Uncertainty Quantification for a Clarifier–Thickener Model with Random Feed

Raimund Bürger, Ilja Kröker, and Christian Rohde

Abstract The continuous sedimentation process in a clarifier–thickener can be described by a scalar nonlinear conservation law for the solid volume fraction. The flux is discontinuous with respect to space due to the feed mechanism. Typically the feed flux cannot be given in an exact manner. To quantify uncertainty the unknown solid concentration and the feed bulk flow are expressed by polynomial chaos. A deterministic hyperbolic system for a finite number of stochastic moments is constructed. For the resulting high-dimensional system a simple finite volume scheme is presented. Numerical experiments cover one- and two-dimensional situations.

Keywords Clarifier–Thickener model, Polynomial chaos, Uncertainty quantification, Galerkin projection, Finite–Volume method
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1 Introduction

Modelling uncertainty is important in many technical applications. Straightforward Monte-Carlo computations are easy but computationally inefficient or even impossible. The quantification of randomness by stochastic Galerkin or collocation methods seems to be more promising in many situations as this leads to deterministic models for at least a finite number of stochastic moments (cf. [MK05] for an overview).

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Roughly speaking, there is by now a well-understood theory for models that can be described by linear partial differential equations. What concerns nonlinear problems –we are interested in hyperbolic conservation laws– first steps have been done just recently [Abg07, PDL09, TLMNE10].

As a prototype model in this field we consider a clarifier–thickener (CT) model for the continuous fluid-solid separation of suspensions under gravity. The CT model provides an idealized description of secondary settling tanks in waste water treatment or of thickeners in mineral processing [BCBT99]. Typically, many input parameters can not be described with deterministic accuracy but behave noisily. We take into account two stochastic dimensions: the uncertainty of the rate of inflow of feed suspension and that of the fraction of solid material. This uncertainty produces a hyperbolic equation with a doubly random flux function. To be precise, consider the longitudinal-infinite vessel $D := \mathbb{R} \times S \subset \mathbb{R}^d$ with the cross-sectional domain $S \subset \mathbb{R}^{d-1}$ and coordinates $\mathbf{x} = (x_1, x_2, \dots, x_d)^T$. The longitudinal direction is aligned with gravity. For a final time $T > 0$ we search then as the unknown the solid volume fraction $u : D_T := D \times (0, T) \to [0, 1]$. According to [BKRT04, BWC00] the sedimentation process can be modelled by the initial value problem

$$\begin{aligned} u_t(\mathbf{x}, t, \omega) + \operatorname{div}\big(\mathbf{h}(\mathbf{x}, t, u(\mathbf{x}, t, \omega))\big) &= \delta(x_1) Q_{\mathrm{F}}(t, \omega_1) u_{\mathrm{F}}(t, \omega_2) && \text{in } D_T \times \Omega, \\ u(., 0) &= 0 && \text{in } D. \end{aligned} \tag{1}$$

The nonlinear flux is given by

$$\mathbf{h}(\mathbf{x}, t, u) = \mathbf{q}(\mathbf{x}, t) u + (\chi_{(-1,1)\times S}(\mathbf{x}) b(u), 0, \cdots, 0)^T,$$

where b is the given nonlinear batch flux density function. The vector field $\mathbf{q} = \mathbf{q}(\mathbf{x}, t) \in \mathbb{R}^d$ is the volume average flow velocity which satisfies a coupled Navier–Stokes-like system [BWC00]. For simplicity, we assume $\mathbf{q}$ to be a given deterministic quantity whose transversal components vanish on $\mathbb{R} \times \partial D$. Furthermore, $\chi_{(-1,1)\times S}$ is the characteristic function for the set $(-1, 1) \times S$. This choice describes the upper overflow boundary and the lower discharge boundary of the vessel. The right-hand side in (1) models the stochastic feed process. For probability measures P_1, P_2 let $\Omega = ((\Omega_1, P_1), (\Omega_2, P_2))$ be the vector-valued probability space. By $Q_{\mathrm{F}} = Q_{\mathrm{F}}(t, \omega_1) > 0$, $\omega_1 \in \Omega_1$, we denote the random feed rate and by $u_{\mathrm{F}} = u_{\mathrm{F}}(t, \omega_2) \in [0, 1]$, $\omega_2 \in \Omega_2$, the feed solid volume fraction. For the idealized vessel we assume that the feed source is distributed over the whole cross section $\{0\} \times S$, i.e. δ denotes the Dirac function in (1). As we will show below, the complete feed term in (1) can be rewritten as part of the flux such that (1) gets the form of a nonlinear conservation law with discontinuous flux. To our knowledge such a situation has not yet been treated in the framework of uncertainty quantification.

In Sect. 2 we detail the model and introduce an approximation for the stochastic process u by a polynomial chaos (PC-) ansatz. A numerical scheme for the PC-system on the base of the Lax–Friedrichs approach is presented. Note that the

Engquist–Osher flux, which is usually applied for problems with discontinuous flux, cannot be used for the higher-dimensional PC-system. Finally, in Sect. 3 numerical experiments are displayed.

2 A Polynomial Chaos Approach for Discontinuous Fluxes

2.1 Formulation of the Model

For notational simplicity we choose $d = 1$ (i.e. $S = \emptyset$) in (1) and use $x = x_1$ for the remaining vertical coordinate. The source term is formally rewritten as

$$\delta(x)Q_{\mathrm{F}}(t,\omega_1)u_{\mathrm{F}}(t,\omega_2) = (H(x)Q_{\mathrm{F}}(t,\omega_1)u_{\mathrm{F}}(t,\omega_2))_x, \tag{2}$$

where H denotes the Heaviside function. Following [BKRT04] we obtain then the flux formulation form

$$u_t(x,t,\omega) + \big(g(x,t,u,\omega)\big)_x = 0 \qquad \text{in } \mathbb{R}\times(0,T)\times\Omega. \tag{3}$$

The flux function g is determined for $t \in (0,T)$ and $\omega \in \Omega$ by the flux in (1) (see assumptions below) minus the flux in (2). This leads to

$$g(x,t,u,\omega) := \begin{cases} q_{\mathrm{L}}(t,\omega_1)(u-u_{\mathrm{F}}(t,\omega_2)) & \text{for } x < -1, \\ q_{\mathrm{L}}(t,\omega_1)(u-u_{\mathrm{F}}(t,\omega_2)) + b(u) & \text{for } -1 < x < 0, \\ q_{\mathrm{R}}(t,\omega_1)(u-u_{\mathrm{F}}(t,\omega_2)) + b(u) & \text{for } 0 < x < 1, \\ q_{\mathrm{R}}(u-u_{\mathrm{F}}(t,\omega_2)) & \text{for } x > 1. \end{cases} \tag{4}$$

To obtain this representation, firstly we have made for $q = q(x,t)$ the ansatz

$$q(x,t) = \begin{cases} q_{\mathrm{L}}(t,\omega_1) & \text{for } x < 0, \\ q_{\mathrm{R}} & \text{for } x > 0, \end{cases} \qquad q_{\mathrm{L}}(.,\omega_1) \in C^1([0,T)), q_{\mathrm{L}}(.,\omega_1) < 0,\ q_{\mathrm{R}} > 0.$$

Stochasticity is solely attached to q_{L}. Secondly, to ensure global conservativity, we have chosen $Q_{\mathrm{F}}(t,\omega_1) = q_{\mathrm{R}} - q_{\mathrm{L}}(t,\omega_1)$.

The flux (4) has discontinuities for $x \in \{-1,0,1\}$. We will not directly work with (3) but expand the equation to a system. For $x \in \mathbb{R}$, $t \in [0,T)$, $\omega_1 \in \Omega_1$ we define

$$\gamma^1(x,t,\omega_1) := \begin{cases} q_{\mathrm{L}}(t,\omega_1) & \text{for } x < 0, \\ q_{\mathrm{R}} & \text{for } x > 0, \end{cases} \qquad \gamma^2(x,t) := \begin{cases} 1 & \text{for } x \in (-1,1), \\ 0 & \text{for } x \notin (-1,1). \end{cases} \tag{5}$$

With the flux $f(t,u,\gamma^1,\gamma^2,\omega_2) := \gamma^1(\cdot,\omega_1)(u - u_{\mathrm{F}}(t,\omega_2)) + \gamma^2 b(u)$ we can understand (3), (4) as a (only seemingly trivial) system of balance laws

$$\begin{aligned} u(x,t,\omega)_t + \big(f(t,u,\gamma^1,\gamma^2,\omega_2)\big)_x &= 0, \\ \gamma_t^1(x,t,\omega_1) = H(-x)q_{\mathrm{L},t}(t,\omega_1), \qquad \gamma_t^2(x,t) &= 0 \end{aligned} \tag{6}$$

for the unknown vector $(u,\gamma^1,\gamma^2)^T \in [0,1]\times\mathbb{R}^2$.

2.2 Polynomial Chaos Representation

Let $\theta = \theta(\omega) = (\theta_1(\omega_1),\theta_2(\omega_2))^T \in \mathbb{R}^2$ be a vector of i.i.d. (independent identically distributed) random variables. Define

$$\psi_{jk}(\theta) = \phi_j(\theta_1)\phi_k(\theta_2) \quad (j,k\in\mathbb{N}_0),$$

where ϕ_k is the k-th Legendre polynomial. Then $\{\psi_{jk}(\theta)\}_{j,k\in\mathbb{N}_0}$ is a family of $L^2(\Omega_1\times\Omega_2)$-orthonormal polynomials in the sense

$$\big\langle\psi_{jk}(\theta),\psi_{lm}(\theta)\big\rangle_{L^2(\Omega)} := \int_{\Omega_1}\int_{\Omega_2}\psi_{jk}(\theta)\psi_{lm}(\theta)\,dP_1(\omega_1)dP_2(\omega_2) = \delta_{jk}\delta_{lm}. \tag{7}$$

We recall that for some second order random field $w = w(x,t,\omega)$ the polynomial chaos (PC-) representation

$$w(x,t,\omega) = \sum_{j,k\in\mathbb{N}_0} w^{jk}(x,t)\psi_{jk}(\theta(\omega)),\ w^{jk} := \int_{\Omega_1}\int_{\Omega_2} w\psi_{jk}\,dP_1(\omega_1)dP_2(\omega_2) \tag{8}$$

holds [GS91]. For the sake of a more handsome notation let $w^0,\dots,w^P$ for $P = P(M) = (M+1)(M+2)/2 - 1$ be an arbitrary but fixed re-indexing of the set $\{w^{jk} \mid j,k\in\mathbb{N}_0,\ j+k\le M\}$. The M-th order approximation of $w(x,t,\omega)$ in (8) is given by

$$(\Pi^P w)(x,t,\omega) := \sum_{p=0}^{P} w^p(x,t)\psi_p(\theta(\omega)).$$

The standard stochastic Galerkin approach (for the first equation in (6)) reads as follows. For $M\in\mathbb{N}_0$ find $u^0,\dots,u^P : D\times(0,T)\to\mathbb{R}$ such that

$$\int_{\Omega_1}\int_{\Omega_2}\Big(\Pi^P u + \big(\Pi_2^M\gamma^1\left(\Pi^P u - \Pi_1^M u_{\mathrm{F}}\right) + \gamma^2 b\left(\Pi^P u\right)\big)_x\Big)\,\Psi_q\,dP_1(\omega_1)dP_2(\omega_2) = 0 \tag{9}$$

holds for $q = 0, \ldots, P$. We used for the given, stochastically one-dimensional approximation of u_F the notation $\Pi_1^M u_{\mathrm{F}}$. An analogous formulation holds for the unknown (stochastically one-dimensional) approximation $\Pi_2^M \gamma^1$ of γ^1.
Using now the orthogonality from (7) the equations (9) can be written in the form

$$u_t^p + \left(\sum_{m=0}^{M} \sum_{q=0}^{P} \gamma^{1^m} u^q c_{mqp} - \sum_{m,l=0}^{M} \gamma^{1^m} u_{\mathrm{F}}^l(t) d_{mlp} + \gamma^2 \mathbb{E}\left[b\left(\Pi^P u \right) \psi_p \right] \right)_x = 0, \tag{10}$$

with $p = 0, \ldots, P$. Here $\mathbb{E}$ denotes the expectation value and

$$\begin{aligned} c_{mqp} &= \int_{\Omega_1} \int_{\Omega_2} \phi_m(\omega_2) \psi_q(\omega) \psi_p(\omega) \, dP(\omega_1) \, dP(\omega_2), \\ d_{mlp} &= \int_{\Omega_1} \int_{\Omega_2} \phi_m(\omega_2) \phi_l(\omega_1) \psi_p(\omega) \, dP(\omega_1) \, dP(\omega_2). \end{aligned} \tag{11}$$

Below we choose b to be a polynomial such that the expectation in (10) can be computed exactly.
We obtain finally from (10) and equations for $\gamma^{1^0}, \ldots, \gamma^{1^M}$ the $(P + M + 3)$-dimensional PC-system. Using the definition of the coefficients in (11) and the (weak) hyperbolicity of (6) it can be shown that the PC-system (10) is weakly hyperbolic.

2.3 1D Finite–Volume Method

The PC-system (10) is quite general and it appears hard to construct e.g. a Godunov-type solver. Therefore, at least in this paper, we use the simple Lax–Friedrichs method on a uniform mesh with cells $[x_{i-1/2}, x_{i+1/2})$, $i \in \mathbb{Z}$ and $\Delta x = x_{i+1/2} - x_{i-1/2}$. Restricting to the u-components $u^0, \ldots, u^P$ we have for time step $\Delta t^n > 0$ the scheme

$$u_i^{p,n+1} = u_i^{p,n} - \frac{\Delta t^n}{\Delta x} \left(F_{i+1/2}^{p,n} - F_{i-1/2}^{p,n} \right) \qquad (i \in \mathbb{Z},\ n \in \mathbb{N},\ p = 0, \ldots, P),$$

$$\begin{aligned} F_{i+1/2}^{p,n} := \frac{1}{2} \Big(& f^p(t^n, u_i^{0,n}, \ldots, u_i^{P,n}, \gamma_i^{1^{0,n}}, \ldots, \gamma_i^{1^{M,n}}, \gamma_i^{2,n}) \\ & + f^p(t^n, u_{i+1}^{0,n}, \ldots, u_{i+1}^{P,n}, \gamma_{i+1}^{1^{0,n}}, \ldots, \gamma_{i+1}^{1^{M,n}}, \gamma_{i+1}^{2,n}) \Big) + \frac{\Delta x}{2\Delta t^n} (u_{i+1}^{p,n} - u_i^{p,n}). \end{aligned}$$

The function f^p is defined by

$$f^P(t,u^0,\ldots,u^P,\gamma^{1^0},\ldots,\gamma^{1^M},\gamma^2) =$$
$$\sum_{m=0}^{M}\sum_{q=0}^{P}\gamma^{1^m}u^q c_{mqp} - \sum_{m,l=0}^{M}\gamma^{1^m}u_{\mathrm{F}}^l(t)d_{mlp} + \gamma^2\mathbb{E}\left[b\left(\Pi^P u\right)\psi_p\right].$$

Initial values are obtained from $u_i^0 = \ldots = u_i^{P,0} = \gamma_i^{1^{1,0}} = \ldots = \gamma_i^{1^{M,0}} = 0$ (cf. (1)) and averaging γ^1, γ^2 from (5) for $\gamma_i^{1^{0,0}}, \gamma_i^{2,0}$.

3 Numerical Experiments

Example 1: [1D Computation with one random dimension]
We consider the problem (3) with the batch flux function $b(w) := \frac{27}{4}w((1-w)^2)$ [BKRT04] and $u_0 = 0$. The solid volume feed fraction u_{F} satisfies

$$u_{\mathrm{F}}(t,\omega_1) := 0.6 + 0.2\theta(\omega_2),$$

such that θ is uniformly distributed on $[0, 1]$. Consequently the random variable u_{F} has the expectation 0.7. No further uncertainty is assumed. We choose $q_{\mathrm{L}} = -1$, $q_{\mathrm{R}} = 0.6$. Figure 1 shows (total view and blow-up close to inflow) the numerical solution with $P = 5$ together with the numerical solution of the deterministic problem using $u_{\mathrm{F}} \equiv 0.7$ and the numerical Monte-Carlo approach with 5000 samples computed with $\Delta x = 0.01$. We use Lax–Friedrichs method for our computation. Almost no differences can be detected.

This is confirmed by the subsequent table which displays the $L^1(\mathbb{R})$-difference between the Monte-Carlo sample solution and the PC-approach for $P = 1,\ldots,6$.

P	1	2	3	4	5	6
L^1-Error	1.1372e-02	1.5566e-02	3.2322e-03	1.4975e-03	8.5714e-04	5.0671e-04

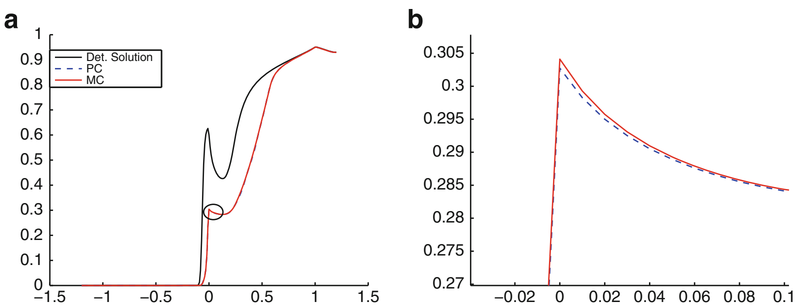

Fig. 1 Solid volume fraction for the deterministic case using the expectation value of the feeding rate, PC-solution, and Monte-Carlo samples. Blow-up in the right figure

We here observe a clear convergence for a reasonable number of stochastic modes.

Example 2: [1D Computation with two random dimensions]
We choose the same setting as in Example 1 but introduce the second random dimension in the suspension feed rate via

$$q_{\mathrm{L}}(t, \omega_1) = -1.2 + 0.4\theta(\omega_1).$$

Again let θ be uniformly distributed on the interval $[0, 1]$. Figure 2 shows the numerical solution with $M = 3$ and $P = 9$. This is compared with the numerical solution of the deterministic problem using the expectation values $q_{\mathrm{L}} = -1$ and $u_{\mathrm{F}} \equiv 0.7$, and the numerical Monte-Carlo approach with 50000 samples at time $T = 1$.

Already for this low random (and spatial) dimension we immediately attain the limits of available computing power. The table below shows the computing time of the PC-approach.

M (P)	1 (2)	2 (5)	3 (9)	4 (14)	5 (20)
cpu-time [s]	1.3721e+03	3.9463e+03	1.2037e+04	3.5001e+04	6.6399e+04

Example 3: [2D Computation with one random dimension]
Let us consider the CT problem (1) for $d = 2$ and $S = (-1.2, 1.2)$, with flux components $h_1(\mathbf{x}, t, u, \omega) = g(x_1, t, u, \omega)$ defined in (4) and $h_2(\mathbf{x}, t, u, \omega) = 0.02 * \cos(\frac{\pi x_2}{0.6}) u$ This corresponds not to a realistic velocity field $\mathbf{q}$ but we understand this example as a test case for the uncertainty quantification. The batch flux function b, solid volume feed fraction $u_F(t, \omega_1)$, and q_L, q_R are as in Example 1. For the numerical approximation we use an adaptive finite-volume method based on

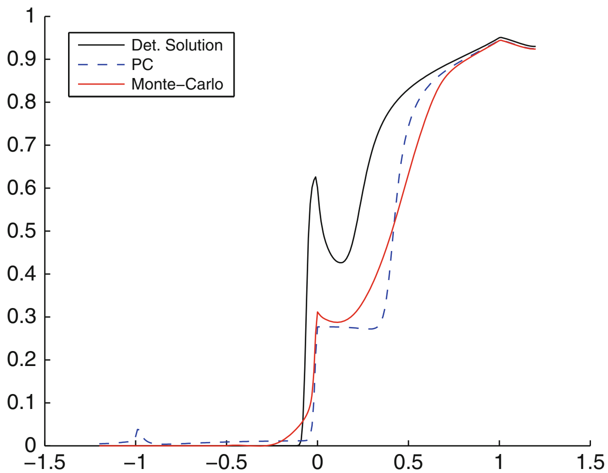

Fig. 2 Solid volume fraction for the deterministic case using the expectation values for solid fraction feeding rate and suspension feeding rate, PC-solution, and Monte-Carlo samples

unstructured triangular meshes with the Lax–Friedrichs flux (cf. [Krö08]). Initially 4608 triangles are used.

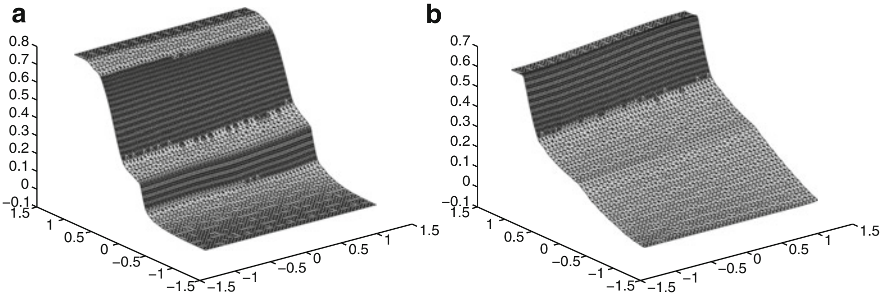

Fig. 3 Solid volume fraction for the deterministic case using the expectation values for solid fraction feeding rate and suspension feeding rate (a), and PC-solution (b) at time $T = 1$

Figure 3(a) shows a deterministic computation with $u_F = 0.7$ and the PC-solution with $P = 7$ (Fig. 3(b)). As in the 1D computations the PC-solution is much smoother and does not develop a peak close to the inlet. As a consequence the adaptive algorithm uses a coarser grid for the PC-solutions. To be specific, at $T = 1$ we had 11826 triangles for the deterministic computation, 8280 for $P = 7$, and 4608 for $P = 1$ (no refinement). Because of the long computation time of each deterministic solution, the computational effort of the Monte-Carlo simulation with a considerable number of samples significantly is higher then the computational effort of the PC approach.

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The paper is in final form and no similar paper has been or is being submitted elsewhere.