Robust simulation of nonclassical gas-dynamics phenomena

By P. M. Congedo†, P. Colonna‡, C. Corre†, J. Witteveen AND G. Iaccarino

A computational study of the occurrence of rarefaction shock-wave (RSW) in a dense gas shock-tube is presented. The approach is based on the characterization of experimental variability and uncertainties in the thermodynamic properties of the fluid to investigate the realizability and reproducibility of a RSW in the FAST shock-tube at Delft University of Technology. The weakness of the RSW makes its occurrence highly sensitive to uncertainties on the initial conditions and on the equation of state. In this work, computational fluid dynamics (CFD) and uncertainty quantification tools are combined to predict the probability of the RSW to occur and also to define experimental error levels required to ensure the reproducibility of the measurements.

1. Introduction

The experimental confirmation of nonclassical gas-dynamic effects in flows of dense vapors is one of the unanswered questions in fluid mechanics, since the initial theory was formulated by Bethe (1942) and later by Zel'dovich (1946) and Thompson (1971). For dense-vapor transonic flows of substances formed by complex organic molecules, phenomena such as rarefaction shock waves and compression fans are theoretically possible. Fluids that might exhibit nonclassical gas-dynamic phenomena are called BZT fluids from the name of the three scientists who first theorized their existence. These anomalies occur when the fundamental derivative of gas-dynamics $\Gamma = 1 + \frac{\rho}{a}\left(\frac{\partial a}{\partial \rho}\right)_s$ with ρ the fluid density, a the sound speed and s the entropy, becomes negative between the upper saturation curve and the $\Gamma = 0$ contour. Such a region is often referred to as the inversion zone and and the $\Gamma = 0$ contour is called the transition line.

Nonclassical gas-dynamic effects could be exploited to design highly efficient turbine nozzles for small Organic Rankine Cycle (ORC) turbogenerators (Brown & Argrow 2000), whereby the formation of compression shocks in the turbine passages can be highly reduced (or even suppressed) thus considerably increasing the isentropic efficiency of the expander (Monaco *et al.* 1997). ORC technology is among the best options for the conversion into electricity of renewable energy sources (solar radiation, biomass, geothermal heat, industrial waste heat).

An attempt to experimentally prove for the first time the existence of nonclassical gas-dynamics is underway at the Delft University of Technology. A newly realized shock-tube will be used to generate a rarefaction shock-wave (RSW) as depicted in Fig. 1 (Colonna *et al.* 2008c). Within the TU Delft project, several advancements with regard to the fundamental theory, thermodynamic modeling of the fluids (Colonna *et al.* 2006, 2008a; Nannan *et al.* 2007), the maximization of the effects (Guardone *et al.* 2010), and the numerical simulation of the fluid flow (Colonna & Silva 2003; Colonna & Rebay 2004),

† LEGI Lab, INPG (Institut National Polytechnique de Grenoble)
‡ Energy Technology Section, Delft University of Technology

have been performed. A major consideration emerged from these studies: if nonclassical gas-dynamic effects do exist, they are relatively weak, if compared, for instance with compression shock waves, and can occur only in a limited range of conditions. Figure 2 illustrates the inversion zone and transition line for a BZT fluid, called D6.

As shown for instance in Colonna *et al.* (2008a) and Colonna *et al.* (2006a), the accuracy of the thermodynamic model has a strong influence on the simulation of nonclassical phenomena, to the point that their presence can depend on the accuracy with which fluid model parameters are determined. Complex thermodynamic models of heavy organic fluids have been recently developed to this purpose, but their accuracy remains critical and somewhat questionable in the absence of detailed experimental characterization. Colonna *et al.* (2008c), Colonna *et al.* (2006a) and Colonna *et al.* (2009) also discuss how the accurate determination and setting of the initial conditions for the experiment play a crucial role for its success.

The accurate simulation of the rarefaction shock-wave experiment can provide considerable insights both for its design and its interpretation. Moreover, flow simulations can be used to design ORC turbines exploiting nonclassical effects, and, also in this case, the correct evaluation of the uncertainty in the simulation owing to the accuracy of the thermodynamic model and of the turbine inlet conditions, can be of great importance. In Cinnella *et al.* (2010), the influence of uncertainties on the critical properties is evaluated in order to compare different thermodynamic models for typical BZT fluids. This work illustrates how some of the more complex thermodynamic models can become inaccurate when small variations on critical properties are considered.

The purpose of the proposed research is to perform numerical simulations aimed at investigating the dynamics of a BZR fluid in a shock-tube. The computational setup mimics an experiment planned at TU Delft. Moreover the objective of our study is to determine the level of accuracy required in the experiment to conclusively demonstrate the presence of rarefaction shocks. For this purpose we analyze the results under variability due our limited ability to measure the initial conditions in the shock-tube. In addition, we also consider the potential uncertainty due to limited accuracy in the gas-dynamic models employed. The paper is organized as follows. Section II is devoted to the description of the various numerical tools needed in the study: the CFD solver for dense gas flows simulations, the thermodynamic models, and the uncertainty quantification approaches. Section III describes the preliminary analysis performed on the baseline configuration showing the necessity for a different choice of initial conditions. In section IV, a forward uncertainty propagation problem is performed comparing different stochastic methods in order to validate the statistics of the numerical solution and analyzing the robustness of the initial point chosen in section III. The closing section summarizes the conclusions that can be drawn from the present work regarding the topic of reproducibility of the rarefaction shock-wave and describes a new approach concerning the application of stochastic numerical solutions to the design of an experiment.

2. Methodology and tools

2.1. *CFD solvers for dense gas flows*

zFlow is a CFD code capable of treating dense gas flows (Colonna & Silva 2003; Colonna & Rebay 2004; Colonna *et al.* 2008b; Harinck *et al.* 2009, 2010; Rebay *et al.* 2009; Turunen-Saaresti *et al.* 2010), and initially developed by Rebay and Colonna. It is linked to the FluidProp thermodynamic library, also developed by the group of Colonna, which

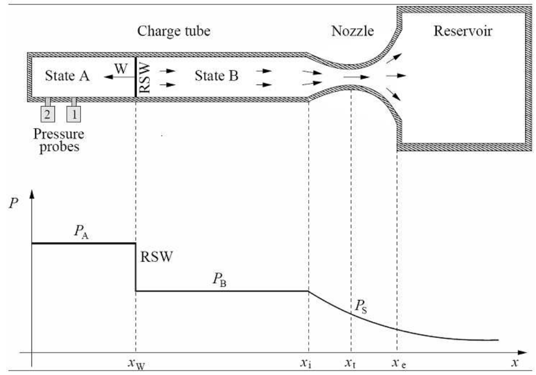

FIGURE 1. Schematic view (top) of the flexible Asymmetric Shock-Tube (FAST) setup and of a rarefaction shock-wave experiment. Qualitative pressure profile (below) along the shock-tube some time after the opening of the valve.

implements a wide variety of thermodynamic models and is based on data for a large quantity of fluids. zFlow can solve the Euler and the RANS equations coupled with the high- or low-Reynolds number k-ω turbulence models in one, two and three dimensions. Other distinguishing features are a high resolution upwind space discretization method for the advective fluxes suited to general unstructured and hybrid grids, and the use of an implicit time integration scheme, which proved to be crucial for the effective computations of fluids characterized by complex and computationally demanding equations of state.

NZDG code developed at LEGI-Grenoble by Congedo and Corre solves the quasi-one-dimensional Euler equations with second-order accuracy in time and space. The convective fluxes are discretized using the Roe numerical flux and a second-order limited MUSCL variable reconstruction. The Roe average for dense gas flows is computed with the simplified approach proposed in Cinnella (2006) and the slope limiter introduced in the linear reconstruction is of the Van Albada type. Second-order accuracy in time and robust time-integration are achieved using a three-level implicit formula to approximate the physical time-derivative, within a dual-time sub-iterative approach to solve the resulting non-linear system.

2.2. *Thermodynamic models*

Siloxane D6 is the fluid chosen for the TU Delft experiment. The Peng-Robinson-Strijek-Vera (PRSV) cubic equation of state (EoS) is considered to describe its thermodynamic behavior. This model is simpler than others, such as the multi-parameter equations of state of the Span-Wagner type (Colonna *et al.* 2006a, 2007a, 2008a), and is chosen here because it is less sensitive to the calibration of the coefficients as shown in Cinnella *et al.* (2010) and Congedo *et al.* (2010). This robustness properties is preferred here to the potential increased accuracy that would result from the use of the Span-Wagner models.

Peng & Robinson (1976) proposed a cubic EoS of the form:

$$p = \frac{RT}{v-b} - \frac{a}{v^2 + 2bv - b^2}. \tag{2.1}$$

where p and v denote, respectively, the fluid pressure and its specific volume, a and b are substance-specific parameters related to the fluid critical-point properties p_c and T_c. To achieve high accuracy for saturation-pressure estimates of pure fluids, the temperature-

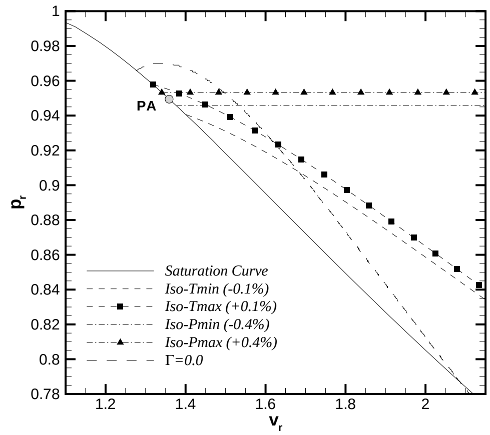

FIGURE 2. Amagat diagram near the saturation curve. Uncertainty region for the point PA.

dependent parameter a in Eq. (2.1) is expressed as

$$a = \left(0.457235 R^2 T_c^2 / p_c^2\right) \cdot \alpha\left(T\right) \tag{2.2}$$

whereas

$$b = 0.077796 R T_c / p_c. \tag{2.3}$$

These properties are not completely independent, since the EoS should satisfy the conditions of zero curvature and zero slope at the critical point. Such conditions allow computing the critical compressibility factor $Z_c = (p_c v_c)/(R T_c)$ as the solution of a cubic equation. The corrective factor α is given by

$$\alpha\left(T_r\right) = \left[1 + K\left(1 - T_r^{0.5}\right)\right]^2, \tag{2.4}$$

with

$$K = K_0 + K_1\left(1 + T_r^{0.5}\right)\left(0.7 - T_r\right)\ for\, T_r < 1\ \ \left(K1 = 0, for\, T_r \geq 1\right), \tag{2.5}$$

and

$$K_0 = 0.378893 + 1.4897153\omega - 0.1713848\omega^2 + 0.0196554\omega^3. \tag{2.6}$$

The parameter ω is the fluid acentric factor and K1 is obtained from saturation-pressure fitting of experimental data. The caloric behavior of the fluid is approximated through a power law for the isochoric specific heat in the ideal gas limit:

$$c_{v,\infty}\left(T\right) = c_{v,\infty}\left(T_c\right)\left(\frac{T}{T_c}\right)^n, \tag{2.7}$$

with n a material-dependent parameter.

2.3. *Sources of Uncertainty*

2.3.1. *Uncertainties in the initial conditions of the experiment*

The initial conditions (IC) for the experiment (and for the simulation) are prescribed according to the theory described in Guardone *et al.* (2010), to maximize the Mach number of the rarefaction shock-wave and facilitate the wave detection. The maximum achievable precision in controlling the temperature and pressure values in the charge tube has been estimated from the measurement instruments and hardware specifications to be 0.4% for the pressure and 0.1% for the temperature.

2.3.2. *Uncertainties on the thermodynamic model*

In the proposed study, PRSV cubic equation of state (Stryjek & Vera 1986) is chosen as thermal EoS. This equation can be considered a good trade-off between different needs because it simultaneously provides an accurate description of the gas behavior for a reduced computational cost and depends on a limited number of parameters hence a reduced number of uncertainty sources. Previous studies (Colonna *et al.* 2008a, Congedo *et al.* 2010) performed in the context of dense gas flows over airfoils have also demonstrated this EoS exhibits good robustness properties when dealing with uncertainties on thermophysical properties only. On the basis of the work of Colonna *et al.* (2008c), the following sources of uncertainty are retained, listed with their associated error bars: the acentric factor (2%), the factor K1 (2%), the isobaric specific heat in the ideal gas state, and the exponent n of power law (6%).

2.4. *Stochastic methods*

In this work we represent the uncertainties in terms of random variables, and consequently transform the original deterministic problem into a more complex stochastic one. Non-intrusive polynomial chaos, as implemented in the NISP (non-intrusive spectral projection) library, is used to deal with the quantification of the uncertainty effects. The development of NISP has been supported by the French National Research Agency (ANR) in the context of the OPUS (open platform for uncertainty treatment in simulation) project (see Congedo *et al.* (2010) for details). Applying this uncertainty quantification (UQ) tool to a CFD problem, such as the computation of a dense gas shock-tube with zFlow or NZDG, requires that a single conventional computation of the D6 flow in the FAST shock-tube is replaced with an ensemble of such computations, each run for specific values (abscissas) of the uncertain D6 thermodynamic properties and uncertain initial flow conditions. The choice of the abscissa depends on the specific methodology selected, such as polynomial chaos, sparse grid, etc. The size of the abscissa set depends on the number of uncertain parameters required and the accuracy determined. The coupling between the NISP UQ library and the available flow solvers has been performed in an earlier work (Congedo *et al.* 2010).

Polynomial chaos (PC) expansions have been derived from the original theory of spectral representation of stochastic processes using Gaussian random variables by Ghanem & Spanos (1991) and later extended by Xiu & Karniadakis (2002) to non-Gaussian processes. Any well-behaved process y (e.g., a second-order process) can be expanded in a convergent (in the mean square sense) series of the form :

$$y(x,t,\xi) = \sum_{\alpha} y_\alpha(x,t)\Psi_\alpha(\xi), \tag{2.8}$$

where ξ is a set of nx indipendent random variables $\xi = (\xi_1, \xi_2, ..., \xi_n)$, and α a multi-index $\alpha = (\alpha_1, \alpha_2, ..., \alpha_n)$, with each component $\alpha_i = 0, 1, ...$ The multivariate polynomial function Ψ_α is defined by a product of orthogonal polynomials $\Phi_i^{\alpha_i}(\xi_i)$ in relation to the probability density of the random variable ξ_i , i.e. $\Psi_\alpha(\xi) = \prod_{i=1}^{nx} \Phi_i^{\alpha_i}(\xi_i)$. A one-to-one correspondence exists between the choice of stochastic variable ξ_i and the polynomials $\Phi_i^{\alpha_i}(\xi_i)$ of degree α_i. For instance, if ξ_i is a normal/uniform variable, the corresponding $\Phi_i^{\alpha_i}(\xi_i)$ are Hermite/Legendre polynomials of degree α_i ; the degree of Ψ_α

is $|\alpha|_1 = \sum_{i=1}^{nx} \alpha_i$. The multivariate polynomial functions Ψ_α are orthogonal with respect to the probability distribution function of the vector ξ of standard independent random variables $\xi_i, i = 1, 2, ..., nx$.

Coefficients $y_\alpha(x,t)$ are the PC coefficients or stochastic modes of the random process y. Defining the scalar product by the expectation operator yields

$$y_\alpha(x,t) = \langle y(x,t), \Psi_\alpha \rangle \left\| \Psi_\alpha \right\|^{-2}. \tag{2.9}$$

For practical use, the PC expansions are truncated to degree no

$$y(x,t,\xi) = \sum_{|\alpha|_1 \le no} y_\alpha(x,t) \Psi_\alpha(\xi). \tag{2.10}$$

The number of multivariate polynomials Ψ_α , i.e., the dimension of the expansion basis, is related to the stochastic dimension nx and the degree no of polynomials and is given by the formula (nx+no)!/(nx!no!).

Several approaches can be used to estimate PC coefficients. The approach used in this paper is based on a non-intrusive formulation which employes numerical quadrature (see Congedo *et al.* (2010) for details). When the number d of variables is large, quadrature formulae using the tensor product of a one-dimensional integration require too many numerical evaluations, and a Sparse Grids integration derived from Smolyak's construction is preferred. The PC coefficients are evaluated from a set of abscissas and weights (ξ_i, ω_i) by formulae of the form

$$y_\alpha(x,t) = \left\| \Psi_\alpha \right\|^{-2} \sum_{i=1}^{n} y(x,t,\xi_i) \Psi_\alpha(\xi_i) \omega_i. \tag{2.11}$$

From the PC expansion of the random process, it is easy to derive its mean and variance and to estimate sensitivity information using the analysis of variance (ANOVA) decomposition (Congedo *et al.* 2010).

Also the simplex stochastic collocation (SSC) method (Witteveen & Iaccarino 2010) is used for computing the stochastic solutions. This approach is also based on quadrature formula, although uses an unstructured, simplex discretization of the space spanned by the uncertain parameters. The moments are computed as:

$$\mu_{\mathrm{u}_i} = \int_\Xi u(\boldsymbol{\xi})^i f_\xi(\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi} = sum_{j=1}^{n_\mathrm{e}} \int_{\Xi_j} u(\boldsymbol{\xi})^i f_\xi(\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi}, \tag{2.12}$$

with statistical moment μ_{u_i}, output of interest $u(\boldsymbol{\xi})$, vector of uncertain parameters $\boldsymbol{\xi}$ with probability density $f_\xi(\boldsymbol{\xi})$, and n_e disjoint elements Ξ_j in parameter space $\Xi = \bigcup_{j=1}^{n_\mathrm{e}} \Xi_j$. SSC builds local interpolants that are used as basis for the integration rule above; this leads to a reliable approximation of both smooth and discontinuous functions, as the local reconstruction satisfies the well-established local extremum diminishing (LED) robustness concept. The method achieves high efficiency using high degree polynomial interpolation, and by using adaptivity, which is performed as randomized point insertion whithin the unstructured grid (refinement sampling). The combination of the various techniques used in the SSC method results in a superlinear convergence rate and a linear increase of the initial number of samples with dimensionality.

3. Preliminary analysis on the reference configuration and setup conditions

Previous studies on the FAST tube have been performed by Colonna *et al.* (2008c) and Guardone *et al.* (2010) with an initial left state as reported in the *p*-*v* plane on Fig. 2, denoted PA and located on the saturation curve. These conditions were originally chosen to maximize BZT effects (Colonna *et al.* 2008c). Other initial left states have been discussed in Guardone *et al.* (2010), corresponding to more elevated pressures, closer to the critical region. Because the robustness or even validity of the thermodynamic model (TD) near critical conditions can be questionable, we retain point PA as reference left state. Since our goal is to account for the full set of physical uncertainties when investigating the FAST tube setup, stochastic methods are first applied to compute the variability of the saturation curves with respect to the uncertainties on the TD model parameters.

Monte Carlo sampling was used and it appeared that the point PA was probably located in the liquid-vapor mixture, an undesirable situation when performing the experiment. In the same p-v plane, the computed variability is plotted in Fig. 2 when the 0.4% and 0.1% uncertainties on the initial pressure and temperature are accounted for. Point PA is clearly not a robust left initial condition (IC) if single-phase conditions are to be guaranteed during the experiment.

A new initial left state can be found by ensuring initial single-phase conditions when the uncertainties on IC and TD are taken into account. Moreover, this initial left state should also be selected to maximize the strength of the RSW occurring in the FAST tube. In order to better understand the effect of the left state on the RSW characteristics, a parametric study is first performed by varying the IC: whereas the left state (pressure p_L and temperature T_L) varies in a region between the saturation curve and the $\Gamma = 0$ curve, the right state is obtained by fixing a pressure ratio p_R/p_L consistent with the value used in Colonna *et al.* (2008c) and a right temperature $T_R = T_L$. A CFD computation using NZDG for each combination of $(p_L, T_L), (p_R, T_R)$ is performed and the Mach associated to the RSW is stored. The resulting Mach contours are plotted in the *p*-*v* plane in Fig. 3 and demonstrate that a left state close to the saturation curve is required in order to obtain a high Mach number for the RSW. Consequently, the choice of a new initial left state must meet the following requirements: i) be insensitive to the uncertainties present, ii) remain in the single-phase region and iii) be close to the saturation.

An automatic procedure has been set up to compute such a state, which relies on an a priori analysis based on thermodynamic considerations only; an a posteriori analysis based on CFD computations is discussed in the next section. The algorithm used to automatically detect an initial left state satisfying the aforementioned requirements is based on three steps: in the first step, a discretization of the *p*-*v* plane is generated by moving along isobaric and isentropic curves; in the second step, the uncertainty region is computed using the given uncertainty levels on initial pressure and temperature and a Monte Carlo approach; in the third step, the uncertainty region should not cross the saturation curve (to avoid liquid-vapor mixture), but the chosen point should be located as close as possible to the saturation curve. This analysis yields a new initial left state, now denoted P1, represented in Fig. 4. The uncertainty region for P1 has a single point in common, without crossing, with the maximal allowed saturation curve computed with the TD uncertainties taken into account. The robustness of point P1 for performing the FAST experiment is assessed in the following a posteriori analysis.

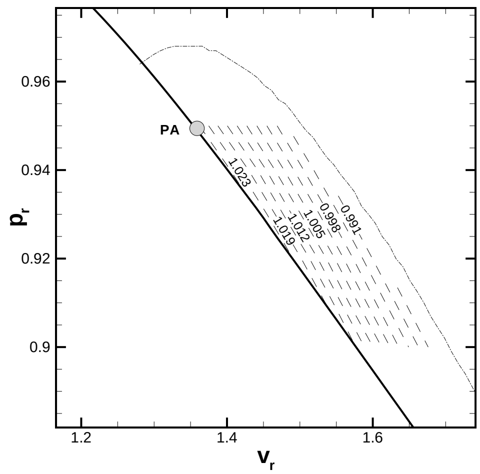

FIGURE 3. Dashed lines: iso-Mach contours of RSW, where each point of the contour represents the shock-tube left state in the Amagat diagram; solid line: saturation curve; dashdotted line: $\Gamma = 0$ line.

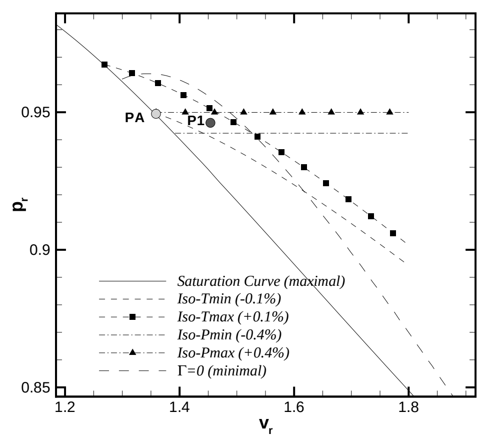

FIGURE 4. Robust point (P1) obtained by means of the automatic procedure, and uncertainty region.

4. Forward uncertainty propagation problem

The stochastic properties of the RSW generated in the shock-tube with uncertain IC and TD are computed in order to assess the probability of occurrence. A detailed cross-validation of the two numerical codes used to compute the dense gas flows is first described and the convergence of the stochastic method is analyzed; the occurrence of RSW for P1 initial conditions is discussed next.

The deterministic solution has been verified by means of comparisons between the zFlow and NZDG numerical codes. In this first numerical study, the initial conditions are taken from Colonna *et al.* (2008c), and the Riemann problem solutions provided by both codes are compared at several consecutive time steps. As shown in Fig. 5, for a non-

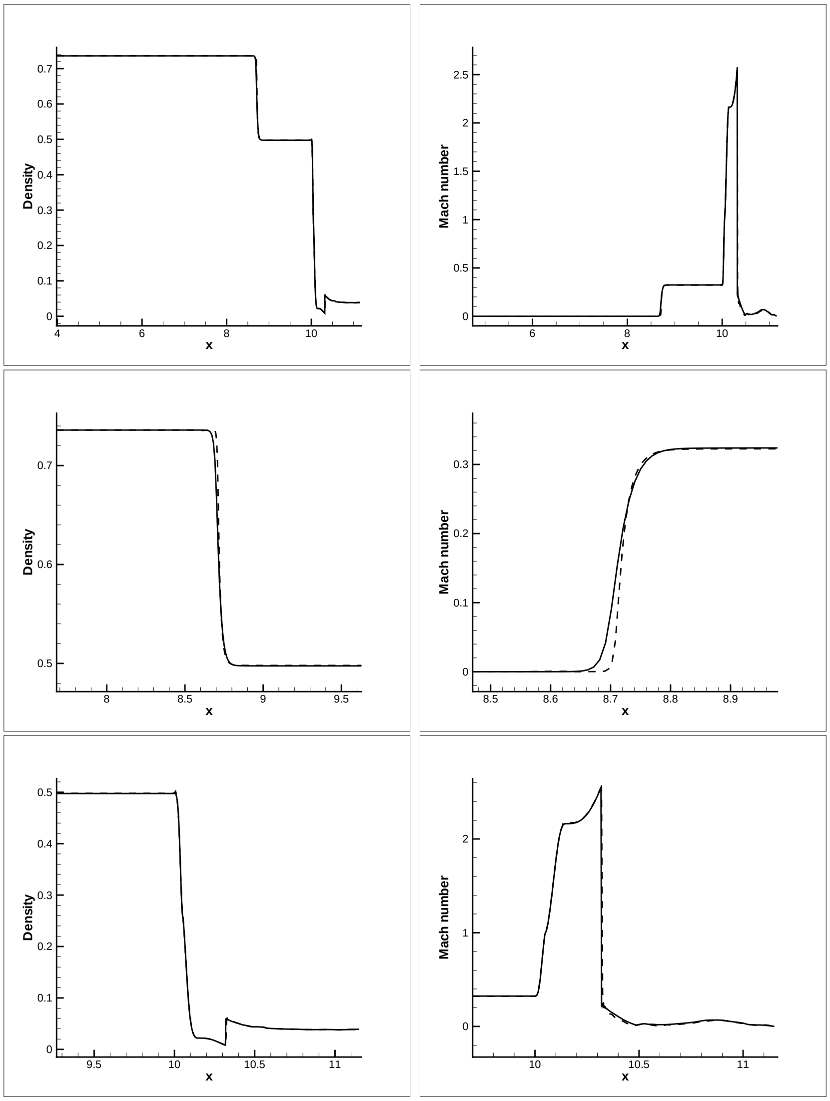

FIGURE 5. Solid line: zFlow; dashed line: NZDG. Left: density; right: Mach number. From top to bottom, solution along the tube, close-up on the expansion shock region, close-up on the nozzle region.

dimensional time t=2.5, solutions are very similar with only a slight difference near the expansion shock. In this region, the NZDG solution appears a bit less dissipative than the zFlow solution. Both numerical solutions are superimposed in the nozzle region. The same trends are observed for the density and Mach number distributions. The NZDG code has been used in the following computations. A mesh of 2000 cells have been chosen, after a convergence study not reported here for brevity. A deterministic computation takes 5 min on a Intel Westmere-EP processor.

Statistic computations have been performed for various sources of uncertainty (on initial conditions IC and/or thermodynamic model TD) and with various stochastic methods for a comprehensive validation of the results. The stochastic solutions provided by the PC method have been compared with Monte Carlo computations taken as reference. Comparisons have been made at different time steps with uncertainty sources taken into account separately (IC or TD) and together (IC+TD).

The P1 conditions produced by the a priori analysis have been retained for the left initial state. The reference solution obtained for the pressure distribution using a Monte Carlo technique for uncertain IC and TD is reported in Fig. 6. The mean stochastic solution and the deterministic solution differ near the RSW, the latter being sharper as expected. In Fig. 6, the region between the maximal and minimal pressure distributions along the tube represents the variability region for the stochastic solution when all the uncertainty sources are taken into account. Comparison between PC method and Monte Carlo shows that a good accuracy is obtained, with the former at a much reduced computational cost, because only 64 computations are necessary (when only four uncertain parameters are considered) with respect to 5000 Monte Carlo evaluations. In Fig. 7, the pressure standard deviation along the tube is compared for PC, SSC and Monte Carlo at a non-dimensional time of 2.5, when only IC uncertainties are taken into account. Monte Carlo and PC solutions show a great similarity, with a difference of 1% on only the computed standard deviation peak, as shown in Fig. 7. The SSC method is found less accurate in the peak region with a difference of 7.5% with respect to Monte Carlo; note, however, the SSC results have been obtained with fewer computations (only 35).

In Table 1, comparisons of Monte Carlo and PC results are reported in terms of the RSW position, velocity, and Mach number at a non-dimensional time of 2.5. The values provided in Table 1 express the difference on the computed coefficient of variation (standard deviation divided by the mean value). These variations have been computed when each source of uncertainty (IC or TD) is considered separately and when they are simultaneously taken into account. The difference between Monte Carlo and PC remain below 0.5% in all cases, which again confirms that accurate statistics can be computed with very few solution evaluations using PC. Note that the differences in statistic computations have been compared at several non-dimensional time steps, 1.5, 2.0, 2.5, and the same trends have been systematically observed.

The influence of each source of uncertainty on RSW properties is now analyzed using PC stochastic results. The coefficients of variation for the RSW properties are reported in Table 2. The uncertainties on initial conditions are clearly dominant for the shock position and velocity; when analyzing the shock Mach number, uncertainties on IC and TD are of comparable level. In Fig. 8, the distribution of the non-dimensional pressure standard deviation is reported along the tube, where uncertainties on IC and TD are considered separately or simultaneously. The solutions for IC and IC+TD are almost coincident (see in particular the close-up on the shock region displayed in Fig. 8). The same analysis has been performed at different times (1.5, 2.0, 2.5) and similar conclusions can be drawn.

Since Monte Carlo computations have been performed in this study, owing to the reduced computational cost of the quasi-one-dimensional flow, it is now possible to compute the probability distribution for the Mach number of the left-running wave. Specifically we are interested in evaluating the probability that the Mach number is less than unity because this is the necessary condition to observe a RSW. As shown in Fig. 9, this probability is equal to 27.8%, clearly an unsatisfactory prospect for the reproducibility of the experiments: the RSW will likely be observed roughly once in four shock-tube shots. In order to increase the probability for the Mach number to be greater than unity, it is necessary to reduce the level of variability on the IC and TD sources.

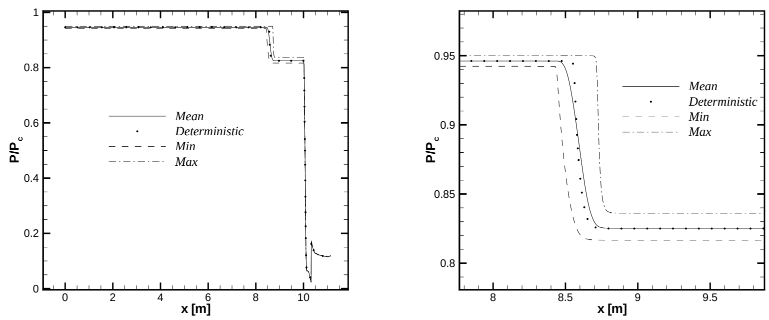

FIGURE 6. left: Mean, maximal, and minimal pressure along the tube computed by means of Monte Carlo computation (uncertainties on initial conditions and thermodynamic model); right: close-up on the expansion shock region.

	IC	TD	$IC + TD$
X_s	0.12	0.09	0.14
U_s	0.45	0.31	0.49
M_s	0.38	0.50	0.46

TABLE 1. A % variation between Monte Carlo and Chaos Collocation on position X_s, velocity U_s and Mach number M_s of the shock, when uncertainties on initial conditions and thermodynamic models are considered separately (IC and TD) and together (IC+TD).

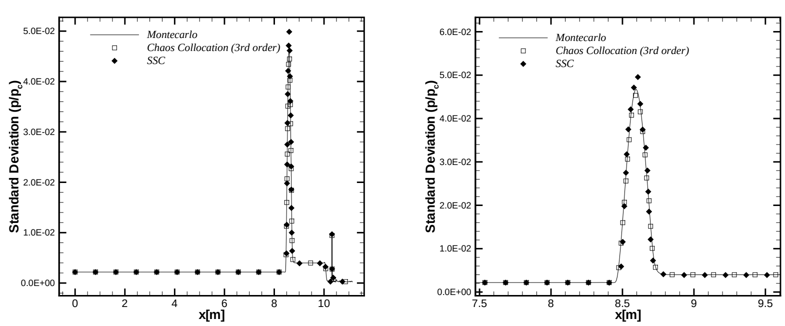

FIGURE 7. left: Comparison of pressure standard deviation between Monte Carlo and Chaos Collocation (uncertainties on initial conditions); right: close-up on the expansion shock region.

5. Conclusions

The objective of this work is to merge CFD codes with stochastic methodologies in order to aid the design of a dense gas flow experiment planned at TUDelft: FAST.

	IC	TD	$IC + TD$
X_s	0.58	0.06	0.59
U_s	3.21	0.31	3.24
M_s	0.80	0.39	0.90

TABLE 2. Coefficient of variation (%) for the position of the shock X_s, the velocity U_s and the Mach number M_s of the shock, when sources of uncertainties are considered separately (IC and TD) or together (IC+TD), adimensional time of 2.5.

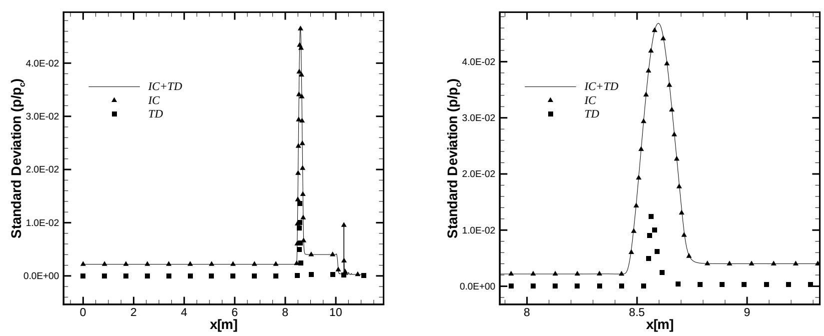

FIGURE 8. left: Standard deviation of pressure along the shock-tube , when uncertainties on initial conditions (IC) and thermodynamic model (TD) are considered separately and together (IC+TD); right: close-up on the expansion shock region.

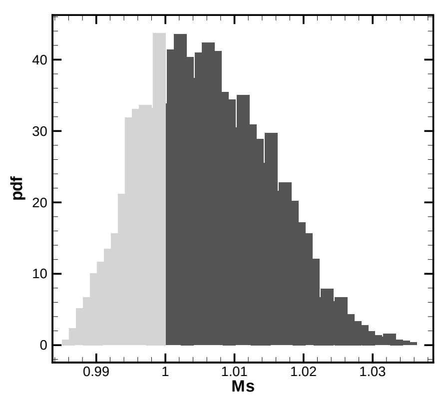

FIGURE 9. Probability density function for the left-running wave Mach number, computed from Monte Carlo results. Probability for the Mach to be inferior to unity equal to 27.8%.

Uncertainties are characterized in both the initial conditions and the thermodynamic models to increase the confidence in the predictions.

The numerical deterministic solution for the FAST geometry has been carefully verified by performing cross-validation between two available dense gas codes. Regarding the stochastic computations, the good accuracy provided by the PC approach for a reduced computational cost has been demonstrated by comparison with a Monte Carlo strategy. By considering only the thermodynamic model and its uncertainties, we first defined a robust initial condition for the shock-tube experiment: an initial condition that maximizes the strength of the RSW while keeping the flow in a single-phase region. Using this initial condition, on the basis of full CFD simulations a forward uncertainty propagation problem was considered, accounting for variability in both the initial conditions and the thermodynamic model. The probability for the RSW Mach number to be less than unity was found equal to 72.2%, a value considered too high for ensuring the reproducibility of the phenomenon. An inverse analysis will be performed in the future to determine how much the input uncertainties have to be reduced to increase this probability to a higher level.

REFERENCES

Bethe, H. A. 1942 The theory of shock waves for an arbitrary equation of state. Technical Report No. 545, Office of Scientific Research and Development.

Brown, B. P. & Argrow, B. M. 2000 Application of Bethe-Zel'dovic-Thompson fluids in organic Rankine cycle engines. *J. Power Sources* **16**, 1118.

Cinnella, P. 2006 Roe-type schemes for dense gas flow computations. *Computers & Fluids* **35** (10), 1264-1281.

Cinnella, P.,Congedo P.M., Pediroda, V., Parussini, L. 2010 Quantification of thermodynamic uncertainties in real gas flows. *International Journal of Engineering Systems Modelling and Simulation* **2**, 12-24.

Colonna, P. & Silva, P. 2003 Dense gas thermodynamic properties of single and multicomponent fluids for fluid dynamics simulations. *J. Fluid Eng.-T. ASME* **125** (3), 414-427.

Colonna, P. & Rebay, S. 2004 Numerical simulation of dense gas flows on unstructured grids with an implicit high resolution upwind Euler solver. *Int. J. Numer. Meth. Fl.* **46** (7), 735-765.

Colonna, P., Nannan N. R., Guardone A., Lemmon E. W. 2006 Multiparameter equations of state for selected siloxanes. *Fluid Phase Equilib.* **244**, 193-211.

Colonna, P., Guardone A., Nannan N. R. 2007 Siloxanes: a new class of candidate Bethe-Zel'dovich-Thompson fluids. *Phys. Fluids* **19** (8), 086102.

Colonna, P., Nannan N. R., Guardone A. 2008 Multiparameter equations of state for siloxanes: [(CH3)3-Si-O1/2]2-[O-Si-(CH3)2]i = 1...3, and [O-Si-(CH3)2]6. *Fluid Phase Equilib.* **263** (2), 115-130.

Colonna, P., Rebay S., Harinck, J., Guardone A. 2008 Real-gas effects in organic Rankine cycle turbine nozzles. *J. Propul. Power* **24**, 282-294.

Colonna, P., Guardone A., Nannan N. R., Zamfirescu C. 2008 Design of the dense gas flexible asymmetric shock-tube. *J. Fluid Eng.-T. ASME* **130**, 034501.

Colonna, P., Guardone A., Nannan N. R., Van der Stelt T. P. 2009 On the computation of the fundamental derivative of gas dynamics using equations of state. *Fluid Phase Equilib.* **286**, 43-54.

Congedo, P. M., Corre, C., Cinnella, P. 2007 Airfoil shape optimization for transonic flows of Bethe-Zel'dovich-Thompson fluids. *AIAA J.* **45** (6).

Congedo, P. M., Corre, C., Martinez, J. M. 2010 Shape optimization of an Airfoil in a BZT flow with multiple-source uncertainties. *Comput. Meth. Appl. Mech. Engrg.*, doi:10.1016/j.cma.2010.08.006.

Ghanem, R. G. & Spanos, S. D. 1991 Stochastic Finite Elements : a Spectral Approach. Springer Verlag.

Guardone A., Zamfirescu C., Colonna, P. 2010 Maximum intensity of rarefaction shock waves for dense gases. *J. Fluid Mech.* **642**, 127-146.

Harinck, J., Colonna, P., Guardone A. 2009 The influence of molecular complexity on expanding flows of ideal and dense gases. *Phys. Fluids* **21** (8), 086101-1-14.

Harinck, J., Colonna, P., Guardone A., Rebay S. 2010 Influence of thermodynamic models in 2D flow simulations of turboexpanders. *J. Turbomach.* **132**, 011001-17.

Monaco, J. F., Cramer, M. S. & Watson, L. T. 1997 Supersonic flows of dense gases in cascade configurations. *J. Fluid Mech.* **330**, 375–409.

Nannan N. R., Colonna, P., Tracy C. M., Rowley R. L., Hurly J. J. 2007 Ideal-gas heat capacities of dimethylsiloxanes from speed-of-sound measurements and ab initio calculations. *Fluid Phase Equilib.* **25** (7), 102-113.

Rebay S., Colonna, P., Pasquale D., Ghidoni A. 2009 Simulation of the turbulent dense gas flow through the nozzle of an organic Rankine cycle turbine. Proceedings of the 8th European Turbomachinery Conference, F. Heitmeir, F. Martelli, and M. Manna, eds., 1137-1148.

Stryjek, R. & Vera, J. H. 1986 PRSV: an improved Peng-Robinson equation of state for pure compounds and mixtures. *Can. J. Chem. Eng.* **64**, 323-333.

Thompson, P. A. 1971 A fundamental derivative in gas dynamics. *Phys. Fluids* **14** (2), 1843–1853.

Turunen-Saaresti, T., Harinck, J., Colonna, P., van Buijtenen, J. 2010 Computational study of a high-expansion ratio radial ORC turbine stator. *J. Eng. Gas Turb. Power.* **132**, 054501.

Xiu, D. & Karniadakis, G. E. 2002 The Wiener-Askey polynomial chaos for stochastic differential equations. *Journal of Science Computing* **26**.

Witteveen, J. A. S. & Iaccarino, G. 2010 Simplex elements stochastic collocation in higher-dimensional probability spaces. *12th AIAA Non-Deterministic Approaches Conference, Orlando, Florida*, AIAA20102924.

Zel'dovich, Y. B. 1946 On the possibility of rarefaction shock waves. *Zh. Eksp. Teor. Fiz.* **4**, 363.