On The Calibration of a Two-phase Flow Model under Uncertain Inlet Conditions

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Introduction

- Calibration consists on inferring the best values of the parameters to fit the observed data.
- Simulations are subject to different types of uncertainties (parameter uncertainty, model error, experiment uncertainty, code uncertainty)
- Need to acknowledge different sources of uncertainty in the calibration process.

Presentation Outline

Presentation Outline

Motivating example

Experimental data

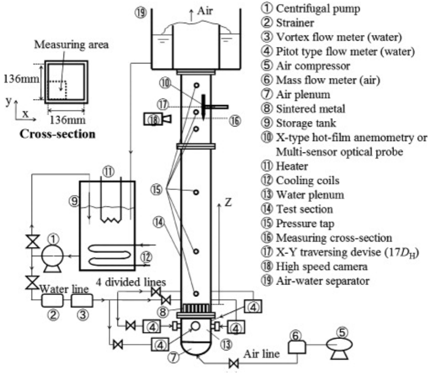

Figure 1: Experimental setup from Sun experiment.

- Sun experiment [1] : Development of gaz-liquid bubbly flow for a vertical square duct.
- Measurements of the void fraction and the liquid velocity.

$\langle J_l \rangle$ (m/s)	$\langle J_g \rangle^*$ (m/s)	$\langle \alpha \rangle^*$ (–)	$\langle W \rangle^*$ (m/s)
1.00	0.089	0.075	1.19
	0.134	0.103	1.25
	0.179	0.134	1.35
	0.226	0.154	1.45
0.75	0.067	0.075	0.85
	0.090	0.108	0.92
	0.135	0.142	1.02
	0.180	0.153	1.09
0.50	0.045	0.069	0.61
	0.090	0.139	0.68
	0.137	0.172	0.75

[1] Sun et al. "Upward air–water bubbly flow characteristics in a vertical square duct" (2014).

Motivating example

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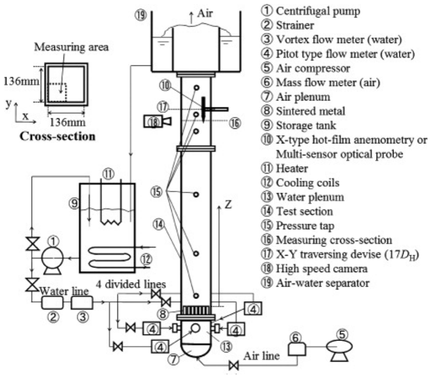

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Motivating example

Mathematical model: (Two-phase RegIme TransitiON Model)[2]

- The TRITON model considers 3 fields: a continuous liquid field, a dispersed gaz field (group 1) and a continuous gaz field (group 2)
- Continuity and moment equations are solved for each field.
- The change in bubble diameters is described by the two-group interfacial area transport equations

$$\frac{\partial a_{i1}}{\partial t} + \nabla.(a_{i1} v_{i1}) = \frac{2}{3}\frac{a_{i1}}{\alpha_{g1}}\left[\frac{\partial \alpha_{g1}}{\partial t} + \nabla.(\alpha_{g1} v_{g1})\right] - \chi\left(\frac{D_{sc}}{D_{sm}}\right)^2 \frac{a_{i1}}{\alpha_{g1}}\left[\frac{\partial \alpha_{g1}}{\partial t} + \nabla.(\alpha_{g1} v_{g1})\right] + \boxed{\sum_j \phi_{j,1}}$$
$$\frac{\partial a_{i2}}{\partial t} + \nabla.(a_{i2} v_{i2}) = \frac{2}{3}\frac{a_{i2}}{\alpha_{g2}}\left[\frac{\partial \alpha_{g2}}{\partial t} + \nabla.(\alpha_{g2} v_{g2})\right] + \chi\left(\frac{D_{sc}}{D_{sm}}\right)^2 \frac{a_{i1}}{\alpha_{g1}}\left[\frac{\partial \alpha_{g1}}{\partial t} + \nabla.(\alpha_{g1} v_{g1})\right] + \boxed{\sum_j \phi_{j,2}}$$

- For Bubbly flow,

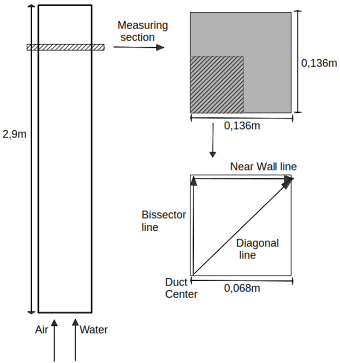
$$\sum_j \phi_j = \phi^1_{RC}(C^{(1)}_{RC}, C_{RC1}) + \phi^1_{WE}(C^{(1)}_{WE}) + \phi^1_{TI}(C^{(1)}_{TI}, We_{cr1})$$

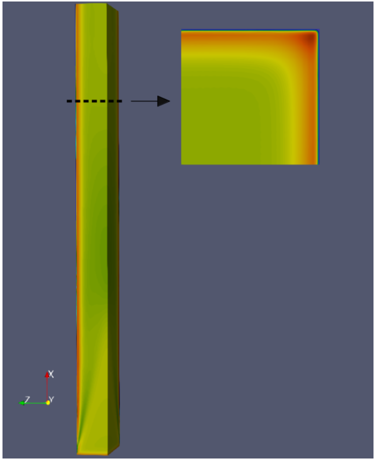
[2] Kuidjo et al. “Comparison of bubbles interaction mechanisms of two-group Interfacial Area Transport Equation model”. International Journal of Multiphase Flow(2023).

Motivating example

Simulation with Neptune CFD

- 3D simulation of the quarter section of the domain with a mesh of 3256000 cells





Motivating example

Simulation with Neptune CFD

The void fraction is underestimated!

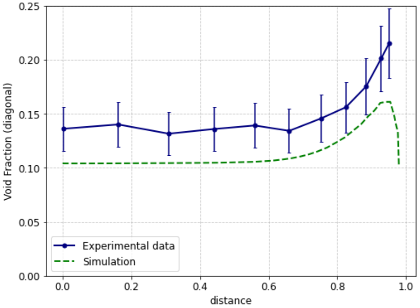
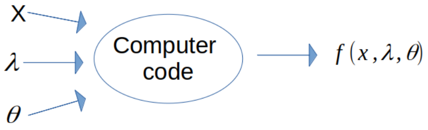


Figure 2: Comparison of the simulation results with experimental data along the diagonal line for the void fraction of the gaz.

Motivating example

The computer code needs several parameters to be run:

- Control variables X: Variables that define the physical system independently from the environment
- Calibration parameters θ : unknown parameters that depend only on the model
- Unknown inlet conditions λ



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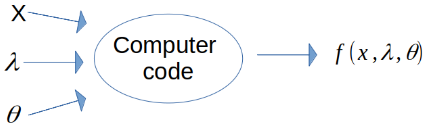
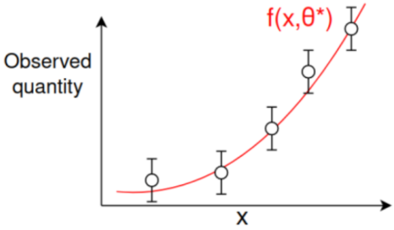


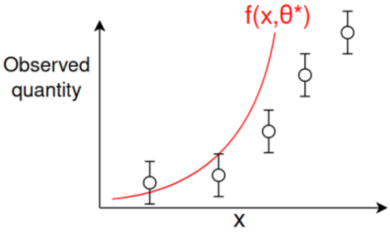
Problem: How to infer the values of the calibration parameters when the inlet conditions are uncertain?

Presentation Outline

Bayesian Calibration with model error

Model predictions after calibration





Some parameter values fit the data well

Best values are not consistent with the observations

Need to consider model error in the calibration.

Bayesian calibration with model error

Statistical Assumptions

$$y_{obs}(x) = f(x, \theta) + \delta(x, \theta) + \varepsilon$$

- Model discrepancy depends on model parameters [3]. It is modeled as a Gaussian process $\delta(x)|GP(\mu(.), k_\psi(., .))$, the covariance function depends on some hyperparameters ψ
- Measurement error is distributed as $\mathcal{N}(0, \sigma_\varepsilon^2)$
- Model error and measurement error are supposed independent.
- Prior distributions of the parameters and the hyperparameters are independent.

[3]Leoni et al. "Bayesian Calibratiion With Adaptive Model Discrepancy". International Journal for Uncertainty Quantification (2024)

Bayesian calibration with model error

- The problem is solved by a modular approach.
- The hyperparameters $\phi = (\psi, \sigma_\varepsilon)$ are first estimated by solving the following optimisation problem

$$\hat{\phi}_{FMP} = argmax(p(\phi|y,\theta)) = argmax\phi(x)(p(y|\phi,\theta)$$

- The posterior density of the parameters is estimated by

$$p(\theta,\phi|y_{obs}) \propto p(\theta)p(y_{obs}|\theta,\phi = \hat{\phi}_{FMP})$$

- We use Metropolis Hastings algorithm to sample from the posterior distribution.

Bayesian calibration with model error

The case of expensive computer codes

- The code is replaced by a statistical approximation that is cheaper to evaluate.

A priori

$$f_{code} \sim GP(m(.), K(.,.))$$

- $m(.)$ is the mean function
- $k(.,.)$ is the covariance function
- We consider a set of training inputs $X = (x_1, x_2, .., x_n)$ with their corresponding code outputs $Y = (y_1 = f_{code}(x_1), f_{code}(x_2), .., f_{code}(x_n))$
- Let $X_* = (x_{*,1}, x_{*,2}, .., x_{*,n})$ be the test set where we want to make the predictions and Y_* their corresponding outputs.
- We can predict Y_* by

$$Y_* | Y, X_*, X \sim \mathcal{N}(\mu_* - K_* K^{-1}(Y - \mu(X)), K_{**} - K_*^T K^{-1} K_*)$$

Presentation Outline

Calibration of the TRITON Model

First approach: Fix the inlet conditions to a specific value and then calibrate model parameters

- Fixed value for the liquid velocity based on expert knowledge
- Infer the posterior distribution of the void fraction based on a Bayesian analysis and then fix the inlet value to the MAP
- Infer model parameters θ

Second approach: Learn the inlet conditions jointly with model parameters

- Consider the vector of parameters $\Theta = (\theta, \lambda)$ for the calibration.
- The relationship between the observations, code output and model error is

$$y_{obs}(x) = f(x, \Theta) + \delta(x, \Theta) + \varepsilon$$

Calibration of the TRITON model

The inlet conditions

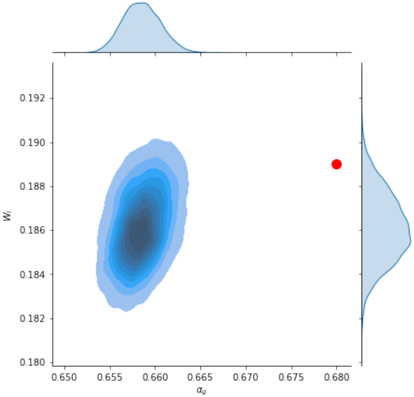
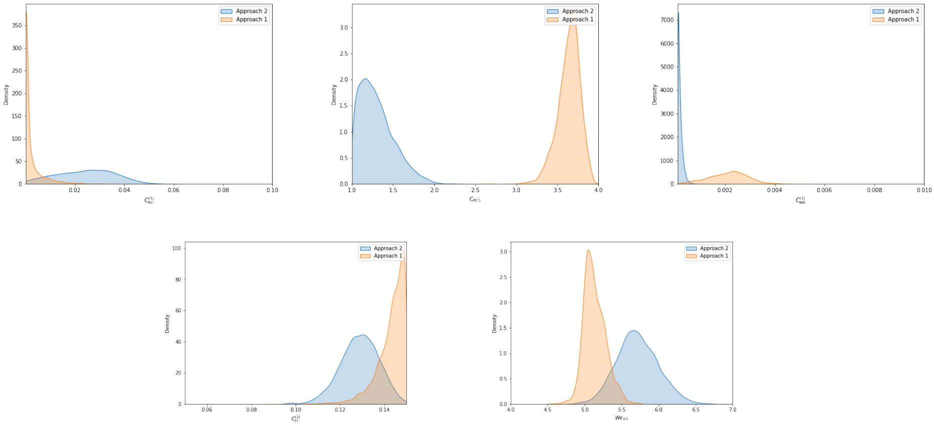


Figure 3: The joint distribution of the injected liquid velocity and the void fraction. The red dot correpond to the values injected for the first approach.

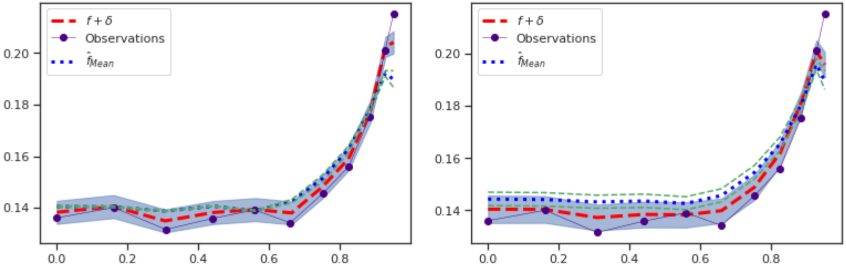
Calibration of the TRITON Model

Comparison of the Posterior distributions of model parameters



Calibration of the TRITON Model

Predictions of the void fraction along the diagonal line: first approach (left), second approach (right)



Presentation Outline

Conclusions and perspectives

- Calibration results depend strongly on the way we handle the inlet conditions
- It is important to consider the uncertainties in the control variables for the calibration
- Further investigations of the choice of model error kernel are needed.
- Incorporating the uncertainty on the inlet conditions with a hierarchical Bayesian formalism where the associated error is modeled using a latent variable.

Thank you for your attention!
Any questions?

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