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Numerical Analysis

# A stochastic surrogate model approach applied to calibration of unstable fluid flow experiments

Un modèle approché stochastique pour la calibration d'expériences d'écoulements instables

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#### ABSTRACT

We propose a stochastic approach for calibration of mixing zone lengths in shock tube experiments. The methodology relies on taking into account uncertain initial data propagated through the basic multifluid Euler equations. In this work, the initial interface position is supposed uncertain, modeled by a stochastic process. The size of the mixing zone is then defined as the support of the probability density function of the stochastic process. This time dependent probability density function is estimated with nonintrusive generalized Polynomial Chaos, its support being in this case cheaply evaluated. This methodology relies on the application of an ergodic principle (Wiener, 1938) and generalizes linear perturbations analysis. It is applied in this Note to the calibration of several experimental results.

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#### RÉSUMÉ

Nous proposons une approche stochastique pour la calibration de tailles de zone de mélange d'expériences de tube à choc. La méthodologie repose sur la prise en compte de données initiales incertaines pour les équations d'Euler. Dans ce travail, la position initiale de l'interface est considérée comme incertaine, modélisée par un processus stochastique. La taille de la zone de mélange est alors définie comme le support de la densité de probabilité du processus. Cette densité de probabilité, fonction du temps, est estimée par Chaos Polynomial généralisé non-intrusif, son support pouvant dans ce cas être évalué à moindre coût. Cette méthodologie repose sur un principe d'ergodicité (Wiener, 1938) et généralise l'approche par perturbations linéaires. Elle est appliquée dans ce papier à la calibration de résultats expérimentaux.

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### Version française abrégée

L'étude d'écoulements instables compressibles par méthodes de perturbation a connu un regain d'intérêt ces dernières années [4,11], de telles méthodes restant toutefois limitées à l'étude de perturbations en régime linéaire [8]. Les méthodes de perturbation sont par ailleurs très utilisées en quantification d'incertitudes (UQ) et ont récemment été étendues pour

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l'approximation de variables aléatoires [17]. Le Chaos Polynomial généralisé (gPC), basé sur les travaux de Wiener [21], s'est révélé efficace pour résoudre les EDP stochastiques (SPDE) non linéaires et "contient" les méthodes perturbatives. Dans ce papier, tout comme gPC généralise les méthodes perturbatives en UQ, nous généralisons l'étude d'écoulements perturbés par gPC en réinterprétant des expériences de tube à choc (voir Fig. 1) comme des problèmes de UQ : nous résolvons les équations d'Euler incertaines et calibrons nos résultats numériques sur plusieurs expériences [13,18]. Les étapes du processus que nous proposons sont décrites unes à unes. La méthodologie proposée – modélisation de l'interface initiale incertaine (Section 2), résolution stochastique (Section 3) et définition de la taille de la zone de mélange (Section 5) – peut être considérée comme une application d'un *principe d'ergodicité* et des travaux de Wiener [21].

Initialement, l'interface incertaine est modélisée par un processus stochastique (SP) de noyau de covariance (1) supposé connu [22,7]. L'approximation de ce SP est assurée à t = 0 par un développement (3) de Karhunen–Loève (KL) tronqué à l'ordre Q, permettant son approximation sur une base de fonctions orthogonales définies par les fonctions propres de l'opérateur (2) et par les variables aléatoires (4) : cette décomposition assure le contrôle et la caractérisation de la condition initiale incertaine (moyenne, variance, longueur de corrélation) et fixe la dimension stochastique Q du problème de propagation d'incertitudes.

Lorsque t > 0, la statistique de l'interface incertaine n'est pas connue et reste à estimer. Pour cela, nous résolvons les équations d'Euler stochastiques multifluides (7)–(8)–(9) par Chaos Polynomial non-intrusif [2,10,15]. Le système stochastique est résolu par un schéma numérique 2D directions alternées de type Lagrange + Projection GAIA d'ordre 3 [5] en N points de quadrature, c'est-à-dire par N simulations indépendantes d'un code de calcul hydrodynamique 2D déterministe.

La position de l'interface  $x_{int}$  est alors approchée par son développement gPC (5) tronqué à l'ordre *P* dans chaque direction stochastique : nous choisissons de définir la *taille de la zone de mélange* comme le *support de sa densité de probabilité,* évalué par échantillonnage Monte-Carlo du développement gPC de  $x_{int}$ .

Les résultats expérimentaux de [13,18] associés aux conditions initiales données Fig. 1–(10)–(11) sont calibrés numériquement par la procédure précédente. La Fig. 2 (gauche) illustre la convergence numérique de l'approche et la Fig. 2 (droite) montre qu'un même noyau de covariance à 2 paramètres permet la calibration de trois expériences issues du même dispositif [18] pour des nombres de Mach sensiblement différents.

#### 1. Introduction

Linear perturbation methods have been given a lot of interest in CFD over the last decades [4,11] in order to predict growth rates of instabilities in various compressible fluid flow problems. They correctly estimate the growth rates of small amplitude defaults at early time, but fail at large amplitude and late time [8]. Perturbation methods are also well known in Uncertainty Quantification (UQ) and have been recently generalized for random variable (RV) approximation [17]. Indeed, spectral methods such as generalized Polynomial Chaos (gPC), based on the seminal work of Wiener<sup>1</sup> [21], have proven to be efficient for solving nonlinear Stochastic Partial Differential Equations (SPDE) and "contain" perturbation methods in the sense that solutions obtained with perturbation methods can be recovered with gPC. In this paper, just as gPC generalizes perturbation methods in UQ, we aim at generalizing the study of perturbed flow thanks to gPC. We directly follow the methodology described in [12] and deepen the study by reinterpreting shock tube experiments from [13,18] as uncertainty driven experiments. Such flows are subject to Richtmyer-Meshkov Instabilities (RMI) generated by shock waves interacting with interfaces between different materials. Initial perturbations on the interface grow in size and cause the materials to mix at late times. RMI plays an important role in Inertial Confinement Fusion (ICF). Fig. 1 presents a schematic of the planar version of the experiment where two fluids, one at rest (right fluid), and the other shocked (left fluid), are initially separated by a perturbed interface. When the shock hits the perturbed interface, hydrodynamic instabilities grow with time creating a mixing zone (MZ). In this paper, we aim at computing the temporal MZ size and comparing the numerical results to experimental ones inferred from flow visualizations. The effect of compression and nonlinearity combined to the interfacial perturbations strongly affect the MZ size [22,7]. In order to model and capture the dynamics, we suggest to model the initial interface by a stochastic process (SP) with known statistics and propagate this uncertainty through the flow field modeled by the basic Euler equations in order to quantify the effect on the MZ.

The paper is organized as follows: in the first section, we present two ways of approximating SPs. The first way, **K**arhunen–Loève (KL) expansions, is convenient when one has *a priori* information on the SP to represent. We suppose it is the case for the initially uncertain interface position as in [12]. The second way, gPC, allows accurate SP approximations relaxing the need for the *a priori* information on the covariance kernel of the SP. We will rely on this approximation scheme for the MZ size as soon as t > 0. In a second section, we briefly describe the multimaterial Euler equations and recall its main properties with the held discretization scheme. The stochastic counterpart of the system will be solved *non-intrusively*. In the last section, we define the MZ length in term of stochastic features of the uncertain interface position, we solve the stochastic multimaterial Euler equations in shock tube configurations and compare our numerical results to experimental ones. The suggested methodology – modelization of the SP (Section 2), stochastic resolution (Section 3) and definition of the size of the MZ (Section 5) – generalizes the linear perturbation approach and can be considered as an application of an *ergodic principle* as suggested by Wiener in [21].

<sup>&</sup>lt;sup>1</sup> Wiener proposed the use of *Gaussian* RVs, leading to *Hermite polynomial* approximations. The use of *arbitrary* RVs, with its *adapted gPC basis*, can be considered as an extension of Wiener's framework toward a better convergence rate for the stochastic resolution, see [3,19].



Fig. 1. Initial conditions for the four experiments from [13] (Poggi Thorembey Rodriguez (PTR)) and [18] (Vetter Sturtevant (VS)). Fig. 1. Conditions initiales pour les quatre expériences de [13] (Poggi Thorembey Rodriguez (PTR)) et [18] (Vetter Sturtevant (VS)).

#### 2. Modeling and representation of the uncertain initial interface

In this paper, we model the initial interface position by a SP. A SP, here the initial position of the uncertain interface  $x_{int}^0$ , is a collection of RVs indexed by a parameter  $y \in I \subset \mathbb{R}$ ,  $\{x_{int}^0(y,\omega), y \in I, \omega \in (\Omega, \mathcal{A}, \mathcal{P})\}$  where  $(\Omega, \mathcal{A}, \mathcal{P})$  is a probability space. For fixed y, referring to the vertical component of the interface spatial position (cf. Fig. 1),  $x_{int}^0(y,\omega)$  is a RV. The covariance kernel (1) of the SP is supposed known. This kernel partly describes the statistics of the uncertain interface.

$$K(y,\zeta) = \mathbb{E}\left[x_{int}^{0}(y,\cdot)x_{int}^{0}(\zeta,\cdot)\right] = \int x_{int}^{0}(y,\omega)x_{int}^{0}(\zeta,\omega)\,\mathrm{d}\mathcal{P}(\omega),\tag{1}$$

$$T_{K}f(y) = \int K(\zeta, y)f(\zeta) \,\mathrm{d}\zeta, \quad \forall f \in L^{2}(I).$$
<sup>(2)</sup>

In order to represent a SP of given covariance kernel, we rely on its Karhunen–Loève expansion [16] defined by (3) allowing the approximation of  $x_{int}^{0}(y, \omega)_{y \in I, \omega \in (\Omega, \mathcal{A}, \mathcal{P})}$  by a linear combination of orthonormal functions, eigenvectors  $(e_i)_{i \in \mathbb{N}}$  and eigenvalues  $(\lambda_i)_{i \in \mathbb{N}}$  of the covariance operator (2), and where  $\mu(y)$  is the mean of the SP.

$$x_{int}^{0}(y,\omega) = \mu(y) + \sum_{n=1}^{\infty} \Xi_{n}(\omega) \sqrt{\lambda_{n}} e_{n}(y),$$
(3)

$$\forall i \in \mathbb{N}, \quad \Xi_i(\omega) = \frac{1}{\sqrt{\lambda_i}} \int_{I} x_{int}^0(y, \omega) e_i(y) \,\mathrm{d}y. \tag{4}$$

The quantities  $(\Xi_n(\omega))_{n\in\mathbb{N}}$  are centered,<sup>2</sup> normalized<sup>3</sup> and orthogonal RVs defined by (4).

In practice, (3) is truncated up to an order Q which denotes the stochastic dimension of our UQ problem. Consequently, we consider an initial condition approximated by  $x_{int}^{0,Q}(y, \Xi(\omega)) \approx x_{int}^{0}(y, \omega)$  where  $\Xi(\omega) = (\Xi_1(\omega), \ldots, \Xi_Q(\omega))^t$ . The initial uncertainty being modeled by a SP, the uncertainty propagation step now consists in the resolution of a SPDE. Notice that the unknowns of the stochastic model we solve explicitly depend on the RV  $\Xi(\omega) = (\Xi_1(\omega), \ldots, \Xi_Q(\omega))^t$ . This resolution is described in the two next sections. We first describe the main features of gPC (Section 3), applied non-intrusively for the stochastic resolution and the deterministic model we are interested in (Section 4).

#### 3. Stochastic resolution by non-intrusive generalized polynomial chaos

In this work, when the covariance of the SP to represent is not known – i.e., as soon as t > 0 – our alternative is the application of gPC theory [21,19]. The gPC expansion provides a general representation of any square-integrable RV in term of standard RVs. Let us consider a RV  $\Xi(\omega) = (\Xi_1(\omega), \ldots, \Xi_Q(\omega))^t$  of independent components and denote by  $d\mathcal{P}^l(\omega)$  the probability measure of the *l*th component of  $\Xi(\omega)$  for all  $l \in \{1, \ldots, Q\}$ . Note that the independence of the RVs can be relaxed in this resolution step, see [9]. We denote by  $(\phi_k^l)_{k \in \mathbb{N}}$  the normalized one-dimensional polynomial associated to the RV  $\Xi_l(\omega)$  orthonormal with respect to  $d\mathcal{P}^l(\omega)$  i.e.,  $\mathbb{E}[\phi_k^l(\Xi_l)\phi_t^l(\Xi_l)] = \int \phi_k^l(\Xi_l(\omega))\phi_t^l(\Xi_l(\omega)) d\mathcal{P}^l(\omega) = \delta_{k,t}$ ,  $\forall l \in \{1, \ldots, Q\}$ ,  $\forall (k, t) \in \mathbb{N}^2$ . We denote by  $(\psi_k(\Xi(\omega)))_{k \in \mathbb{N}}$  the multidimensional normalized gPC basis of  $L^2(\Omega, \mathcal{A}, \mathcal{P})$  obtained by tensorization of the  $(\phi_k^l)_{k \in \mathbb{N}, l \in \{1, \ldots, Q\}}$  taken in  $(\Xi_l(\omega))_{l \in \{1, \ldots, Q\}}$ . This basis is orthonormal with respect to the probability measure  $d\mathcal{P}(\omega) = \prod_{i=1}^{Q} d\mathcal{P}^l(\omega)$ . The result is the following, see [1,19]: let  $u(y, \Xi(\omega))$  be a stochastic random process, such that  $\mathbb{E}[u^2(y, \Xi)] < \infty$ ,  $\forall y \in I$ , then

$$u^{P}(y, \Xi(\omega)) = \sum_{k=0}^{P} u_{k}(y)\psi_{k}(\Xi(\omega)) \stackrel{L^{2}(\Omega, \mathcal{A}, \mathcal{P})}{\underset{P \to \infty}{\longrightarrow}} u(y, \Xi(\omega)),$$
(5)

<sup>2</sup>  $\mathbb{E}[\Xi_n] = 0, \forall n \in \mathbb{N}.$ 

<sup>&</sup>lt;sup>3</sup>  $\mathbb{E}[\Xi_n^2] = 1, \forall n \in \mathbb{N}.$ 

$$u_k(y) = \mathbb{E} \left[ u(y, \Xi) \psi_k(\Xi) \right],$$

where  $(u_k(y))_{k \in \mathbb{N}}$  are the projections of  $u(y, \Xi(\omega))$  on the components of the gPC basis (6).

Consequently, once the basis  $(\psi_k)_{k \in \mathbb{N}}$  built – associated to the input RVs  $\Xi(\omega) = (\Xi_1(\omega), \dots, \Xi_Q(\omega))^t$  – the practical application of gPC implies estimating the coefficients  $(u_k(y))_{k \in \mathbb{N}}$ . For this, we rely on non-intrusive gPC: the approximation of the coefficients (6) for fixed  $y \in I$  is ensured by the introduction of quadrature rules with N points  $(w_j, \xi_j)_{j \in \{1, \dots, N\}}$  (for numerical integration see [15,10,2]), so that  $\forall k \in \{0, \dots, P\}$  we have  $u_k(y) = \int u(y, \xi)\psi_k(\xi) d\mathcal{P}(\xi) \approx \sum_{j=1}^N w_j u(y, \xi_j)\psi_k(\xi_j)$ . In the next section, we describe the stochastic model we solve at the quadrature points  $(w_j, \xi_j)_{j \in \{1, \dots, N\}}$  in order to

In the next section, we describe the stochastic model we solve at the quadrature points  $(w_j, \xi_j)_{j \in \{1,...,N\}}$  in order to estimate the size of the MZ with respect to time.

#### 4. Euler equations and deterministic hydrodynamic solver

Supposing uncertain initial conditions, we want to propagate uncertainty through the 2D multifluid Euler equations

$$\begin{cases} \partial_t \rho \alpha + \partial_x \rho u \alpha + \partial_y \rho v \alpha = 0, \\ \partial_t \rho + \partial_x \rho u + \partial_y \rho v = 0, \\ \partial_t \rho u + \partial_x (\rho u^2 + p) + \partial_y (\rho u v) = 0, \\ \partial_t \rho v + \partial_x (\rho u v) + \partial_y (\rho v^2 + p) = 0, \\ \partial_t \rho e + \partial_x (\rho u e + p u) + \partial_y (\rho v e + p v) = 0, \end{cases}$$

$$p(\rho, \varepsilon, \alpha) = \left( \Gamma(\alpha) - 1 \right) \rho \varepsilon \quad \text{with} \qquad (8)$$

$$\Gamma(\alpha) = \frac{\gamma_0(\gamma_1 - 1) + \alpha(\gamma_0 - \gamma_1)}{\gamma_1 - 1 + \alpha(\gamma_0 - \gamma_1)}, \qquad (9)$$

where all quantities depend on  $(x, y) \in \mathcal{D} \subset \mathbb{R}^2$ ,  $t \in [0, T] \subset \mathbb{R}^{+,*}$  and  $\mathcal{E}(\omega) = (\mathcal{E}_0(\omega), \dots, \mathcal{E}_Q(\omega))^t \in (\Omega, \mathcal{A}, \mathcal{P})$  denoting a random vector allowing the representation through KL development of Section 2 of the initial uncertain interface, modeled by a SP with given covariance kernel. The first equation corresponds to a closure equation for the mixture **e**quation **of s**tate (EoS), the quantity  $\alpha$  denotes the volume fraction of fluid 1. The quantity  $\rho$  is the mass density, u and v are the components of the velocity, p is the pressure, e is the specific total energy such that  $e = \varepsilon + \frac{u^2}{2} + \frac{v^2}{2}$  with  $\varepsilon$  the specific internal energy. The other equations correspond to – respectively – mass, momentum and total energy conservation. The closure is given by (8)–(9): we consider a perfect gas EoS (8) relying on the additivity of internal energies and isobaric hypotheses (9).

System (7)–(8)–(9) is hyperbolic [14] under conditions  $\varepsilon > 0$  and  $0 \le \alpha \le 1$ . From a numerical point of view, each system obtained for a fixed RV  $\Xi(\omega)$  is solved thanks to a directionally split 3rd order GAIA finite volume scheme with TVD limiters: all details concerning the deterministic numerical discretization are given in [5].

#### 5. Calibration of shock tube experiments

In this section, we apply the above surrogate strategy – i.e., modelization of an uncertain interface through a SP approximated by a KL expansion, resolution of the stochastic Euler equations (7) at quadrature points with GAIA scheme and approximation of the SP for t > 0 thanks to non-intrusive gPC – in order to calibrate the evolution with time of the size of the MZ in the experiments from [13,18]. Fig. 1 presents the initial conditions of the shock tube experiments given in papers [13] (PTR) and [18] (VS). We apply periodic boundary conditions at the top and bottom of the simulation domain and neutral and wall type boundary conditions on the left and right sides of the domain as in Fig. 1. Paper [18] (VS) presents results obtained with the same experimental device in three different configurations.<sup>4</sup>

The only calibration device of our surrogate approach consists in the initial SP (Section 2). We consequently have to "explore" the space of all SPs in order to calibrate the four shock tubes of [13,18]. The exploration space being large, we restrain our attention to an astutely chosen subclass of SPs. The following choices for the restrictions rely on mechanical engineering arguments. First, we consider homogeneous SPs [21,7,22]. Second, we focus on exponential covariances. This choice is motivated by the trigonometric form of eigenfunctions of exponential kernels, see [16], in agreement with what is considered in numerical and experimental mechanical designs [7,22,8]. The choice of the covariance kernel is not enough so as to fully characterize the initial SP, it remains to define the RVs (4). Always in order to avoid exploring a large space, we restrict ourselves to independent<sup>5</sup> uniformly distributed RVs on [-1, 1]. Uniformity is in agreement with initially very localized uncertainties in the experiments [13,18]. The truncation order of the KL expansion Q remains also a calibration parameter. In practice, the calibration of the experimental results with the above initial SPs was performed using *brute force* methods on the variances, correlation lengths and truncation order of the KL expansion. The held *two-coefficient* covariance

<sup>&</sup>lt;sup>4</sup> Same fluids and Atwood numbers, for different initial volumes of fluids and/or Mach numbers, see Fig. 1 top-right, bottom-left and bottom-right.

<sup>&</sup>lt;sup>5</sup> Note that the independence is also common, see [7,8,22].



Fig. 2. Comparisons between experimental (circles) and numerical results (dots). Left: experiment from [13]. Right: experiments from [18]. Fig. 2. Comparaisons entre expériences (cercles) et résultats numériques. Gauche : expérience de [13]. Droite : expériences de [18].

kernels for the simulations are given by (10) for [13] and by (11) for [18].

$$K_{PTR}(x, y) = 0.002 \exp\left(-\frac{|x-y|}{2.5}\right),$$
(10)  

$$K_{VS}(x, y) = 0.002 \exp\left(-\frac{|x-y|}{0.8}\right).$$
(11)

After some preliminary convergence tests and calibration, we decided to truncate the KL representations after the three main modes (Q = 3). For PTR, order Q = 3 ensures 90% of the statistics of the SPs is resolved, for VS, Q = 3 ensures 97% of resolution (see [16] for more details). Better results could probably be obtained by relaxing several of the previous hypothesis.

Let's now denote by  $x_{int}(t, y, \Xi(\omega)), t > 0$  the uncertain interface position.<sup>6</sup> We approximate  $x_{int}(t, y, \Xi(\omega)), t > 0$  thanks to gPC applying materials of Section 3 i.e., we have  $x_{int}(t, y, \Xi(\omega)) \approx x_{int}^{P}(t, y, \Xi(\omega)) = \sum_{k=0}^{P} x_{l,k}(t, y)\psi_{k}(\Xi(\omega))$ . Adopting an ergodic hypothesis, we evaluate the MZ length  $\Delta x_{int}(t)$  with respect to time by estimating the support of the probability density function of  $x_{int}^{P}(t, y, \Xi(\omega))$  and by taking its mean over y, the later being consistent with the information available in [13,18]. Therefore, we introduce

$$\Delta x_{int}(t) = \int_{I} \left( \max_{\Xi(\omega)} (x_{int}(t, y, \Xi(\omega))) - \min_{\Xi(\omega)} (x_{int}(t, y, \Xi(\omega))) \right) dy$$
(12)

where the max and min over the stochastic space are estimated by **M**onte-**C**arlo (MC) sampling of  $\Xi(\omega)$  in  $x_{int}^P(t, y, \Xi(\omega))$ . The latter estimation is cheap thanks to the gPC approximation.<sup>7</sup> The practical choice of the gPC order *P* as well as the choice of the number *N* of sampling points for integration are crucial for an accurate approximation. It is known gPC approximations suffer slow convergence rates when dealing with discontinuous solutions. We here want to emphasize that instead of looking for a polynomial approximation of the RV "mass density" in the vicinity of the interface, which is discontinuous, we focus on the RV "position of the discontinuity" which is continuous. Consequently, a low order gPC expansion is sufficient. In the following computations, we take an order 3 in each stochastic directions, hence  $P = (3 + 1)^3 = 64$ . For numerical integration, we take a fully tensorized Gauss–Legendre quadrature with 3 points in each stochastic directions leading to N = 27 deterministic independent runs of the hydrodynamic code for one curve.

Fig. 2 shows the evolution of the MZ lengths with respect to time. It presents a comparison between the experimental results of [13] (left) and [18] (right) and the numerical results obtained applying our stochastic approach and computing (12). The large circles correspond to an evaluation of the confidence in the experimental results [13,18]. The MZ lengths extracted from experiments are subject to experimental uncertainties together with uncertainties associated to the interpretation of the photographs plus our retranscription errors.

On Fig. 2 (left), three curves are displayed together with the experimental results of [13]. The first numerical curve comes from a linear theory calculation in Lagrangian coordinates with planar transverse perturbations also solved with a

<sup>&</sup>lt;sup>6</sup> Note that  $x_{int}(0, y, \Xi(\omega)) = x_{int}^{0,Q}(y, \Xi(\omega)) \approx x_{int}^{0}(y, \omega)$ .

<sup>&</sup>lt;sup>7</sup> Note that this MC estimation is licite. Indeed, the convergence in the  $L^2$  sense of gPC ensures the convergence in law hence the convergence of the characteristic function (according to Levy's continuity theorem) hence of the support of the approximation.

3rd order GAIA scheme, see [4]. Let's consider an infinitesimal perturbation  $\varepsilon$  of the interface position  $\Delta x$  at t = 0, then  $\Delta x(t = 0) = \Delta x_0 + \varepsilon \Delta x_1$ . Numerically, the amplitude of the perturbation has been set with  $\Delta x_0 = 0$ ,  $\Delta x_1 = 1$  together with planar transversal mode  $k_{\perp} = 4.82$ , see [4]. Note that this transversal mode is in agreement with the highest mode  $(\lambda_1, e_1(y))$  of the KL development (3) of the covariance kernel given by (10), see [16]. The curve obtained from the linear theory fits the experiment as long as the regime is linear but fails at later times i.e., after the second reshock here. The two other numerical curves are from our stochastic surrogate approach and are obtained with spatial discretizations of 8 and 16 cells per amplitude of the finest mode<sup>8</sup> of the initial perturbation<sup>9</sup> in (10). Both numerical results fit the experimental ones in the linear regime together with the nonlinear one and can be considered converged: the slight difference between the two curves can be explained by the use of a MC method in order to estimate the support of  $x_{int}^{P}(t, y, \Xi(\omega))$ .

Fig. 2 (right) shows the same kind of results obtained for the three shock tube experiments of paper [18]. We calibrated the approach on the VS85 experiment, corresponding to Mach number 1.5, and fed the two other studies with this same co-variance kernel (11) as an uncertain initial interface position. We observe that the same *two-coefficient* covariance kernel also allows the calibration of experiments VS87 and VS89 (Mach 1.98 and 1.24) and obtained from the same experimental device.

For VS85 and VS87, our surrogate approach seems to saturate earlier than the experimental results as the two last points are not reached. Several hypothesis can be made. First, it is known that gPC suffers long term integration problems [6,20]. Besides, it could also be due to 3*D* effects whereas in this paper, we only performed 2*D* simulations. Finally, we should also mention an eventual inadequacy of our stochastic surrogate model, which propagates the uncertainty on the initial interface position through the basic Euler equations.

#### 6. Conclusion

A stochastic surrogate model approach has been proposed to *calibrate* the nonlinear development of *mixing zones* in shock tube experiments. This stochastic approach is general and could be applied to other fluid flow problems. It is based on (i) modeling the uncertain initial interface position by a stochastic process and (ii) solving non-intrusively the resulting nonlinear stochastic Euler equations *via* several independent unstable flow simulations. The statistics of the uncertain interface position with respect to time, including mean value, variance and support of the probability density function – assimilated to the mixing zone length – are estimated by applying non-intrusive generalized Polynomial Chaos approximations. Such a stochastic approach embodies both a generalization of the *linear perturbation theory* and an application of an *ergodic principle* (Wiener, 1938). Numerical results for several multifluid shock tube experiments have been given: a reasonably good agreement is reached, provided the parameters of the covariance kernel characterizing the initially uncertain interface position are properly calibrated.

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<sup>&</sup>lt;sup>8</sup> Computations using  $500 \times 500$  and  $1000 \times 1000$  cells.

<sup>&</sup>lt;sup>9</sup> On these problems, the modal discretization can be considered fully resolved.