Bayesian quantification of thermodynamic uncertainties in dense gas flows

Xavier MERLE
Paola CINNELLA

DynFluid Laboratory - Arts et Metiers ParisTech Paris
151, Bvd. de l'Hôpital - 75013 Paris, France

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Context

- Flows of complex organic fluids close to saturation conditions are encountered in many engineering applications:
  - high-Reynolds wind tunnels to chemical transport,
  - refrigeration,
  - energy conversion cycles,
  - ...
- For compressible single-phase flows occuring in thermodynamic conditions close to the liquid-vapor coexistence curve, the fluid thermodynamic behaviour differs significantly from that of a perfect gas and can no longer be represented by the polytropic perfect gas law.

Consequences

We have to find other Equations of State (EOS) to represent this particular thermodynamic behaviour!

Main Issues

- Countless EOS have been proposed in the literature, diversified according to the substance to be modelled.
- EOS based on theoretical and analytical criteria,
  - van der Waals,
  - Redlich-Kwong,
  - Peng-Robinson,
  - Martin-Hou,
  - ...

  provided that some thermodynamic inputs are available for the substance of interest.
- However, such data are typically affected by more or less significant experimental errors.

Consequences

Several uncertainties related to the use of such complex EOS coming from:

- the values taken by the substance-specific coefficients,
- the functional form of the model.

Main Issues

In these conditions, an interesting work to do is:

- to evaluate the response of the system to the uncertainties in the input parameters (Cinnella *et al.* [1]),
- to calibrate the input parameters, thanks to some experimental data, to improve the way an EOS represents the thermodynamic behaviour (this work).

Problem: no experimental data available up to now!

Consequences

Reference data generated by using a more complex EOS ⇒ investigation of the feasibility of the calibration procedure.

Side effect: calibration of simple, cheap EOS on a more complex, accurate and expensive one.

For this study, we use:

- Span-Wagner EOS as the reference,
- Redlich-Kwong (RKS), Peng-Robinson (PRSV) and Martin-Hou EOS to be calibrated.

[1] **Paola Cinnella, Pietro Marco Congedo, Valentino Pediroda and Lucia Parusini, "Sensivity analysis of dense gas flow simulations to thermodynamic uncertainties," Phys. Fluids, 23, 116101, 2011.**

Bayesian Inference - framework

The Bayesian inference framework is employed to perform the calibration.
In our case, the Bayes rule takes the form:

$$\underbrace{p(\theta|d,y)}_{\text{posterior}} \propto \underbrace{p(d|y,\theta)}_{\text{likelihood}}\underbrace{p(\theta)}_{\text{prior}}$$

where

- θ is a random vector of parameters,
- y is the dense gas solver output quantity of interest (model),
- $\mathbf{d}$ is the experimental (numerical) data.

The quantity of interest is the criterion used for the calibration and is therefore chosen according to the experimental data.

- the calibration is performed from simulations of transonic dense gas flows (D5, siloxane) around a NACA0012 airfoil,
- quantity of interest: the pressure coefficient $C_p = \dfrac{p - p_\infty}{\frac{1}{2}\rho_\infty U_\infty^2}$, at 17 locations along the airfoil wall (simulated pressure taps).

Bayesian Inference - simulations

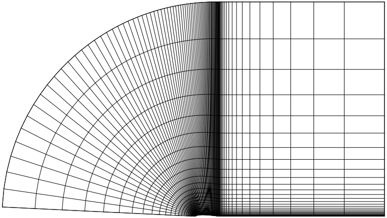


Figure: Mesh around a NACA0012 profile.

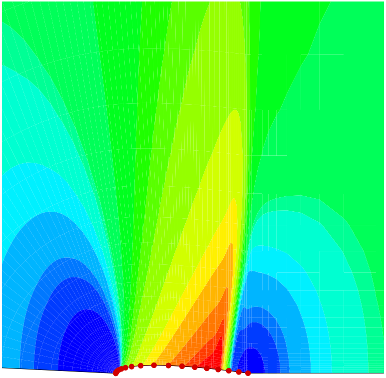


Figure: Iso-contours of pressure coefficient. ●: numerical pressure sensors.

Bayesian Inference - prior and likelihood

A common practice, when no particular informations are available about the parameters, is to impose uniform distributions for prior:

$$p(\theta) \sim \mathcal{U}([a, b])$$

For the likelihood, we modelled the data d as:

$$d(x_i) = \hat{d}(x_i) + e_i$$

- e_i, the experimental noise; e_i is assumed to be independant and normally distributed with mean zero and a standard deviation of 10% of the observed value.
- $\hat{d}(x_i)$, the true pressure coefficient value at x_i. $\hat{d}(x_i)$ is assumed to be equal to the modelled value $y(x_i)$, multiplied by an error coefficient η_i:

$$\hat{d}(x_i) = \eta_i y(x_i, \theta)$$

which takes into account the discrepancy between the simulation and the actual system.
η is assumed to be well represented by a correlated Gaussian model of the form: $\eta \sim \mathcal{N}(1, K_M)$

Bayesian Inference - prior and likelihood

Finally, the likelihood can be written under the form:

$$p(d|y,\theta) = \frac{1}{\sqrt{(2\pi)^n |K|}} \exp\left[-\frac{1}{2}(d-y)^T K^{-1}(d-y)\right]$$

- $K = K_e + K_M$, with K_e a diagonal matrix with corresponding variance and

$$K_M = \sigma^2 \exp\left[-\left(\frac{x-x'}{10^\alpha X}\right)^2\right]$$

  where x and x' are two subsequent observations abscissa separated by the length scale $10^\alpha X$ ($X \approx 1$).
  σ and α become new parameters (known as hyper-parameters)
- $\theta = (\theta_p, \theta_h)$.

The inference is done using sampling techniques of the prior and the likelihood:

- *pymc* python library, based on a Markov-Chain Monte-Carlo sampler and the Metropolis-Hastings algorithm,
- samples of 200 000 draws are used, the first 50 000 of which are rejected.

Dense gas solver

Dense gas effects essentially influence the inviscid flow behaviour

- analysis of single-phase compressible inviscid flows, governed by the Euler equations and completed by a real-gas thermodynamic model.

More specifically:

- 2-D flows (100×32 grid),
- cell-centred finite volume scheme for structured multi-block meshes of third-order accuracy,
- scalar dissipation (to reduce the computational costs),
- local time stepping, implicit residual smoothing and multigrid are used to efficiently drive the solution to the steady state.

The computation is about 10 minutes long on a classical personal computer:

- need for a surrogate model,
- in this work: piecewise multidimensional Lagrange interpolations.

Equations of state

- thermal equation: functional relation between thermodynamic variables

$$\text{e.g } p = \frac{RT}{\nu - b} - \frac{a/T^{0.5}}{\nu(\nu + b)}$$

- caloric equation: temperature dependence of internal energy or heat capacity

$$\text{e.g } c_{\nu,\infty}(T) = c_{\nu,\infty}(T_c)\left(\frac{T}{T_c}\right)^n$$

- these relations involve a lot of parameters and variables: pressure temperature, specific volume...
- for the EOS we are interested in:

Redlich-Kwong and Peng-Robinson:
- the exponent n
- the reduced ideal-gas isocoric heat $c_{\nu,\infty}$
- the acentric factor ω

Martin-Hou:
- the critical temperature T_c
- the reduced ideal-gas isocoric heat $c_{\nu,\infty}(T_c)$
- the critical pressure p_c

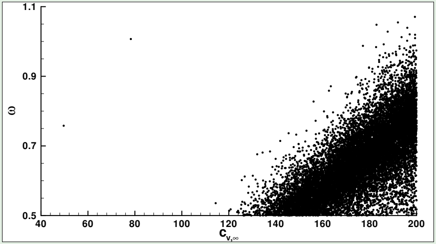
Preliminary analyses

- Sobol analysis (Monte-Carlo):

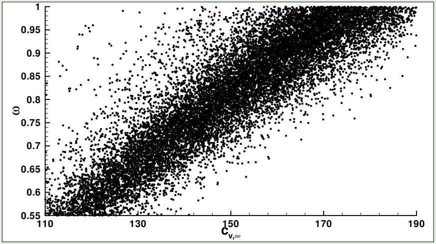
	Strong influence on C_p	Weak influence on C_p
RKS	ω, $c_{\nu,\infty}(T_c)$	n
PRSV	ω, $c_{\nu,\infty}(T_c)$	n
MAH	T_c, p_c, $c_{\nu,\infty}(T_c)$	

- correlations:

Redlich-Kwong



Peng-Robinson



Preliminary analyses

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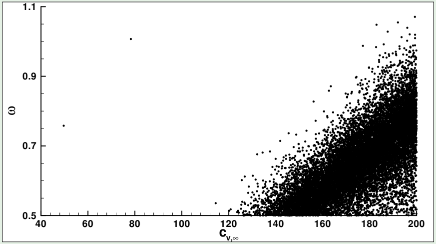
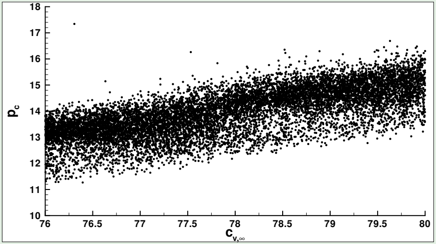


Martin-Hou



Preliminary analyses - preliminary conclusion

The previous observations allow to reduce the number of parameters:

- Redlich-Kwong: the calibration is performed with only one parameter (ω) whereas n and $c_{\nu,\infty}(T_c)$ are taken at fixed values

$$\begin{cases} n = 0.5 \\ c_{\nu,\infty}(T_c) = 180.0 \end{cases}$$

- Peng-Robinson: the calibration is performed with only one parameter (ω) whereas n and $c_{\nu,\infty}(T_c)$ are taken at fixed values

$$\begin{cases} n = 0.5 \\ c_{\nu,\infty}(T_c) = 150.0 \end{cases}$$

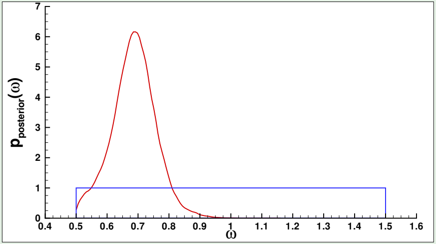
- Martin-Hou: the calibration is performed with the two parameters T_c, p_c whereas $c_{\nu,\infty}(T_c) = 78.0$

Calibration - Redlich-Kwong

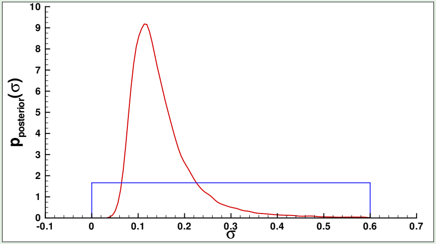
- legend:
  - prior
  - posterior
- statistics:

	Mean	Standard deviation
ω	0.68609	0.07180
σ	0.15079	0.07028
α	-0.97095	0.19811

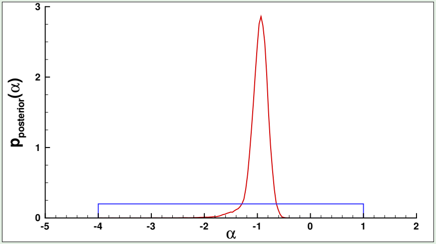
$p_{\text{posterior}}(\omega)$



$p_{\text{posterior}}(\sigma)$



$p_{\text{posterior}}(\alpha)$

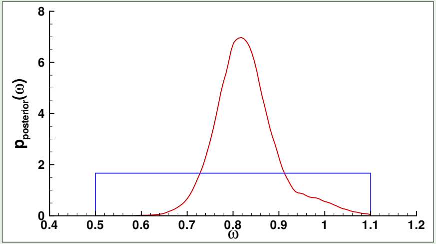


Calibration - Peng-Robinson

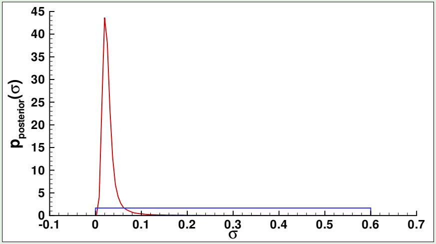
- legend:
  - prior
  - posterior
- statistics:

	Mean	Standard deviation
ω	0.82925	0.06900
σ	0.03050	0.02872
α	-1.58707	0.56775

$p_{\text{posterior}}(\omega)$



$p_{\text{posterior}}(\sigma)$



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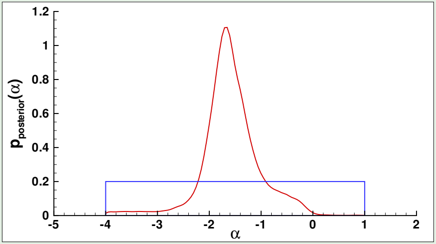
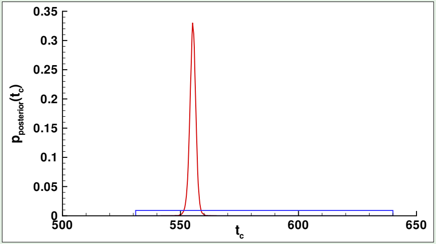


Calibration - Martin-Hou

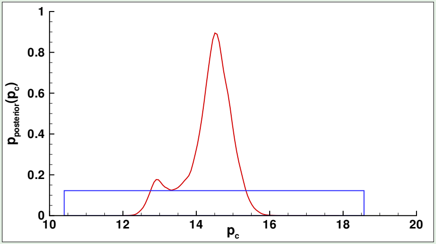
- legend:
  - prior (blue)
  - posterior (red)
- statistics:

	Mean	Standard deviation
T_c	555.20456	1.37210
p_c	14.33245	0.64496
σ	0.07523	0.02481
α	-1.60219	0.33949

$p_{\text{posterior}}(T_c)$



$p_{\text{posterior}}(p_c)$



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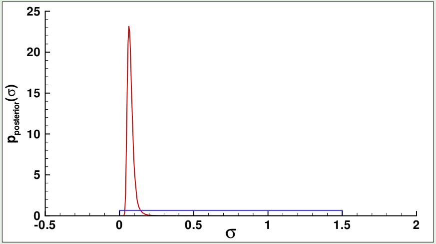
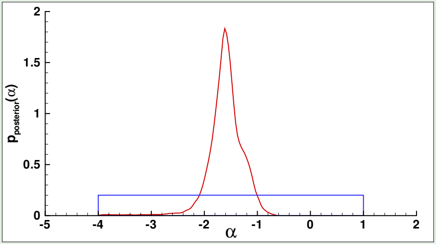
$p_{\text{posterior}}(\sigma)$

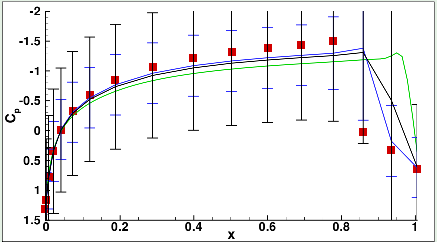


$p_{\text{posterior}}(\alpha)$

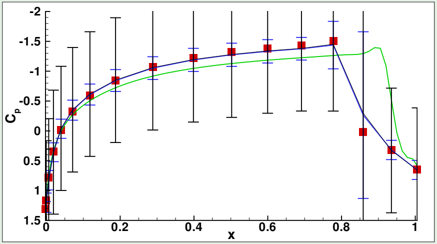


Calibration

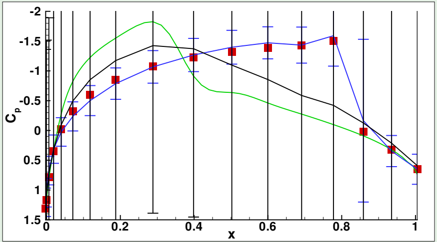
Redlich-Kwong



Peng-Robinson



Martin-Hou



- legend:
  - reference (red squares)
  - classical values (green line)
  - calibrated solution (blue line)
  - prior solution (black line)

- Good agreements between calibrated and reference data,
- The study seems to show that there is not only one parameter set which best fit the experimental data since some parameters are found to be correlated to each other,

$\Rightarrow$ to be confirmed,

- Future work: perform Bayesian model averaging to take into account several model forms and scenarios.

Bayesian inference

e_i is assumed to be independant and normally distributed with mean zero and a standard deviation of 10% of the observed value. Then we can write that:

$$p(d|\hat{d}) = \frac{1}{\sqrt{(2\pi)^n |K_e|}} \exp\left[-\frac{1}{2}(d-\hat{d})^T K_e^{-1}(d-\hat{d})\right]$$

η is assumed to be well represented by a correlated Gaussian model of the form:

$$\eta \sim \mathcal{N}(1, K_M)$$

A common used choice for K_M is:

$$K_M = \sigma^2 \exp\left[-\left(\frac{x-x'}{10^\alpha X}\right)^2\right]$$

where x and x' are two subsequent observations abscissa separated by the length scale $10^\alpha X$ ($X \approx 1$).

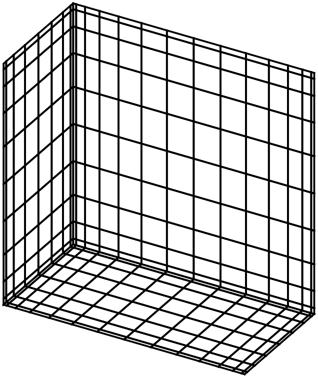
σ and α become new parameters (known as hyper-parameters) to be calibrated and representing the magnitude of the error variance and the magnitude of the correlation length.

Response surface

- multi-dimensional lagrange interpolations

$$\Pi f(v_1, ..., v_m) = \sum_{i_1=0}^{n_1} ... \sum_{i_m=0}^{n_m} \alpha_{i_1...i_m} l_{i_1}(v_1)...l_{i_m}(v_m),$$

where the l_i's are the 1-D caracteristic lagrange polynomials,
- Gauss-Lobatto grids to minimize the interpolation error,
- in this study $m \leq 3$.



Preliminary analyses

- Interpolation: 10 random points inside the mesh for each EOS (total: 170 points)

	Parameter range	$< 1\%$	$> 10\%$
RKS	$\omega \in [0.5, 1.1]$ $c_{\nu,\infty}(T_c) \in [30.0, 200.0]$ $n \in [0.0, 1.0]$	163	1
PRSV	$\omega \in [0.5, 1.1]$ (9) $c_{\nu,\infty}(T_c) \in [100.0, 200.0]$ (9) $n \in [0.0, 1.0]$ (9)	166	1
MAH	$\omega \in [a, b]$ $T_c \in [a, b]$ $p_c \in [a, b]$	X	Y

Main discrepancies are in the vicinity of the shock.

- Sobol analysis:

	Strong influence on C_p	Weak influence on C_p
RKS	ω, $c_{\nu,\infty}(T_c)$	n
PRSV	ω, $c_{\nu,\infty}(T_c)$	n
MAH	T_c, p_c, $c_{\nu,\infty}(T_c)$	

Redlich-Kwong

Thermal equation:

$$p = \frac{RT}{\nu - b} - \frac{a/T^{0.5}}{\nu(\nu + b)}$$

- p pressure,
- T absolute temperature,
- ν the specific volume,
- R the gas constant,
- a and b two material dependant parameters.

The Soave modification[1]:

- $a(T) = a_c\alpha(T); a_c = 0.42747R^2\frac{T_c^2}{p_c}, \alpha(T) = [1 + m(1 - T_r^{0.5})]^2,\ Tr = \frac{T}{T_c}$ and $m = 0.480 + 1.57\omega - 0.176\omega^2$
- $b = 0.08664R\frac{T_c}{p_c}$

where the subscript c denotes critical-point values and ω is the substance acentric factor.

[1] **G. Soave, "Equilibrium constants from a modified Redlich-Kwong equation of state," Chem. Eng. Sci., 27, 1197, 1972.**

Redlich-Kwong

Caloric equation:

$$c_{\nu,\infty}(T) = c_{\nu,\infty}(T_c)\left(\frac{T}{T_c}\right)^n.$$

where $c_{\nu,\infty}(T)$ is the ideal-gas-limit isocoric specific heat.

Those equations can be written in a normalized form:

$$\begin{cases} p_r = \dfrac{T_r/Z_c}{\nu_r - b_r} - \dfrac{a_r/T_r^{0.5}}{\nu_r(\nu_r + b_r)} \\ \dfrac{c_{\nu,\infty}(T)}{R} = \dfrac{c_{\nu,\infty}(T_c)}{R}(T_r)^n \end{cases}$$

in such a way that the RKS model only depends on the following three factors:

- the acentric factor ω,
- the exponent n,
- the reduced ideal-gas constant-volume specific heat at the critical temperature $c_{\nu,\infty}(T_c)$.

Peng-Robinson

Thermal equation:

$$p = \frac{RT}{\nu - b} - \frac{a}{\nu^2 + 2b\nu - b^2}$$

with

- $a = 0.457235 R^2 \frac{T_c^2}{p_c} \alpha(T)$,
- $b = 0.077796 R \frac{T_c}{p_c}$.

To improve the results, the recorrelated m as a function of ω of Stryjek and Vera can be used:

$$m = 0.378893 + 1.4897153\omega - 0.17131848\omega^2 + 0.0196554\omega^3$$

Thanks to same normalization technique as in the RKS case, the PRSV model depends only on three parameters:

- the acentric factor ω,
- the exponent n,
- the reduced ideal-gas constant-volume specific heat at the critical temperature $c_{\nu,\infty}(T_c)$.

Martin-Hou

Thermal equation:

$$p = \frac{RT}{\nu - b} + \sum_{i=2}^{5} \frac{f_i(T)}{(\nu - b)^i}$$

with

- $b = RT_c \dfrac{1 - \beta/15}{pc}$; $\beta = 20.533 - 31.883 Z_c$, $Z_c = \dfrac{p_c \nu_c}{RT_c}$ the critical compressibility factor,
- $f_i(T) = A_i + B_i T + C_i \exp\left(-\dfrac{kT}{T_c}\right)$; $k = 5.475$.

A_i, B_i and C_i can be expressed in terms of T_c, p_c, Z_c, the Boyle temperature (function of T_c) and one point on the vapour pressure curve.

This equation can be reduced in such a way that the MAH model depends only on the following parameters: p_c, T_c, Z_c, the normal boiling temperature T_b, n and $c_{\nu,\infty}(T_c)/R$.

The work of Cinnella *et al.* shows that only T_c, p_c and $c_{\nu,\infty}(T_c)/R$ have a great influence on the outcome.