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Bayesian quantification of thermodynamic uncertainties in dense gas flows

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ABSTRACT

A Bayesian inference methodology is developed for calibrating complex equations of state used in numerical fluid flow solvers. Precisely, the input parameters of three equations of state commonly used for modeling the thermodynamic behavior of the so-called dense gas flows, – i.e. flows of gases characterized by high molecular weights and complex molecules, working in thermodynamic conditions close to the liquid–vapor saturation curve – are calibrated by means of Bayesian inference from reference aerodynamic data for a dense gas flow over a wing section. Flow thermodynamic conditions are such that the gas thermodynamic behavior strongly deviates from that of a perfect gas. In the aim of assessing the proposed methodology, synthetic calibration data – specifically, wall pressure data – are generated by running the numerical solver with a more complex and accurate thermodynamic model. The statistical model used to build the likelihood function includes a model-form inadequacy term, accounting for the gap between the model output associated to the best-fit parameters and the true phenomenon. Results show that, for all of the relatively simple models under investigation, calibrations lead to informative posterior probability density distributions of the input parameters and improve the predictive distribution significantly. Nevertheless, calibrated parameters strongly differ from their expected physical values. The relationship between this behavior and model-form inadequacy is discussed.

1. Introduction

Flows of complex organic fluids close to saturation conditions are encountered in several engineering applications like energy conversion cycles [1–3], high-Reynolds wind tunnels [4], chemical transport and processing [5], and refrigeration [6]. In thermodynamic regions close to the liquid–vapor coexistence curve, the thermodynamic behavior of fluids with high molecular complexities differs significantly from that of a perfect gas and can no longer be represented by the polytropic perfect gas law. The largest deviations are encountered in the so-called dense gas flows [7–9] – for which a non-ideal dependence of the speed of sound on the fluid density is observed when the flow is submitted to isentropic perturbations – and most of all for a class of fluids known as the Bethe–Zel'dovich-Thompson (BZT) fluids [10–12]. Examples of gases exhibiting this special behavior are given by heavy hydro- and fluorocarbons and siloxanes, for which accurate and comprehensive thermodynamic data are scarce. As a consequence, high-accurate equations of state (EOS), i.e. thermodynamic laws designed to describe the fluid thermal and caloric behavior in the region of interest, are in general not available. Now, numerical simulations of dense gas flows, i.e. flows of molecularly complex gases at pressures and densities of the general order of magnitude of those of the liquid/vapor critical point, can be extremely sensitive to the model used to describe the fluid thermodynamic behavior [13]. This sensitivity is particularly large for BZT fluids, which are theoretically predicted to exhibit non-classical gas dynamic behaviors, like expansion discontinuities and splitting shocks, in a tiny thermodynamic region close to the liquid/vapor coexistence curve [14].

On the other hand, reliable simulations of compressible flows with complex thermodynamic behavior require the quantification of thermodynamic modeling errors, especially for those applications that look for improvements of the order of a few percents of the system performance, e.g. energy conversion cycles (see e.g. [3]).

For a given EOS, uncertainties of two kinds exist. The first source of uncertainty is represented by the mathematical form of the EOS to be used for a given fluid; on the other hand, the

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material-dependent coefficients associated to the EOS have to be calibrated from the available experimental data, which in turn are imperfectly known. Modeling uncertainties can be reduced to levels on the same order of the experimental uncertainty for molecularly simple well known fluids like water, hydrogen, or carbon dioxide (see [15]), i.e. even as low as 0.1%. For molecularly complex fluids reserved essentially to an industrial use, like the dense gases of interest here, high accurate experimental data are more hardly available, so that a significant uncertainty on the closure coefficients may exist. Specifically, critical-point properties and acentric factors are particularly important data for the calibration of EOS, and are commonly used as input parameters in cubic EOS as, e.g., the Soave–Redlich–Kwong [16] and Peng–Robinson–Stryjek–Vera EOS [17], and virial EOS like Martin–Hou [18] and Benedict–Webb–Rubin [19]. However, in the common practice these input parameters are most often used without including statistical uncertainty information. Precisely, they are input to the model to obtain deterministic solutions corresponding to their nominal values, despite that small errors, e.g. in the critical properties, may sometime affect the quality of final results in a quite dramatic fashion [20]. In addition to uncertainties associated to thermodynamic model parameters, previous work [13] shows that for some particularly complex gases the uncertainty associated to the mathematical form of the EOS, or model-form uncertainty, can be even overwhelming with respect to the parametric uncertainty.

In this work, we adopt a Bayesian approach to quantify modeling uncertainty associated to thermodynamic models used for dense gas flow simulations, i.e. we take the point of view that the uncertainty associated to both model parameters and mathematical form can be represented in terms of probability. A similar approach was used in the work of Robinson et al. [21], who investigated the impact of parametric and modeling uncertainties associated to the Mie–Grunheisen thermodynamic model by using, as a first step, Bayesian inference techniques to obtain a posteriori estimates of the closure coefficients associated to the EOS and, as a second step, by propagating posterior distributions through a numerical code for shock hydrodynamics. Precisely, they first calibrated the EOS coefficients using thermodynamic experimental data available for Aluminium 6061, and then propagated the posteriors through the fluid dynamic model. Here, we investigate the possibility of calibrating thermodynamic models by using directly aerodynamic data, i.e. data describing the flow behavior, instead of strictly thermodynamic information. For some engineering applications using complex fluids, this information is expected to be more readily available, e.g. through pressure taps inserted in the flow, than thermodynamic data. Moreover, this approach allows calibrating the model directly on observed data for the output quantities of interest, like velocity, pressure, and temperature fields. The statistical model adopted is similar to that used in [22,23] to calibrate closure parameters of turbulence models for a boundary layer flow. The procedure includes a statistical "model-inadequacy" term accounting for the gap between the model response obtained with the best-fit parameters and the (unobserved) true phenomenon. The feasibility of the proposed approach is investigated for a simple case study, i.e. the transonic flow of a silicon oil, namely cyclopentasiloxane (D5), past an airfoil, as in [13]. Experimental data being not available for this case, and since the scope of the present work is assessing the proposed calibration approach and not solving a realistic flow configuration, "synthetic" calibration data are generated by numerically computing the pressure distribution around the airfoil using a reference EOS based on Helmholtz free energy [24], which is considered as the best available thermodynamic model for the selected fluid. Numerical solutions of the flow equations are generated by means of a finite volume code based on a third-order accurate numerical scheme [25]. Using these synthetic data, we calibrate two well-known cubic EOS, namely, the Peng–Robinson–Stryjek–Vera (PRSV) [17] and the Soave–Redlich–Kwong (RKS) [16], and the five-term virial Martin–Hou (MAH) [18] model , coupled to the numerical flow solver. This results in posterior probability distributions for the model parameters. Moreover, calibration allows quantifying the model-form uncertainty. This information is propagated back through the flow solver for providing posterior predictive distributions of the quantity of interest.

The paper is organized as follows: in Section 2 we introduce the physical problem, the governing equations used to model the fluid flow of interest, and the thermodynamic models used to describe the fluid thermodynamic behavior, as well as the numerical methods used to solve them. In Section 3 we present the reference data used for calibration. Section 4 introduces an analytical model used to replace the costly numerical flow solver to speed up prior and posterior uncertainty quantification analyses. A preliminary sensitivity analysis is carried out in Section 5 to identify the most influential parameters and interactions between them. Section 6 sets the Bayesian calibration framework, including a discussion of the surrogate model used to represent the CFD code response to changes in the input parameters. Finally, Section 7 illustrates and discusses the numerical results, with focus on the role played by the model-inadequacy term to capture the calibration data.

2. Problem statement

In this study, we develop a methodology for calibrating thermodynamic models for the numerical simulation of dense gas flows, with focus on dense gas flow through energy conversion machines, and namely turbines of Organic Rankine Cycles (ORC). These are characterized by the presence of bladed disks. Blade sections can be roughly seen as airfoils. Hereafter, we investigate the feasibility of our calibration methodology for a simplified configuration, roughly representative of a blade section, i.e. an isolated airfoil. Such kind of configuration was often used in the past to investigate qualitatively dense gas effects in turbomachinery [26,27]. Moreover, for this simplified problem sensitivity studies of the impact of thermodynamic uncertainties on flow simulation results were carried out in [13].

Precisely, the selected case study is represented by the steady transonic flow of a dense gas over a wing section, namely, a NACA0012 airfoil. The working fluid is a siloxane (silicon oil), known with the commercial name of D5 (chemical formula $((CH_3)_2SiO)_5$).

The free-stream conditions of the flow, i.e. flow velocity and thermodynamic conditions at the far field, are treated in the following as deterministic and correspond to a value of the Mach number $M_\infty = 0.95$, an angle of attack equal to 0^0, a reduced pressure $p_{r,\infty} = 0.92$ and $\rho_{r,\infty} = 0.5263$.

Hereafter, we briefly describe the main features of dense gas flows, then introduce the equations used to model the flow, as well as the thermodynamic submodels used to describe the gas thermodynamic behavior, and finally provide some information about the flow solver used to generate numerical solutions.

2.1. Dense gas flows

Dense gas flows are flows of gases at thermodynamic conditions close to the liquid/vapor critical point, where the perfect gas law is invalid. In the dense regime, some heavy polyatomic fluids, referred to as the Bethe–Zel'dovich–Thompson (BZT) fluids, can exhibit non-classical nonlinearities, such as expansion shock waves, mixed shock/fan waves, and splitting shocks (see, e.g. [27] and