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# Bayesian calibration of the Peng-Robinson fluid model for siloxane MDM vapor flows in the non-ideal regime

G. Gori *, O. Le Maître †and P. M. Congedo ‡

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## ABSTRACT

Non-Ideal Compressible-Fluid Dynamics (NICFD) investigates the gas dynamics of a special class of fluids, typically (but not limited to) vapors of molecular complex compounds, characterized by a thermodynamic state space containing a *non-ideal* region. In the non-ideal regime, the fluid no longer behaves as an ideal gas with state equation $Pv = RT$ (whereas $P$ is the gas pressure, $v$ the specific volume, $R$ the gas constant and $T$ the temperature) and more complex fluid models are required. Currently, the community is racing to develop reliable and predictive tools to investigate the non-ideal dynamics and to ultimately improve the design of devices involving NICFD flows. A global perspective including experiments, computations, and theory is needed in order to develop sophisticated physical models as well as a systematic and comprehensive treatment of calibration and validation procedures.

This work focuses on the calibration of the polytropic Peng-Robinson (PR) fluid model [Peng and Robinson, 1976] for siloxane MDM (Octamethyltrisiloxane, $C_8H_{24}O_2Si_3$) vapor flows in the non-ideal regime. Specifically, the goal is to calibrate the material-dependent parameters appearing in the equations of state by combining experimental NICFD flows measurements with numerical simulations. The calibration process relies on a standard Bayesian inference framework and it takes advantage of the first-ever experiments on non-ideal expanding flows of siloxane MDM vapor [Spinelli et al., 2018]. The Bayesian framework to infer the polytropic PR model parameters accounts for uncertainties in the test-rig operating conditions (treated as nuisance parameters). Specifically, the inference considers the total pressure $P_t$ and total temperature $T_t$ at the inlet of the test section (uncertain operating conditions) and the fluid critical pressure $P_{cr}$,

*giulio.gori@inria.fr, DeFI Team, CMAP Lab (Ecole Polytechnique, Inria Saclay - Ile de France), 1 rue Estienne d'Orves, 91120 Palaiseau, France
†LIMSI, CNRS, Université Paris-Saclay, Bât. 508, rue John von Neumann, Campus Universitaire, F-91405 Orsay, France
‡DeFI Team, CMAP Lab (Ecole Polytechnique, Inria Saclay - Ile de France), 1 rue Estienne d'Orves, 91120 Palaiseau, France

critical temperature $T_{cr}$, acentric factor $\omega$ and specific heat ratio $\gamma$ (fluid model parameters of interest).

The Bayes' theorem reads

$$\mathcal{P}\left(\mathbf{q} \mid \mathbf{o}\right) \propto \mathcal{P}\left(\mathbf{o} \mid \mathbf{q}\right) \, \mathcal{P}\left(\mathbf{q}\right), \tag{1}$$

where $\mathbf{q} = (P_t, T_t, P_{cr}, T_{cr}, \omega, \gamma)^T$ is the vector of the unknown parameters and $\mathbf{o}$ is the vector containing the experimental measurements. Uniformly distributed prior distributions $\mathcal{P}\left(\mathbf{q}\right) \sim \mathcal{U}_{\mathbf{q}}[\mathbf{q}_{min}, \mathbf{q}_{max}]$ are considered. The prior bounds for the operating conditions were provided by the experimentalists. For the PR model parameters, the priors were set to largely encompass reference values reported in the literature and to satisfy thermodynamic stability criteria and physical limits. The likelihood $\mathcal{L} \triangleq \mathcal{P}\left(\mathbf{o} \mid \mathbf{q}\right)$ is considered Gaussian. The measurements set compounds $N_c$ experiments at different operating conditions and we explicitly define

$$\mathcal{L} = \Pi_{j=1}^{N_c} \mathcal{L}_j, \quad \mathcal{L}_j = \Pi_{i=1}^{N_{p,j}} \exp\left(-\left(O_{ij} - U_{ij}(\mathbf{q})\right)^2 / 2\sigma_{ij}^2\right), \tag{2}$$

where $N_{p,j}$ is the number of measurements in the $j$-th experiment, $O_{ij}$ is the measurement of probe $i$ in experiment $j$, $\sigma_{ij}^2$ is the measurement variance and $U_{ij}$ is the measured value predicted by the Computational Fluid Dynamics (CFD) model. SU2 is an open-source suite capable of dealing with non-ideal, fully turbulent, flows and it now embodies the reference among NICFD solvers [Economon et al., 2015, Gori et al., 2017]. The measurement variances were provided by the experimentalists. The resulting posterior distribution is sampled via a Markov-Chain Monte-Carlo (MCMC) approach based on the Metropolis-Hastings (MH) algorithm [Hastings, 1970]. As the sampling requires many model evaluations, we rely here on surrogate models for the $U_{i,j}(\mathbf{q})$.

Results reveal an inherent inconsistency between numerical predictions based on the model and the measurements. Indeed, the sole variation of the PR model parameters does not allow for significant mitigation of the discrepancy between computational results and experimental data. The inconsistency possibly arises from a bias error in the available measurements, from an epistemic uncertainty affecting the PR model, and (or) form using an inadequate computational model to reproduce the experimental flows. We discuss future investigations that could help clarifying the sources of inconsistency.

## References

[Peng and Robinson, 1976] Peng, D. Y. and Robinson, D. B. (1976). A New Two-constant Equation of State. *Ind. Eng. Chem. Fundam.*, 15:59–64.

[Spinelli et al., 2018] Spinelli, A. and Cammi, G. and Gallarini, S. and Zocca, M. and Cozzi, F. and Gaetani, P. and Dossena, V. and Guardone, A. (2018). Experimental evidence of non-ideal compressible effects in expanding flow of a high molecular complexity vapour. *Experiments in Fluids*, 59.

[Economon et al., 2015] Economon, T.D. and Palacios, F. and Copeland, S.R. and Lucaczyk, T.W. and Alonso, J.J. (2015). SU2: An Open-Source Suite for Multiphysics Simulation and Design. *AIAA Journal*, 54:828–846.

[Gori et al., 2017] Gori, G. and Zocca, M. and Cammi, G. and Spinelli, A. and Guardone, A. (2017). Experimental assessment of the open-source SU2 CFD suite for ORC applications. *Energy Procedia*, 129:256–263.

[Hastings, 1970] Hastings, W.K. (1970). Monte Carlo sampling methods using Markov chains and their applications. *Biometrika*, 57:97–109.