model this may be the case, care must be taken that the extended stochastic model also satisfies this constraint. This implies that the variations induced by the stochastic model should be bounded. In the definition of the stochastic models for the uncertainty in the concentration distribution (and/or a boundary condition) this can be achieved by choosing the spread of the random noises sufficiently small. Taking the spread as a small fraction of model’s prediction is another (and even better) possibility. This would represent a multiplicative formulation of the system noise.

3. **Non-negative dispersion coefficients.** Dispersion coefficients must be non-negative as well. In the deterministic and stochastic modelling of this coefficient the same issues must thus be considered as mentioned above for concentration distributions.

4. **Numerical aspects.** Apart from the above physical considerations the user must verify as well that constraints that originate from the numerical solution procedures (stability and accuracy requirements) are still satisfied.

5. **Flow induced errors.** In practice the flow coefficients \( A(\cdot) \) and \( Q(\cdot) \) are often obtained from a simulation of a numerical flow model. These flow coefficients may contain several uncertainties as well, which are then imported in the ADE leading to errors in the prediction of the advective transport. In the calibration or assimilation of the model using observed data, these errors in the advection may then lead to unrealistic/inconsistent estimates or corrections for dispersion coefficients and/or boundary conditions. For practice this means that a proper verification of the flow should be carried out first. This provides another argument that uncertainties in the transport model must be bounded to prevent that their estimates are a correction for advection errors, and thus without a physical meaning, that is, the predictive capability of the model is negatively affected.

6. **Non-identifiable temporal variability.** Within a parameterisation \( E(\cdot|\Theta) \) of a dispersion coefficient it must be realised that temporal dependencies cannot easily be identified. Only in case of high density concentration observations, which are consistent with the ADE model and not noisy, reasonable estimates may be found for parameters \( \Theta \) that are associated to temporal variations.

7. **Non-identifiable spatial variability** Similarly, a dispersion coefficient \( E(\cdot|\Theta) \) cannot be identified accurately at positions with low or absent concentration gradients in the observations.

8. **Smoothness constraints for dispersion coefficients.** Smoothness properties are an important issue for dispersion coefficients, especially in the spatial direction. Theoretically the relevance of this aspect can readily be verified from the term \( \frac{\partial E}{\partial x} \) that arises from the evaluation of the dispersive part \( \frac{\partial}{\partial x} \left( E \cdot A \frac{\partial c}{\partial x} \right) \) in the ADE’s conceptual model. On the other hand, from practical applications of numerical ADE models it is known that discontinuities in a dispersion coefficient can lead to large non-regular effects for the concentration distribution. Therefore smoothness properties must
carefully be verified, both within the deterministic formulation of a dispersion coefficient and within the stochastic modelling of its uncertainties.
3 The HBV-96 Rainfall Runoff model

3.1 Physical problem description

Catchment hydrological models are important tools in addressing a range of problems related to water resources assessment, development, and management. Catchment models simulate the water balance dynamics at the catchment scale. Processes as rainfall, evaporation, infiltration of water into the soil, groundwater flow, river runoff are typical ingredients of these catchment models. Because of the significance of water in terrestrial systems, catchment models are an integrated part of virtually all environmental models at the catchment scale. Their applications range from catchment water, reservoir management, climate studies, flood forecasting and, assessment of nutrient balances to providing water process dynamics to biophysical models. A large number of models have been developed, representing more or less accurately the main physical processes involved in the transformation of rainfall into runoff. Among these models are well known conceptual models such as the Sacramento model and HBV-96 model which are used in several flood forecasting systems worldwide.

3.2 The deterministic model

3.2.1 The conceptual model

The HBV-96 model is a conceptual quasi-distributed precipitation-runoff model. It calculates the runoff of a catchment or a series of catchments as the result of estimated precipitation on the catchment, taking into account catchment properties and intermediate processes. It was developed at the Swedish Meteorological and Hydrological Institute (SMHI) in the early 70s. As the HBV model is a conceptual model it describes the most important runoff generating processes with simple and robust structures. The following points give a short overview of the three main components in the model together with examples for related parameters:

3.2.1.1 Snow Routine

The precipitation is the initial input into the model. It can have the form of rainfall and snowfall. This process is ruled by a threshold temperature (parameter $tt$) below which precipitation is supposed to be snow; the transition from rain to snow can be realised continuously over a temperature interval (parameter $tti$). Snow melt computations are based on a day-degree relation (snow melt factor $cfmax$). The snow distribution is computed separately for different elevation and vegetation zones in the basin.

3.2.1.2 Soil Routine

This part of the model controls which part of precipitation forms excess water and how much water is evaporated or stored in the soil. The runoff coefficient depends on the ratio of actual soil moisture and the maximum water storage capacity of the soil (parameter $fc$) as well as an exponent representing drainage dynamics (parameter $beta$). The parameter $lp$ defines the
water storage in the soil at which actual evaporation starts to be equal to potential evaporation. Values of potential evaporation are required as input data and there is a special correction factor for evaporation in forest areas \((cevpfo)\). Interception in forest areas and open land can also be simulated (parameters \(icfo\) and \(icfi\)).

### 3.2.1.3 Runoff Generation Routine

This routine is the response function which transforms excess water from the soil routine to runoff. The routine consists of one upper, non-linear reservoir (parameters \(khq\), \(hq\) and \(alpha\)) and one lower, linear reservoir (recession coefficient \(k4\)). The upper one represents direct runoff. The lower reservoir represents the base flow which is fed by groundwater. Groundwater recharge is ruled by a maximum amount of water that is able to penetrate from soil to groundwater (parameter \(perc\)). Timing and distribution of the resulting runoff is further modified in a transformation function by means of a retention parameter (\(maxbas\)); this routine is a simple filter technique with a triangular distribution of the weights.

Figure 3.1 shows a schematic overview of the HBV-96 model. It shows how the model states denoted by \(S\) (\(S_{ic}\): interception storage, \(S_{snow}\): content of melt water in snow pack states (sp) & liquid water in snow pack (wc), \(S_{uz}\): upper zone, \(S_{lz}\): lower zone) are affected by the rainfall (\(P_{input}\), model forcing) and evapo-transpiration from the wet leaves (\(E_{ic}\)) and the soil (\(E_{act}\)). Finally, the water leaves the catchment as river runoff (\(Q_{fast}\), \(Q_{slow}\), \(Q_{out}\)). Above, below and alongside the arrows the parameters are displayed that affect the processes that occur.

### 3.2.2 Model forcing

Input data (model forcings) are observations of rainfall, air temperature and estimates of the potential evapo-transpiration. The time step is usually 1 day, but it is possible to use shorter time steps (one or several hours). The evaporation values are normally monthly averages although it is possible to use daily or hourly values. Air temperature data are used for calculations of snow accumulation and melt. It can also be used to adjust the potential evapo-transpiration when the temperature deviates from normal values, or to calculate potential evaporation.
Conversion of deterministic models into stochastic models

Figure 3.1. Simplified calculation scheme of the HBV model (Federal Institute of Hydrology (BfG), 2001) (for explanation see text).

\[ S_{\text{uz}} = \left( \frac{S_{\text{sm}}}{f_c} \right)^{\beta_{\text{sm}}} \cdot P_{\text{HBV}} \]

\[ S_{\text{uz}} = c_{\text{flex}} \]

\[ S_{\text{uu}} = \text{perc} \]

\[ S_{\text{uz}} = k_{\text{h}, q_{\text{h}}, \alpha} \]

\[ Q_{\text{fast}} = k \cdot (S_{\text{uz}})^{1-\alpha} \]

where \( k \) is computed of \( k_{\text{h}, q_{\text{h}}, \alpha} \)

\[ Q_{\text{slow}} = S_{\text{iz}} \cdot k^\alpha \]

\[ Q_{\text{out}} = S_{\text{iz}} \cdot k^\alpha \]

\[ S_{\text{snow}} = \text{cfmax} \cdot (t - t_t) \]

\[ P_{\text{HBV}} = P_{\text{input data}} \cdot p_{\text{corr}} \pm \Delta S_{\text{sen}} - \Delta S_{\text{el}} \]

\[ \Delta S_{\text{el}} = S_{\text{uz}} \cdot \text{Pfc} \]

\[ \Delta S_{\text{en}} = P_{\text{HBV}} - \Delta S_{\text{el}} \]

\[ \Delta S_{\text{iz}} = \text{perc} \] when \( S_{\text{iz}} = \text{perc} \)

\[ \Delta S_{\text{iz}} = S_{\text{iz}} \] when \( S_{\text{iz}} < \text{perc} \)
3.3 Uncertainties in the HBV-96 model

3.3.1 Main sources of uncertainties

3.3.1.1 Conceptual model

The most important issue is the representation of the physical reality. It is evident that a conceptual model such as HBV-96 has to make a large concession in this respect and it can be stated that the resemblance of the modelling of the processes in the model with the detailed processes in physical reality is limited. Nevertheless, in the aggregated sense of representing the key links of transforming precipitation into runoff, given the key catchment properties, these conceptual models are capable of reproducing the rainfall-runoff process at the spatial and temporal scales of interest very well. In other words, there is inevitable uncertainty associated with the simplistic soil, evaporation, snow, and runoff routines. Unfortunately, these uncertainties are difficult to quantify in detail.

3.3.1.2 Algorithmic implementation

In practice, the model algorithm and model structure can be also a source of uncertainties. However, as the implementation of these transfer-like functions does not involve complex discretisation approximations, it can be assumed that these type of uncertainties are smaller than uncertainties in the model concept and model parameters and therefore neglected.

3.3.1.3 Model empirical parameters

It is evident that for a hydrological rainfall-runoff model, and probably for most models, the impact of the choice of the model parameters has a large impact on the outcome of the modelling. The HBV model parameters are normally obtained after calibration/history matching. Errors in input, model structure and output can make the identification of model parameters complex. The uncertainty in the model parameters can be large.

3.3.1.4 Model domain parameters

Uncertainties can also occur due to the spatial and temporal aggregation level that is used. The division in sub-basins, altitude zones, soil groups and land use may vary with the application. One should be aware that these choices are not unique and therefore likely non-optimal, and therefore associated with uncertainties.

3.3.1.5 Model forcings

The errors in the model forcings such as rainfall, evaporation and temperature can be large. Uncertainties in the model forcings can have an effect (biased parameter estimates) on the calibrated model parameters if these uncertainties are not taken into account during model calibration (Willems, 2002 and reference therein). Evaporation is often not measured and is often estimated using very simple relationships or derived from monthly mean values and is therefore very uncertain. Rainfall uncertainty depends on the density of the rain gauge network and the type of interpolation used and is can be quite large (up to 50%). Temperature
can affect both evaporation and snow fall and melt. One can make the assumption that errors in temperature are relatively small compared to errors in rainfall. Errors in temperature measurements may have an influence on the amount of snowfall due to the choice of the altitude zones because of the temperature variation with altitude.

### 3.3.2 Parameterisation of uncertainties

For the parameterisation of model structural error we refer to Evensen (Evensen, 2003) and to Appendix A. The uncertainties of model parameters can be estimated during calibration. In hydrology, there are two major approaches for estimating the model parameter uncertainties by deriving parameter values that give overall better representation in some a priori defined criterion. These are the GLUE approach (Beven and Binley, 1992) and an MCMC approach (Thiemann et al., 2001; Vrugt et al., 2003).

Parameterisations for the model forcings are not widely available. Willems (Willems, 2002) is one of the few that parameterised the uncertainty of the rainfall. He found that conditional to the point rainfall estimates (\(X_p\)), the uncertainty of the spatially averaged rainfall \(X\) can be described using a lognormal distribution. It corresponds to a normal distribution for \(\ln(X/X_p)\):

\[
P\left( \ln \left( \frac{X}{X_p} \right) \mid X_p \right) \sim N\left( \mu_{\ln(X/X_p)} \mid X_p, \sigma_{\ln(X/X_p)} \mid X_p \right)
\]

(3.1)

where \(X_p\) denotes that everything is conditional to the value of \(X_p\) and the \(N\) denotes a normal distribution with mean

\[
\mu_{\ln(X/X_p)} \mid X_p = c_1 \exp(-X_p)
\]

(3.2)

and standard deviation

\[
\sigma_{\ln(X/X_p)} \mid X_p = \sqrt{c_2 + c_1 \exp(-X_p)}
\]

(3.3)

with \(c_1=1.2\) and \(c_2=0.2\) (Willems, 2002). Koster et al. (Koster et al., 2004) and Weerts and Serafy (Weerts and El Serafy, 2005) both used white noise to model the uncertainty in rainfall (using a standard deviation of \(0.15 P_{\text{measured}} + 0.02 \text{ mm}\)) and temperature (using a standard deviation of 2°C). Depending on the formulation of the evaporation (monthly mean, measured daily or hourly values) a parameterization can be chosen. Weerts and Serafy (2005) used a multiplicative error model since the evaporation was available in the form of monthly means. Koster et al. (2004) used an additive error model. However, the effect of the uncertainties in the evaporation showed little influence on the runoff compared to the effect of the uncertainties in the rainfall and those in the temperature. In both cases, the winter time was considered when the evaporation is low. Both parameterizations might be suitable in summer time when the evaporation error is more important.
3.4 Practical user aspects

3.4.1 Maxbas

In the deterministic HBV-96 model a smoothing parameter (maxbas) of the discharge per sub-basin is used. In practise, this parameter is used to ensure that occurrence of the modelled runoff peaks occur at the same time as the measured runoff peaks. Due to this parameter, the modelled discharge signal is also somewhat smoothed. A larger parameter value means a lower peak over a wider stretched base. Smoothing over fewer days may mean a high peak over a very short time. This smoothing over several hours can be an obstacle for the sequential data assimilation filters that require that the discharge process is a Markov process: state $x_n$ only depends on state $x_{n-1}$. Therefore, it is advised to set maxbas to zero and shift the rainfall instead.

3.4.2 Temperature

When the temperature is far below zero and precipitation occurs, this will fall as snow and will not reach the soil moisture stores or the upper and lower zone. During such a period a snow pack will form. Consequently, the discharge signal does not contain any information about the different amounts of snow that are fed into the model. Therefore, depending on what types of measurements are being assimilated the estimated build-up of the snow pack can be unrealistic. Obviously, measured snow pack information is required, in addition to the runoff measurements, for the filters to be able to account for snow fall as well. If this information is not available and discharge measurements are the only data to be assimilated, it is advised to limit the uncertainty of the rainfall during periods of frost to prevent an unrealistic build-up of a snowpack.

3.4.3 Correction factors

In the HBV-96 conceptual model several correction factors are defined (see paragraph 3.2.1). When applying sequential data assimilation the corrections are implicitly carried out through assimilation of measured data. Therefore, it is advised to set these correction factors to unity.

3.4.4 Physical and practical constraints

It is clear that limits to both the values of the model forcings and the model parameter exist. For the model forcings it is clear that the precipitation cannot be negative ($\leq 0$), the same applies to the evaporation ($\geq 0$). Table 3.1 provides an overview of practical ranges and default values on some of the most important model parameters. These limits are not hard limits but were chosen based on reported values in the literature and author’s experience and must by no means taken as hard limits. These limits are provided to give the user a starting point when calibrating the model.

<table>
<thead>
<tr>
<th>parameter</th>
<th>description</th>
<th>min</th>
<th>default</th>
<th>max</th>
</tr>
</thead>
<tbody>
<tr>
<td>icfo (mm)</td>
<td>interception storage</td>
<td>0</td>
<td>1.5</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>forest zone</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>fc (mm)</td>
<td>field capacity</td>
<td>100</td>
<td>200</td>
<td>500</td>
</tr>
</tbody>
</table>
### Conversion of Deterministic Models into Stochastic Models

#### Parameters Table

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>perc (mm/d)</td>
<td>Percolation capacity from upper to lower zone</td>
<td>0, 0.6, 1</td>
</tr>
<tr>
<td>khq (1/d)</td>
<td>Recession coefficient</td>
<td>0.15, 0.2, 0.24</td>
</tr>
<tr>
<td>alfa (-)</td>
<td>Recession coefficient</td>
<td>0, 1.6, 3</td>
</tr>
</tbody>
</table>
4 One Dimensional flow model (Sobek-River)

4.1 Physical problem description

The study of the behaviour of a river or a river system is very essential in solving problems in river management, flood protection, design of canals, irrigation systems and navigation. Many river systems have been changed by engineering measures such as embankments, groynes, and hydraulic structures that change its behaviour. To describe the flow in such a system and predict its behaviour due to imposed changes, modelling systems are often used. Sobek is a one dimensional hydrodynamic flow (i.e. open channel dynamic) modelling system that is capable of simulating and forecasting the water discharge and water levels through an open channel. Two examples of applications are the modelling of the peak river flow of the river Rhine downstream of Maxau as the result of a specific peak flow in Maxau due to upstream rainfall, and the modelling of the effects of the use of flow regulating structures such as locks and barrages on the distribution of the river flow at river junctions. For the sake of illustration, the river Rhine system is shown in Figure 4.1.

![Figure 4.1 The Rhine basin](image-url)
4.2 The conceptual model

4.2.1 Governing differential equations

The one dimensional hydrodynamic flow in open channels is described by two equations which together describe the continuous spatial (x) and temporal (t) flow variation. The flow variations are represented by variations in the discharge and the water level dependent cross sectional area. The equations are the continuity equation and the momentum equation.

The continuity equation describes the mass conservation and is described as follows:

\[
\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = q_{lat}
\]  

(4.1)

Where

\( A \)  
total cross section area (m\(^2\));

\( Q \)  
discharge (m\(^3\)/s);

\( q_{lat} \)  
lateral discharge (m\(^2\)/s).

In the above continuity equation the total mass (i.e. total cross section \( A \)) is used. The total cross section area includes the flow cross section area and the storage cross section.

The momentum equation describes the momentum conservation law. Since this equation describes the momentum of the moving bulk of water, the flow cross section \( A_f \) is used in the equation. The non conveying part of the cross section in which water is only stored (i.e. storage cross section) is excluded.

To describe the conservation in the water momentum, the sum of the changes in the main terms describing the momentum of the moving bulk of water should be equal to zero. Those terms in the same order as appearing in the equation (4.2) are: the acceleration or the inertia, the convection, the water level gradient, the bottom friction, the wind friction, the extra head loss, and the density gradient.

\[
\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x} \left( \alpha_B \frac{Q^2}{A_f} \right) + gA_f \frac{\partial h}{\partial x} + gQ\frac{\partial h}{\partial x} + W_f \frac{\tau_{wi}}{\rho_w} + gA_f \left( \eta + \xi Q \right) + \frac{g}{\rho_w} \frac{\partial \rho}{\partial x} A'_f = 0
\]  

(4.2)

where

\( \alpha_B \)  
Boussinesq constant (-);

\( A_f \)  
flow cross section area (m\(^3\));

\( g \)  
gravity acceleration (m/s\(^2\));

\( h \)  
water level (m);

\( C \)  
Chézy coefficient (m\(^{1/2}\)/s);

\( R \)  
hydraulic radius (m);

\( W_f \)  
Flow width (m);

\( \tau_{wi} \)  
wind shear stress (kg/m.s\(^2\));

\( \rho_w \)  
water density (kg/m\(^3\));

\( \eta \)  
first additional resistance coefficient (-);

\( \xi \)  
second additional resistance coefficient (s\(^2\)/m\(^6\));

\( A'_f \)  
first order moment cross section (m\(^2\) m).

In the water level gradient, the slope of the river bed is neglected. Due to this approximation, the equations are not valid for steep bottom gradients.
4.2.2 Hydraulic structures equations

In Sobek several hydraulic structures are available. The flow through the structures is computed based on upstream energy level, upstream and downstream water level and the hydraulic structure dimensions. As an example, the flow equation for the free gate flow describing the discharge and relating it to the water levels across the gate is as follows:

\[
Q = \mu_{gf} c_{gf} W_s d_g \left[ -\sqrt{2g dh_{stru}} + \sqrt{2g \left( dh_{stru} + H - (z_s + \mu_{gf} d_g) \right)} \right] \tag{4.3}
\]

Where
- \( H \) the downstream energy level (m);
- \( dh_{stru} \) structure head difference (m);
- \( d_g \) gate depth (m);
- \( z_s \) the structure height with respect to the model reference level (m);
- \( W_s \) the structure width (m);
- \( \mu_{gf} \) free gate flow contraction coefficient (-);
- \( c_{gf} \) free gate flow correction coefficient (-);

Similar equations are used for drowned gate, free weir, drowned weir and advanced weir flow, each having a contraction and a correction coefficient.

4.2.3 Examples of model parameters and their parameterization

4.2.3.1 Chézy coefficient

To compute the bed friction term in the momentum equation (4.2), Sobek uses the Chézy coefficient in one of the following roughness formulation options:
- Chézy coefficient constant;
- A function of the hydraulic radius, \( R \), as in White Colebrook formula using the Nikuradse roughness coefficient, \( k_n \), Manning’s formula using the Manning coefficient, \( n_m \), or Strickler formula using the Strickler roughness coefficient, \( k_s \);
- Engelund-like roughness predictor using the Chézy coefficient with respect to the bed material, the Shields parameter, and that of the bed material,

The Chézy, Nikuradse, Manning or the Strickler coefficients may be constant, spatially varying or a tabulated function of the water level \( h \) or the total discharge \( Q \). In general, the formulation is very well accepted from the accuracy point of view; however, the values of the coefficient can vary in space and time. These variations in space and time within a section, sometimes even a branch, are generally not considered by the modeller.

4.2.3.2 The boussinesq coefficient

The boussinesq coefficient in equation (4.2) accounts for the non-uniform velocity distribution in a cross section and it is computed by Sobek. There are two options: either the boussinesq coefficient is a constant equal to unity or a function of the of the Chézy coefficients \( C_r \), the hydraulic radii \( R_n \) and the cross section flow areas \( A_j \). For a channel consisting of a main channel (index \( i=0 \)) and two floodplain (index \( i=1 \) and \( i=2 \)), the boussinesq coefficient is calculated as follows:

\[
\alpha_p = \left( \frac{C_0^2 A_{i=0} R_0 + C_1^2 A_{i=1} R_1 + C_2^2 A_{i=2} R_2}{C^2 A_j R} \right) \tag{4.4}
\]
If the boussinesq coefficient is defined as a function of the Chézy coefficient, it will contain all the variability described in section 4.2.3.1. If it is taken as a constant equal to unity means the velocity distribution in a cross section is uniform.

4.2.3.3 Wind friction coefficient and the wind hiding factor

The wind shear stress induces extra friction term in the momentum equation. It is expressed as a function of the density of air, wind hiding factor, wind friction coefficient, and the wind driving forces (i.e. velocity and direction). The wind friction coefficients and the wind hiding factors are used to dampen or amplify the effect of the wind on the wind shear stress. The wind friction coefficient can be also defined as a function of the wind velocity field. Those coefficients are very difficult to quantify since they don't have a profound physical meaning. Their effect can be only justified through the model output.

4.2.3.4 First and second resistance coefficients

The first and second resistance coefficients as defined in equation (4.2) are used to define the additional local head losses at the location of structures. If hydraulic structures are not defined, those coefficients can be used to model local head losses in a simpler approach as a constant value or a function of the local water level.

4.2.3.5 Hydraulic structures correction and contraction coefficients

As described in section 4.2.2 and given in the free gate flow equation (4.3), the hydraulic structure correction and contraction coefficients are incorporated in the discharge equation to incorporate the simplifications normally assumed by the user in the dimensions and location of a structure as well as the shifting in the flow conditions from free flow to submerged flow. Those coefficients are defined as a constant value which might be true for the location and dimensions, but not for the temporal variations in the flow conditions.

4.2.4 Driving and governing forces

4.2.4.1 Boundary conditions

In order to solve the discretised set of water flow equations for a specific (limited area) model domain, information on the water flow at the boundaries of the model domain should be specified. The boundary conditions are normally given as

- Discharge $Q$ as a constant, tabulated function of time, periodic functions;
- Water level $h$ as a constant, tabulated function of time, periodic functions, tidal components, Fourier series;
- Rating curves (i.e. $Q-h$ relation) in tabulated form.

The boundaries are normally represented by controlling points, like water gauges at upstream river model boundary or tide gauges at the estuary mouth, which is a common location for a downstream model boundary. The information on the boundary is assumed to be well defined, i.e. matching the requirements of the equations. This implies that they define a well posed problem, which according to theory has a (unique) solution.
4.2.4.2 Lateral discharge as sources

A lateral discharge may be a point source (Example: power station, a secondary branch) or a source across a specified reach (such as ground water seepage). Specifying a lateral discharge indicates that a certain volume of water is exchanged at that location and/or reach. This volume of water is included in the continuity equation only. It is assumed that the momentum entering or leaving the model can be neglected. In order not to violate this assumption in the momentum conservation law, the lateral discharge should not become too large (i.e. less than 10%) compared to the discharge in the main channel at that location and/or reach where the lateral discharge is exchanged.

4.2.4.3 Wind Field

The wind field in one dimension is specified through its velocity and its direction with respect to the polar direction. The wind velocity and direction can be specified as a constant value in time or a temporal function. However, the wind velocity and the wind direction are assumed to be spatially uniform over the whole river system. This might induce problems for large networks.

4.2.5 Discretisation of the conceptual model

The flow equations as in (4.1) and (4.2) are discretised using the Preissmann box scheme. The discretisation of the different terms connects variables at neighbouring grid points in time and in space. The resulting set of equations is solved by means of a modified Newton method. The solution to the set of the equations is a function of the spatial (i.e. at every grid point) and temporal description of the discharge \( Q(x,t) \) and water levels \( h(x,t) \) and the boundary conditions at time \( t+1 \). The flow equations are initialized by prescribing discharges and water levels on the whole domain at time level \( t=t_{\text{init}} \). In general, the exact detailed information on the hydrodynamic initial conditions is not available. Plenty of assumptions can be used for the initial conditions (Example: uniform discharge, constant water levels, etc.). As a relaxation to those rough assumptions, an adaptation period to the imposed initial conditions is required for most of the hydrodynamic numerical models (i.e. the so-called spin up period).

Most of the terms in the set of the discretised equations are being linearised. The hydraulic coefficients, \( a_B, C, \) and \( R \) and the channel flow width, \( W_f \), are not linearised because of the complexity of their expressions. Underrelaxation is applied to ensure convergence. The Sobek model consists of a network of branches connected to each other at nodes. Each node is a location where two or more branches join. In each branch a number of grid points are defined. These grid points represent the spatial numerical grid on which the continuity and the momentum equation are numerically solved.

At the nodes, a grid point is defined for each branch. The water level at those grid points is identical, while the discharge satisfies the continuity equation (i.e. total incoming discharge is equal to total outgoing discharge). Hydraulic structures are located at grid points. Internally, Sobek makes a copy of this grid point upstream and downstream the hydraulic structure. Those two points are used for the application of structure formulas discussed in section 4.2.2 which relate the discharge and the water levels across the hydraulic structure.
4.3 Uncertainties in Sobek

In general, hydrodynamic models often contain several uncertainties, which can occur at several stages. The model’s equations may contain errors due to lack of knowledge about the complex physical processes and their interaction. Often, simplifications are made in the derivation of the differential equations and its discretisation. These simplifications will increase the model’s uncertainty. Uncertainties in the output of the model can also occur due to incorrect, estimated or incomplete input data of the model, such as boundary conditions, meteorological data, and driving forces, or due to uncertain and/or lumped model parameters. The uncertainties in Sobek are described as uncertainties in the model parameters (i.e. coefficients), the sources or driving forces (i.e. lateral discharge, boundary conditions and driving wind forces), in the temporal and spatial state (i.e. water level and discharge), and in the equation definition and/or discretisation due to the assumptions often used for simplifying the phenomena at hand. The latter is normally skipped due to lack of experience in quantifying its effects.

4.3.1 Uncertainties in model parameters

In general, the uncertainty in the parameters must be limited. They may vary within a margin that is considered to be physically realistic. If this is not the case, they often include a compensation for other model errors that are not explicitly accounted for in the model error term. Realistic estimation of parameter estimation can be beneficial for long term prediction.

4.3.1.1 Friction parameters

The bed friction is the friction between the flowing water and the river bed. The bed friction may dependent on the dynamic flow properties and the characteristics of the soil. Thus, the bed friction will be neither uniform nor constant in space and time. The formulation for the calculation of the Chézy coefficient depends on the user definition of Chézy, Nikuradse, Manning or the Strickler coefficients. Even with complex expressions for those coefficients, those coefficients may be still a source of uncertainties in the hydrodynamic equations. There are many ways to account for uncertainties in the coefficients, one of which is to assign a distributed uncertainty field to those coefficients. The definition of a distributed uncertainty field is given in Appendix A.2. As expressed in equation (A.2.4), the spatial dependency can be established by means of a covariance matrix $\Gamma(z)$. The main uncertainty parameters that define this covariance are the variance of the uncertainty $\sigma^2$, and the spatial correlation length $R$. Depending on the characteristics of the soil, the correlation scale can be defined. For highly heterogeneous soil, the spatial correlation length is small almost equal to zero. For homogeneous soil, the spatial correlation scale is large and almost equal to the whole modelled domain. On the other hand, since the error in defining the Chézy coefficient is higher in a heterogeneous soil, the variance should be high. From practice, the standard deviation of the error in Chézy coefficients is in the order of magnitude of 0.5% to 1% of the Chézy coefficient value (i.e. if the Chézy coefficient is defined to be 35 m$^{1/2}$/sec, the variance of the error is about 0.5 m$^{1/2}$/sec).

The boussinesq coefficient accounts for the non-uniform velocity distribution in a cross section and plays an important role in the convection part of the momentum equation. It can be regarded as an extra friction parameter across the cross section of the flow. The user can define the boussinesq coefficient as a function of the Chézy coefficient. If uncertainties are
assumed on the bed friction term (i.e. Chézy coefficient) this would directly imply that no extra uncertainties should be attached to the Boussinesq coefficient. The latter might lead to physically unacceptable variation in the momentum equation due to friction parameters.

4.3.1.2 Wind friction parameters

In Sobek applications, the wind field is assumed to be spatially uniform. This might be a source of uncertainties for large networks. Uncertainties in the first and second wind friction coefficient and the wind hiding factor as explained in section 4.2.3.3 can be a way to represent the uncertainties on the wind velocity and direction. In practice, it is very difficult to define the spatial and temporal variations of such uncertainties. It is easier to apply the uncertainties directly on the wind field as a driving force (i.e. wind velocity and direction).

4.3.1.3 Head loss and structure parameters

In a hydraulic structure, the discharge through the structure is dependent on the upstream and downstream water level and of parameters that define the dimension and location of the structure. The hydraulic behaviour of a structure can be defined as the discharge head loss relation. This relation for different types of structures is expressed as in the equation (4.3) for the free gate flow. Contraction and correction coefficients are used to account for the errors in the very coarse modelling of the structures and flow conditions through a structure. Those coefficients are normally defined by the user and they are a source of uncertainties attached to any hydraulic structure (uncorrelated in time and space). The uncertainty in those parameters that are flow dependent is temporally correlated. The temporal correlation length can be taken more or less the same as the flow time scale.

To define the additional local head losses at the location of structures, an extra head loss term in the momentum equation (i.e. equation (4.2)) is defined. This term is dependent on the first additional resistance coefficient and a second resistance coefficient and also on the discharge. If hydraulic structures are not defined, those coefficients can be used to model local head losses in a simpler approach as a constant value or a function of the local water level. This assumption might induce uncertainties in the momentum equation. The uncertainties in the first and second additional resistance coefficient are physically unlikely to be correlated in space and time.

4.3.2 Uncertainties in driving and governing forces

The lateral discharge, boundary conditions, and wind information are driving forces for the hydrodynamic flow. This information is generally available through measurements at gauges (boundary conditions), other models such as rainfall-runoff (lateral discharge), and satellite information (wind field). Measurements of water level at gauges are available in the form of time series. However, in some cases, the measurement interval is longer than the required discretised time interval used in solving the hydrodynamic equations. Interpolation between measurements is often used to provide the boundary conditions for water levels. In case of using models to provide boundary conditions and or lateral discharges, the driving forces provided through the model inherit the uncertainties of that model. Furthermore, the models are used in prediction mode which increases the uncertainty in their output (i.e. the boundary conditions for the hydrodynamic model and the lateral discharges at specific locations in the hydrodynamic model). Though the satellite wind data are generally accurate, the spatial scale
is in most cases much larger than the spatial scale in the hydrodynamic models. This implies that smaller variations of the wind velocity and direction that might affect the hydrodynamics in open channels are not represented. The simplification made in the driving forces of 1D hydrodynamic model, such as a constant value or a temporal function of the wind velocity and direction, or the assumption of zero momentum entering or leaving the model with lateral discharge, would also lead to errors in the driving forces.

It follows from section 4.2.4.2, that the uncertainties in the lateral discharge should not become too large compared to the uncertainties in the modelled local discharge (i.e. less than 10%). The uncertainties in the wind field can be accounted for as explained in section 4.3.1.2 or directly as uncertainties on the wind velocity and direction. Assigning uncertainties to the boundary conditions is a very critical issue. This can create an unrealistic water level gradient that can propagate downstream or upstream the modelled domain. Time variation and correlations in the uncertainties in the boundary conditions have to be limited in order not to violate the “smooth” solution of the 1D hydrodynamic equations.

4.3.3 Uncertainties in the schematization

The bottom topography data should be having a reliable level of accuracy. However, specifying the bottom topography in great detail does not necessarily lead to more accurate results but may generate small scale flow phenomena that cannot be modelled adequately. Inducing uncertainties on the bottom topography would have the same effect. The cross sectional area and/or its shape also contain uncertainties. Simplifications on the shape and the dimensions of the cross section are also made. The spatial variability of a cross section is also not taken into account. In practice, it is very difficult to assign an uncertainty measure on the geometry of the main channel at hand. However, the effect of uncertain geometry will be mirrored on the model output.

4.3.4 Uncertainties in the model output

The modelling assumptions can result in uncertainties in the spatial and temporal water levels and the discharges calculated by the model. Typical variations of channel geometry take place over a length assumed to be large with respect to its depth and width. The radius of curvature of each channel is assumed to be large compared to its width. The length of a branch that contains structures is assumed large with respect to the structure dimensions. Unsteady flow fluctuations within a structure are neglected. Due to those assumptions, the flow phenomena near the structures, nodes, and through relatively large lateral discharge and through channels with rapidly varying geometry, can locally not be modelled accurately.

The Preissmann scheme that is used in Sobek may introduce oscillations in the order of $2\Delta x$. $\Delta x$ being the spatial resolution of the grid. In order to guarantee a smooth solution, spatial correlation scales on the model output should be larger than $2\Delta x$. Spatially uncorrelated noise should not be used on the water level and or discharge with an exception at the structure grid points.

The simulation of flow and thus the non-linear interactions may generate fluctuating errors that have time scales smaller than the time scale used in the model forcing. As a result of the numerical temporal discretisation, those errors can become large and significant creating wiggles in time. To smooth those errors, a numerical dissipation mechanism is required.
Using temporally correlated uncertainties on the model output equal to or longer than the time scale at the boundaries may create the same wiggles in time.

The discretisation procedure in Sobek explained in section 4.2.5 also induces conditions on the uncertainties if applied on the model output. At connecting nodes, the uncertainties on the water level of the connected branches have to be fully correlated for the first grid point on each connected branch, while the uncertainties on the discharge have to satisfy the continuity conditions applied on the discharge. For the hydraulic structures, the correlation between uncertainties in the water levels and in the discharge upstream and downstream has to be chosen very careful to follow the law of the conservation of energy.
5 References

5.1 References for the advection dispersion model


5.2 References for the flow model (Sobek River)


5.3 References for the rainfall runoff model


A  Stochastic modelling of uncertainties

The main issue in sequential data assimilation procedures (as for example Kalman Filter based algorithms) is that a model’s estimate of a system state is corrected at every time step at which new observations become available. The corrected model state is propagated forward in time through the numerical model until the next time that observations are available. The updating of the correspondingly predicted model state is then repeated.

The correction of a model’s state is actually a weighted combination of the computed system state and the observed information, and the key issue is that these weights are based on the uncertainties in both. To carry out such an integration of data and model, estimates must then be available for these uncertainties. A common procedure is to construct stochastic models for all involved sources of uncertainty. In this way the originally deterministic (conceptual or numerical) model is embedded into a stochastic environment. This appendix deals with general aspects of this extension of the deterministic model with random components.

For the stochastic representation of uncertainties in a deterministic model three levels of ‘complexity’ are discriminated. Firstly, in Section A.1, uncertainties are considered at the ‘basic’ level of single, and more or less ‘isolated’, model parameters. Secondly, in Section A.2, this is extended to the definition of uncertainties for model coefficients as for example dispersion coefficients in ADE or friction coefficients in flow models. In contrast to model parameters, model coefficients can depend on the spatial and temporal coordinates. Therefore model coefficients are sometimes referred to as distributed parameters. Thirdly, Section A.3 will deal with uncertainties in the model’s state-variables. These state variables can be seen as distributed quantities as well. Note that in these three steps the assignment of uncertainties gradually shifts from very localised ‘entries’ in the model, to a fully global (“integrated, lumped or aggregated”) form.

First a few notes are formulated with regard to the status and assumed properties of the deterministic model. It is assumed that physical and dynamical knowledge of the phenomena has been incorporated as much as possible, or at least reasonably well in the formulation of the model. Preferably, the deterministic model has been calibrated to achieve a best starting point when applying sequential data assimilation facilities. The calibration procedure should provide reasonable estimates for the model parameters and/or the model predictions. It should also provide a quantification or an indication of the uncertainties in those estimates. These can be used as important prior information for a proper initialisation of the parameters in the stochastic models for the uncertainties. Otherwise, it is recommended to apply some sensitivity or uncertainty analysis to the model to get this information.

Throughout this Appendix it will be assumed that the deterministic model (actually the numerical model derived as a discretised version of the conceptual model defined in continuous time and spatial coordinates) is in state space form. This will certainly be the case for conceptual models that are in the form of partial differential equations as e.g. transport models in the form of ADE, and flow models based on the Saint Venant equations.
Recall that in discrete time and space a state space formulation means that the system’s state at time $t + \Delta t$ can be derived from the system’s state of the previous time $t$, and the system’s external forcing within $t$ and $t + \Delta t$ (Markovian property). To ensure the applicability of standard sequential data assimilation procedures this state space property must also be taken into account when constructing stochastic models for the uncertainties.

### A.1 Uncertainties of single model parameters

In this case uncertainties are ‘restricted’ to merely the (one or more) constant model parameters $\Theta$ in the parameterisation of a model coefficient and/or boundary condition. If the uncertainties are assigned only to model parameters, then it is implicitly assumed that the formulation of the model dynamics and the parameterisation of its coefficients are either perfect or are much less uncertain than the model parameters $\Theta$.

The idea is then that the parameters’ initial values (often expert estimates, or a result of calibration) represent a mean value that can still vary somehow in time, and this temporal variation must (indirectly) be retrieved or identified from observed information. These fluctuations are (stochastically) modelled as a random process according to the following state equation for $\Theta$ in discrete time ($t = 0, 1, 2, 3, \ldots$, in units $\Delta t$ following from the discretisation of the conceptual model):

$$\Theta_t = \Theta_{t-1} + W_t \quad (A1)$$

The $W_t$ is a zero mean white random (and usually Gaussian) process, meaning that the random variables $W_s$ and $W_t$ are independent for $s \neq t$. As a result a white noise $W_t$ evolves in time without memory effects. The white noise $W_t$ does not need to be stationary, however. By allowing the spread $\sigma_t$ of $W_t$ to depend on time, one can account for (random) temporal variability in the physical system. This may be desired when confronted with non-stationary system behaviour as for example short or long term temporal trends, daily or seasonal variations, or other quasi-periodicities.

As a consequence of $W_t$ being a white noise, equation A1 has the form of a state equation for $\Theta_t$ (first order in time, i.e. one step memory). The set of original state equations (i.e. the deterministic model equations) must be extended with equation A1 for the new and additional state variable $\Theta_t$. Finally, and merely as a remark, it is noted that equation A1 represents a random walk model in one ‘spatial’ dimension and in discrete time.

Apart from the stochastic state space model of equation A1 several alternative formulations may be feasible or even necessary. For example:

$$\Theta_t = \Theta_{ref} + W_t \quad (A2)$$
The $\hat{\Theta}_{\text{ref}}$ represents a constant reference value for the parameter. This reference may be its value found in a preceding calibration procedure, or some other user prescribed or preferred initial guess. In this case $\Theta_i$ may still vary in time, but it is ‘forced’ to fluctuate around the reference value. In this way the model of equations A2 stays closer to the assumption (within the deterministic model) that the parameter should formally be a constant. To focus further to the situation of constant parameters (and their estimation by means of deterministic model calibration) an other alternative of equations A1 and A2 may be considered:

$$\Theta_i = \hat{\Theta}_{\text{ref}} + W_0 \quad \text{(A3)}$$

In this case $W_0$ is again random variable but now fixed in time. As a result of equation A3 this will also be the case for $\Theta_i$. In this form a sequential assimilation procedure is then actually applied for the calibration of the parameter. In most (Kalman Filter based) assimilation algorithms linear corrections of an estimate are applied. Therefore the ‘risk’ remains that an estimate gets stuck in a local optimum, and/or is biased.

Physical processes such as flow, transport, rainfall and discharge will hardly ever evolve without temporal memory and neither this will be the case for their uncertainties. This suggests replacing the white noise $W_i$ in equations A1 and A2 by another random forcing that includes a temporal correlation. Care must be taken that a state space formulation is satisfied, and therefore AutoRegressive Moving Average (ARMA) models tend to be most suited to define such non-white random processes in discrete time. AR(1) (auto-regressive models of order 1) models are the most simple and commonly used ARMA models in sequential data assimilation procedures. The white noise $W_i$ in equation A1 (and similarly A2) is then replaced by a ‘coloured’ or ‘pink’ noise $Z_i$ according to:

$$\Theta_i = \Theta_{i-1} + Z_i \quad \text{(A4a)}$$

with the following AR(1) model for $Z_i$:

$$Z_i = a \cdot Z_{i-1} + W_i, \quad |a| < 1 \quad \text{(A4b)}$$

The $W_i$ in equation A4b is again a white noise while $Z_i$ is a low pass filtered version of $W_i$ and $a$ represents the time correlation scale. Note that in this case an additional state equation (for the new state variable $Z_i$) must be added to the state equations of the deterministic model. In case $a$ is constant in time, and $W_i$ is a stationary white process, it can be shown that the auto-covariance function $\Gamma^{(Z)}_{\tau} := \mathbb{E}[Z_i \cdot Z_{i+\tau}]$ of $Z_i$ has an exponential form:

$$\Gamma^{(Z)}_{\tau} := \sigma_Z^2 \cdot a^{|\tau|}$$

$$= \sigma_Z^2 \cdot \exp\left(|\tau| \cdot \ln(a)\right) \quad \text{if } a > 0 \quad \text{(A5a)}$$
The integer valued time shift \( \tau \) is in units \( \Delta t \). The auto-correlation time \( T_Z \) is defined as the time shift for which the auto-covariance function is \( \frac{1}{2} \) of its maximum (at zero time shift) and it is easily verified that here \( T_Z = -\frac{\Delta t}{\ln(a)} \). The spread \( \sigma_w \) of \( W_i \) is related to the spread \( \sigma_z \) of \( Z_i \) according to:

\[
\sigma_z = \frac{\sigma_w}{\sqrt{1-a^2}}
\]

(A5b)

In this way the (statistical properties of the) noise \( Z_i \) is characterised by two parameters, the spread \( \sigma_z \) and the auto-correlation time \( T_Z \). The spread represents the size of the uncertainty, and the auto-correlation time is a measure for the temporal memory in the uncertainty of parameter \( \Theta \). In applications this physical interpretation can conveniently be used for a proper initialisation of these parameters. The \( Z_i \) characterised by equations A4ab is a stationary random AR(1) process. Suitable non stationary generalisations of this random process can be constructed by means of a time dependent prescription of parameter \( a \) and/or a non-stationary white noise \( W_i \).

Apart from AR(1) higher order ARMA models can be used as well for the modelling of the uncertainty in a model parameter. Whether to do this or not depends on the (temporal) smoothness properties that are required for the uncertainty. In fact, in case of a white noise realisations of this process are highly non-smooth, and even discontinuous. Time trajectories of an AR(1) process are neither smooth, but continuous. For smooth(er) trajectories higher order AR or ARMA models will then be required. This will be at the cost of more state variables, and also the interpretation of the meaning of the model and (the initialisation of) its parameters will be much more complex. Therefore higher order ARMA-model will not be considered in further detail.

Apart from temporal correlations, mutual dependencies may be necessary when random processes are assigned to two or more different uncertain parameters. This can be the case, for example, when those different parameters are physically correlated. A special type of mutual dependency is spatial dependency. This is used when a single parameter is used in the parameterisation of spatial distributed parameter. Such (spatial) dependencies will be considered in more detail in the next section, when dealing with the stochastic modelling of so called distributed parameters.

### A.2 Uncertainties in distributed model parameters

Model coefficients can be seen as distributed parameters i.e. model entities that are not constant (in time) and/or non-uniform (in the spatial coordinates). As typical examples friction coefficients in flow models and dispersion coefficients in transport models can be mentioned.
For the representation of (random) uncertainties in a distributed parameter, \( E(\cdot) \) say, equation A1 can directly be generalised to

\[
\tilde{E}_t = \tilde{E}_{t-1} + \tilde{W}_t \tag{A6}
\]

The \( t \) is again a discrete time and vector \( \tilde{E}_t \) denotes the values of the coefficient \( E(\cdot) \) at time \( t \) on the discrete spatial positions representing a spatial structured or non-structured grid on which the conceptual model is discretised. Depending on the dimension of the deterministic model, the grid may be 1D, 2D, or even 3D dimensional vectors. Obviously, equation A6 is an \( N \)-dimensional generalisation of equation A1. For higher dimensional models, e.g. 3D, the \( N \) can become ‘extremely’ large.

Following the procedure of Section A.1, the case that the random noise \( \tilde{W}_t \) is white with regard to both the temporal evolution and the spatial direction would be most ‘simple’. The assumption of no temporal memory for modelling the temporal evolution of uncertainties is still debatable as discussed in Section A.1. However, the assumption of spatial independencies for the modelling of the spatial variability of the uncertainties in a model coefficient \( E(\cdot) \) as here formulated is unrealistic.

For the representation of temporal memory, the procedures outlined in Section A.1 using AR(1) models for a univariate parameter \( \Theta \), can be generalised to the case of distributed parameter \( \tilde{E}_t \) as follows

\[
\begin{aligned}
\tilde{E}_t &= \tilde{E}_{t-1} + \tilde{Z}_t \\
\tilde{Z}_t &= A \cdot \tilde{Z}_{t-1} + \tilde{W}_t
\end{aligned} \tag{A7}
\]

The \( A \) is a \( N \times N \) matrix denoting the deterministic part in the time propagation mechanism for the \( N \)-variate pink noise \( \tilde{Z}_t \). The off-diagonal elements of \( A \) represent non-local spatial interactions since the \( A_{m,n} \) provides a ‘transfer’ of the noise \( \tilde{Z}(\cdot) \) of time \( t-1 \) at spatial position \( n \) to the \( \tilde{Z}(\cdot) \) of time \( t \) at another position \( m \). For reasons of stability all eigenvalues \( \lambda_n \) of \( A \) must satisfy \( |\lambda_n| < 1 \).

The \( \tilde{W}_t \) is an \( N \)-dimensional zero mean random time series. It behaves as a white noise when seen as a function of time. The \( N \)-components of \( \tilde{W}_t \), however, can include spatial dependencies in the modelling of the uncertainties. Such spatial dependency can be established by means of a non-trivial covariance matrix \( \Gamma^{(w)} \) of \( \tilde{W}_t \) with its entries \( \Gamma_{m,n}^{(w)} \) defined by:

\[
\Gamma_{m,n}^{(w)} := \mathbb{E}[W_t(x_m) \cdot W_t(x_n)] \tag{A8}
\]
In applications care must be taken that $\Gamma^{(W)}$ is a symmetric and positive definite $N \times N$ matrix. Clearly this $\Gamma^{(W)}$ is an essential new issue when considering the stochastic modelling of distributed parameters as an extension of ‘single’ model parameters.

On the basis of equations A7 and A8, the statistical properties can be computed for a multivariate (spatial) pink noise $\tilde{Z}_i$. Omitting details it can be derived that $\tilde{Z}_i$ is a zero mean noise with the following auto-covariance function $\Gamma^{(Z)}_{\tau}$, $\tau$ denoting a discrete time shift in units $\Delta t$ ($\tau \in \mathbb{Z}$):

$$
\Gamma^{(Z)}_{\tau} := \mathbb{E} \left[ \tilde{Z}_i \cdot \tilde{Z}_i^T \right] = \begin{cases} 
\Gamma_0^{(Z)} \cdot A^T, & \tau \geq 0 \\
(\Gamma_0^{(Z)} \cdot A^T)^T, & \tau < 0
\end{cases} \quad (A9)
$$

With regard to time this auto-covariance covariance has again an exponential form. The $\Gamma_0^{(Z)} := \mathbb{E} \left[ \tilde{Z}_i \cdot \tilde{Z}_i^T \right]$ is the auto-covariance function at shift $\tau = 0$. It can be shown that it is related to $A$ and $\Gamma^{(W)}$ according to:

$$
\Gamma_0^{(Z)} = A \cdot \Gamma_0^{(Z)} \cdot A^T = \Gamma^{(W)} \quad (A10a)
$$

This provides an implicit definition of $\Gamma_0^{(Z)}$ as function of $A$ and $\Gamma^{(W)}$. In an explicit (and analytical) form $\Gamma_0^{(Z)}$ can equivalently be written as:

$$
\Gamma_0^{(Z)} = \sum_{\ell=0}^{\infty} A^\ell \cdot \Gamma^{(W)} \cdot (A^T)^\ell \quad (A10b)
$$

Equations A9 and A10 are then a multivariate generalisation of the univariate case as worked out in Section A1, leading to the equations A5.

We conclude this assessment of stochastic models for uncertainties in distributed parameters with a few additional notes and comments. In more or less an arbitrary order:

1. Instead of the ‘fluctuation’ equation $\tilde{E}_i = \tilde{E}_{i-1} + \tilde{Z}_i$ one may again choose the alternative state equations $\tilde{E}_i = \tilde{E}_{\text{Ref}} + \tilde{Z}_i$ or $\tilde{E}_i = \tilde{E}_{\text{Ref}} + \tilde{Z}_0$ to take into account that the variations/uncertainties of the model coefficient $E(\cdot)$ are with respect to a preferred constant reference value $\tilde{E}_{\text{Ref}}$.

2. In practice it will often not be easy to find a proper formulation for the transfer matrix $A$. Simplification of $A$ to a diagonal matrix, or even a constant times the unit matrix, will often be applied.

3. Non-stationarities can again be included by means of time dependent formulations for the transfer matrix $A$ and/or the covariance matrix $\Gamma^{(W)}$. In this way, one can adapt to...
changing system conditions, as e.g. short or long term trends or temporal periodicities. In practice, however, it will be usually not easy to describe these physical non-stationarities in mathematical terms.

4. Physical knowledge about the spatial scales of the process must be used for a proper formulation of the covariance matrix $\Gamma^{(W)}$ (or $\Gamma^{(Z)}$). Here several alternatives are feasible. Formulations are often based on the distance of the grid points. The distance measure can be the standard Euclidean metric, or a ‘physical’ metric that is based on travel times of the process that is considered (flow, waves, concentration, etc.). For a metric distance $r_{m,n}$, a metric based covariance function $\Gamma$ is

$$
\Gamma_{m,n} = \sigma^2 \cdot \exp\left(-\frac{r_{m,n}}{R}\right) , \quad \alpha \geq 1
$$

(A11)

The $\alpha$ is a shape parameter that must be 1 or larger than 1 to ensure that $\Gamma$ is a well defined covariance matrix (i.e. symmetric and positive definite). $R$ represents a spatial correlation length. For a standard Euclidean distance in 1D, $r_{m,n}$ is the distance between the spatial positions $m$ and $n$.

The variances (i.e. the $N$ diagonal entries $\Gamma_{n,n}$) of the $\Gamma$ of equation A11 are all equal to $\sigma^2$ and thus constant as function of the spatial coordinate. In practice non uniform (here: spatially varying) prescriptions will often be more realistic. For an example where such a non-uniform covariance structure is constructed one is referred to Section 2.4.4.

5. In the model’s formulation of equation A7 it is silently assumed that the dimension of the white noise $\hat{W}_t$ is the same as the number of spatial grid points ($N$) of the numerical model. This means that $N$ univariate (but correlated) noises are defined, one for each grid point. In practice, especially when dealing with scarce observed data sets and/or dense spatial grids, there may soon be a discrepancy in the amount of observed data and the ‘degrees of freedom’ in the model for $\hat{W}_t$. To overcome this mismatch, a noise $\tilde{Z}_t$ is often defined on a coarser grid (with $M$ grid points; $M < N$) and this $\tilde{Z}_t$ is then interpolated to the computational grid. In this way $\tilde{Z}_t = B \cdot \tilde{Z}_t$ with $B$ the $N \times M$ matrix that governs the (linear) interpolation. This leads to the following alternative formulation of equation A7.

$$
\begin{align*}
\tilde{E}_t &= \tilde{E}_{t-1} + B \cdot \tilde{Z}_t \\
\tilde{Z}_t &= A \cdot \tilde{Z}_{t-1} + \tilde{Z}_t
\end{align*}
$$

(A12)

This generalised form, with a lower dimensional noise $\tilde{Z}_t$ to reduce the number of noise components, can also be the result of other simplifications than merely interpolation.
Finally, it must be remarked that so far only random noises of type AR(1) were considered. More generally higher order AR(MA)-models may be used as well. For such multivariate random models, it will be much more difficult to derive analytically the statistical properties and control the stability. Moreover, the physical interpretation and the effects of corrections in the data assimilation procedures may become highly unclear.

A.3 Uncertainties in the model’s state equations

In Sections A1 and A2, model uncertainties were assigned to one or a few particular components in the model. In “complexity” these model components varied from single model parameters (Section A.1) to distributed parameters, Section A.2). In this way uncertainties were localised to well-defined model entities, and usually these entities are on one to one basis associated to physical (sub)processes. For examples: advection coefficients for the flow induced displacement of substances, dispersion coefficients for the temporal increase of the size of patches, model inputs representing external system forcing, etc. Actually, this localisation of uncertainties within the model concept is often the starting point in model calibration. In this section, the extension of the deterministic model with stochastic formulations for its uncertainties is carried out in a more global (or lumped or aggregated) way and in a wider sense. In fact, uncertainties are now assigned to the model’s state equations or to the state variables (i.e. solution of the state equations) directly. When the uncertainties are formulated for the state equations there is the alternative to do this for the (continuous) equations of the conceptual model, or the equations of the numerical model that follows from the conceptual model after discretisation. The latter are the equations that are actually solved in the numerical procedures (“algorithmic model”) and here aspects such as implicit or explicit numerical integration schemes can play a role as well.

A.3.1 Uncertainties for the state variables

The model’s state variables at a discrete time \( t \) are denoted by a vector \( \tilde{\xi}_t \) with \( \tilde{\xi}_t = (\xi_1, \xi_2, \xi_3, \ldots, \xi_N) \). The dimension \( N \) depends on the number of physical quantities in the model and the number of grid points \( M \) (e.g. \( N=2*M \) for a 1D numerical flow model describing the joint temporal evolution of water levels and longitudinal flow velocities, or \( N=3*M \) when dealing with a 2D depth averaged flow model) and the number of grid points in the spatial discretisation. In practice \( N \) can be quite large, especially when dealing with large scale 3D (inhomogeneous flow) models.

After the model’s evaluation of \( \tilde{\xi}_t \) at a discrete time \( t \) this state \( \tilde{\xi}_t \) is interpreted as ‘merely’ a mean of a random process. The uncertainty is represented again by random noises. For the modelling of these random noises the same procedures can be followed as described extensively in Section A.2 since the state \( \tilde{\xi}_t \) is also a distributed quantity as a matter of its definition.

An advantage of assigning uncertainties directly to the state variables is that the modelling of these uncertainties can be based rather easily on all kind of prior knowledge about the spatial and temporal scales, and the range/variability of the state variables. This prior information can consist of physical process/system/expert knowledge, and/or measured data.
sets. A further advantage is that the numerical implementation of such a random perturbation of a model state $\tilde{z}_t$ is straightforward and hardly requires any effort.

A disadvantage in this very “explicit” modelling of the uncertainty in the state is that physical constraints may be violated. For example, care must be taken that adapted concentrations do not become negative, or that water levels remain positive when compared to the position of the water system’s bed. It will also be much more difficult to satisfy conservation laws (if necessary). Moreover, even if at time $t$ a randomly perturbed distribution of a state variable satisfies the desired constraints it is not guaranteed that this will hold as well at the times $t+1$, $t+2$, $t+3, \cdots$ when a perturbed state is propagated forward in time via the numerical model. As a further disadvantage it must be mentioned that assignment of random noise to the state $\tilde{z}_t$ can induce large non-smoothness properties, both in the temporal and in the spatial directions. These can be unrealistic in physical sense, and may also lead to undesired numerical effects with regard to stability and accuracy.

### A.3.2 Uncertainties assigned to the state equations

In this case the uncertainties are prescribed for the model’s state equations rather assigned directly to the most recently computed state variables. Here the state equations will be considered that represent the conceptual model, i.e. the mathematical model derived in continuous time and spatial coordinates. It is assumed that the conceptual model is in the form of one or more partial differential equations, as for example advection diffusion equations in transport models, and the St. Venant equations in flow models. For transparency of the discussion below, an advection diffusion equation (ADE) in 1D is considered as a concrete example. In this case the state variable is a concentration distribution $c(\cdot)$ that satisfies the following conceptual model:

$$\frac{\partial (A \cdot c)}{\partial t} + \frac{\partial (Q \cdot c)}{\partial x} = \frac{\partial}{\partial x} \left( E \cdot A \frac{\partial c}{\partial x} \right) + S \quad (A13)$$

For the meaning of the symbols and an extensive discussion of theoretical and practical aspects of the ADE one is referred to Section 2.2.1 of this document.

Because of the physical interpretation (of the meaning and possible effects) a definition of uncertainties at the level of the conceptual model will be most convenient, and the idea is to assign a random noise $Z(\cdot)$ to the right hand side of equation A13 to account for all (remaining) uncertainties in the model:

$$\frac{\partial (A \cdot c)}{\partial t} + \frac{\partial (Q \cdot c)}{\partial x} = \frac{\partial}{\partial x} \left( E \cdot A \frac{\partial c}{\partial x} \right) + S + Z \quad (A14)$$

In this form the term $Z(\cdot)$ can be interpreted as an additional (and random) source term or a model input. In case $Z(\cdot)$ is a (spatially) distributed noise it represents a diffusive source. Alternatively, $Z(\cdot)$ can be defined for merely one or a few spatial positions to deal with local uncertainties in the modelling. These can for example be small external loads or
extractions of substance that were ignored in the source term $S(\cdot)$ of the deterministic model. It must be noted, however, that the $Z(\cdot)$ need not uniquely be associated with $S(\cdot)$ but can be introduced to account for uncertainties in the other (storage, advection, and dispersion) terms of the conceptual model as well.

As a matter of its definition the extension of the deterministic model leading to equation A14 need not be conservative, and mass can be created or removed. Therefore alternative formulations of the uncertainty may be desired that do not affect the total mass balance. For the present example this can be achieved by adding the noise to the mass flux, rather than the source term(s). The total mass flux in equation A13 is $\Phi(\cdot)$ defined by:

$$\Phi := Q \cdot c - E \cdot A \cdot \frac{\partial c}{\partial x}$$

(A15)

With this $\Phi(\cdot)$ we obtain:

$$\frac{\partial (A \cdot c)}{\partial t} + \frac{\partial \Phi}{\partial x} = S$$

(A16)

The idea is then to assign the uncertainties $Z(\cdot)$ to the flux leading to the following (conservative and randomised) transport model:

$$\frac{\partial (A \cdot c)}{\partial t} + \frac{\partial (\Phi + Z)}{\partial x} = S$$

(A17)

In this way the uncertainties are assigned to specific model component(s) to account for one or more constraints that must be satisfied in the random extension of the deterministic model.

Here these issues are illustrated on the basis of an ADE but they can similarly be achieved for, and generalised to, other types of models, as for example (conceptual) flow models based on the St. Venant equations. In that case one may e.g. omit uncertainties in the right hand side of the continuity equation to ensure a closed water mass balance (or again define uncertainties for fluxes as illustrated above). By means of uncertainties assigned to the momentum equations a spatial redistribution of the mass balance can then still be achieved. Such uncertainties in the momentum equations can then be seen as an extra external model forcing. For flow models this extra random forcing may for example represent errors in the meteorological model inputs.

The uncertainties $Z(\cdot)$ can again be a white or non white random noise as considered before and for the mathematical details, comments, and examples see Sections A1 and A2. A few additional aspects must still be mentioned, for example:

1. In case uncertainties are assigned to the state equations, the stochastic models for the $Z(\cdot)$ (including physical aspects such as the magnitude, and spatial and temporal
memory scales) must thus be designed at this ‘level’. Via the model (and the actual case specific values of its parameters and coefficients) and its propagation in time, these uncertainties are converted to the state variables. This translation may involve several linear or non-linear operations and therefore the statistics for the resulting uncertainties in the state variables (\( \Xi(\cdot) \), say) may not be very clear beforehand. In fact, the statistical properties of the \( Z(\cdot) \) and \( \Xi(\cdot) \) may be significantly different and \( \Xi(\cdot) \) may even exhibit an undesired non-physical behaviour. In practice one or more tests, variations, and sensitivity experiments may then be required to establish and verify the statistics of \( \Xi(\cdot) \) in more detail, and the model of \( Z(\cdot) \) must be modified until \( \Xi(\cdot) \) behaves satisfactorily.

2. The extension of the conceptual model with random noise must correspondingly be included in the numerical/algorithmic model. In this way it must be ensured, for example, that assumed physical properties, and/or important constraints (as e.g. conservation laws) are consistently incorporated in the discrete random model. Therefore the discretisation of the new random terms must be carried out with care, and its software implementation may require a significant effort (in contrast to the situation of Section A3.1 where the uncertainties are directly assigned to the state variables).

3. It must also be noted that in case random noise is assigned to the model equations (or parts of these such as fluxes) that this extension may be accompanied with a temporal and/or spatial differentiation of these noises (see equation A17 for a particular example). In order that these differentiations are well defined in the conceptual model and so do not induce undesired effects in applications (i.e. inaccuracies, instabilities, etc., in the numerical/algorithmic model due to large perturbations) the uncertainties should be sufficiently smooth. In such cases uncertainties should not be modelled as a white noise, and AR(1) processes (with an exponential auto-covariance function) may also be less suited. As a guideline for the verification of the smoothness of a random process the following theorem can be mentioned: a stochastic processes (in continuous time) is smooth (more precisely: differentiable in mean square sense) if its covariance function is twice differentiable.