METAMODEL BASED ON EVOLUTIONARY NEURAL NETWORKS FOR THE SOLUTION OF INVERSE PROBLEMS WITHIN THE BAYESIAN FRAMEWORK OF STATISTICS

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1. Introduction and Motivation

- In nowadays complex hydraulic systems, transients in pumps and valves may induce significant variations in pressures and flow rates.
- For example, if the liquid velocity is suddenly reduced by the closure of a valve, pressure waves with large magnitudes and large velocities propagate through the pipelines.
- Such a phenomenon is known as **water hammer** and can seriously affect the pipeline integrity.
- **This work deals with the estimation of parameters of a water hammer model.**

Source: Lüdecke, H. J., Kothe, B., KSB Know- how: Water Hammer Volume 1, KSB, 2006.

Source: Chaudhry, M.H., 2014, Applied Hydraulic Transients, New York, USA, Springer.

2. Mathematical Formulation

- **U** = vector of state variables
- **F** = flux
- **B** = source term
- p = pressure
- q = mass flow rate
- u = velocity
- ρ = density

- A = cross-section area of the pipe
- D = pipe diameter
- f = friction coefficient (Darcy-Weisbach)
- f_u = transient friction coefficient
- a = sound velocity (celerity)

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{U})}{\partial x} = \mathbf{B}(\mathbf{U})$$

$$\mathbf{U} = \begin{pmatrix} p \\ q \end{pmatrix} \qquad \mathbf{F}(\mathbf{U}) = \begin{pmatrix} \dfrac{qa^2}{A} \\ Ap + \dfrac{q^2}{\rho A} \end{pmatrix}$$

$$\mathbf{B}(\mathbf{U}) = \begin{pmatrix} \dfrac{q}{\rho A} \dfrac{\partial}{\partial x}(\rho a^2) \\ \dfrac{-f\,|q|\,q}{2\rho AD} - \rho A g \operatorname{sen}\theta + P \dfrac{\partial A}{\partial x} - f_u \left(\dfrac{\partial q}{\partial t} - a \dfrac{\partial q}{\partial x} \right) + \sum_{b=1}^{B} \Delta P_b \, \delta(x - x_B) \end{pmatrix}$$

2. Mathematical Formulation

Sound velocity (celerity):

$$a = \sqrt{\frac{K}{\rho\left(1+\left(\frac{K}{E}\right)\psi\right)}}$$

where *E* is the Young's modulus of the pipe and *K* is the elastic modulus of the fluid.

- ψ is a nondimensional parameter that depends on the elastic properties of the pipe including its supports:

- Rigid pipe: $\psi = 0$
- Thick-wall elastic pipe with frequent expansion joints: $\psi = 2\left(\frac{R_o^2 + R_i^2}{R_o^2 - R_i^2} + \upsilon\right)$
- Thin-wall elastic pipe with frequent expansion joints: $\psi = \frac{D}{e}$

3. Solution of Direct Problem

The system of equations is split at each time step Δt with the initial condition given by the solution at the previous time instant.

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{U})}{\partial x} = \mathbf{B}(\mathbf{U})$$

$$\mathbf{U} = \mathbf{U}^n$$

$$\left.\begin{array}{l} \dfrac{\partial \mathbf{U}}{\partial t} + \dfrac{\partial \mathbf{F}(\mathbf{U})}{\partial x} = 0 \\ \mathbf{U} = \mathbf{U}^n \end{array}\right\} \Rightarrow \overline{\mathbf{U}}^{n+1}$$

WAF-TVD

$$\left.\begin{array}{l} \dfrac{d\mathbf{U}}{dt} = \mathbf{B}(\mathbf{U}) \\ \mathbf{U} = \overline{\mathbf{U}}^{n+1} \end{array}\right\} \Rightarrow \mathbf{U}^{n+1}$$

$$\mathbf{U}^{n+1} = \overline{\mathbf{U}}^{n+1} + \mathbf{B}\Delta t$$

4. Solution of the Inverse Problem

BAYES' THEOREM

$$\pi_{posterior}(\mathbf{P}) = \pi(\mathbf{P}|\mathbf{Y}) = \frac{\pi_{prior}(\mathbf{P})\pi(\mathbf{Y}|\mathbf{P})}{\pi(\mathbf{Y})}$$

$\pi_{posterior}(\mathbf{P})$ = posterior probability density (conditional probability of the parameters **P** given the measurements **Y**)

$\pi_{prior}(\mathbf{P})$ = prior density (information about the parameters prior to the measurements)

$\pi(\mathbf{Y}|\mathbf{P})$ = likelihood function (expresses the likelihood of different measurement outcomes **Y** with **P** given)

$\pi(\mathbf{Y})$ = probability density of the measurements, evidence (normalizing constant)

$$posterior \propto prior \text{ x } likelihood$$

4. Solution of the Inverse Problem

Markov Chain Monte Carlo (MCMC) methods

Metropolis-Hastings Algorithm

1. Sample a *Candidate Point* $\mathbf{P}^*$ from a proposal distribution $q(\mathbf{P}^*|\mathbf{P}^{(t-1)})$.

2. Calculate the acceptance factor:

$$\alpha = \min\left[1, \frac{\pi(\mathbf{P}^* \mid \mathbf{Y})\, q(\mathbf{P}^{(t-1)} \mid \mathbf{P}^*)}{\pi(\mathbf{P}^{(t-1)} \mid \mathbf{Y})\, q(\mathbf{P}^* \mid \mathbf{P}^{(t-1)})}\right]$$

3. Generate a random value U that is uniformly distributed on (0,1).

4. If $U < \alpha$, set $\mathbf{P}^{(t)} = \mathbf{P}^*$. Otherwise, set $\mathbf{P}^{(t)} = \mathbf{P}^{(t-1)}$.

5. Return to step 1.

4. Solution of the Inverse Problem

- Vector of model parameters: $\mathbf{P}^T = [f_u, \psi, D, e, E, K, \rho_0]$
- The parameters $[D, e, E, K, \rho_0]$ are fairly known with small uncertainties from other experiments or even tabulated data. Hence, they were modeled with truncated Gaussian priors.
- $[f_u, \psi]$ depend on the construction characteristics of the pipeline, as well as on the fluid and flow conditions. These parameters were modeled with uniform priors, with bounds provided by positivity constraints and expressions available in the literature for their calculations.
- Measurement errors were additive, Gaussian, with zero mean, uncorrelated and with known variances.

4. Solution of the Inverse Problem

Parallel version of the Metropolis-Hastings algorithm

Cui, T., Fox, C., Nicholls, G. K., O'Sullivan, M. J., 2019, Using Parallel Markov Chain Monte Carlo to Quantify Uncertainties in Geothermal Reservoir Calibration, International Journal for Uncertainty Quantifications, vol. 9, pp 295-310

- **This algorithm parallelizes the Markov chain, taking advantage from the fact that rejection of candidates generated with the Metropolis-Hastings algorithm is much more often than their acceptance as samples of the posterior distribution.**
- Theoretical results available in the literature revealed that the optimal acceptance rate with Gaussian random-walk proposals is 23.4% for a large number of parameters.
- Although the statistical efficiency of the algorithm is considered high with acceptance rates between 10% and 60%, numerical experiments are commonly used to obtain acceptance rates around 30%.

4. Solution of the Inverse Problem

Metamodel

- **Evolutionary Neural Network Algorithm (EvoNN)** applies a multi-objective evolutionary algorithm on a population of Neural Networks of flexible topology and architecture. One hidden layer is used.
- **The multi-objective evolutionary algorithm attempts to simultaneously optimize the accuracy and complexity of the neural net population, which ultimately leads to a Pareto frontier containing a set of optimum models showing the best possible tradeoffs between these conflicting objectives.**
- The complexity of the EvoNN is measured with the **Modified Akaike's Information Criterion (AICc)** based on the total number of connections (C) between neurons in the network:

$$\mathrm{AIC}_C = 2C + N_{\mathrm{tr}} \ln\left(\frac{S_{\mathrm{LS}}}{N_{\mathrm{tr}}}\right) + \frac{2C(C+1)}{N_{\mathrm{tr}} - C - 1}.$$

$$S_{\mathrm{LS}} = \sum_{i=1}^{N_{\mathrm{tr}}} (y_i - y_{\mathrm{tr},i})^2$$

- Helle M, Petterson F, Chakraborti N, Saxen H (2006) Modelling noisy blast furnace data using genetic algorithms and neural networks. Steel Res Int 77(2):75–81.
- PyRVEA (2019) Research Group in Industrial Optimization. https://github.com/industrial-optimzation-group/ pyRVEA/tree/master/pyrvea.

4. Solution of the Inverse Problem

APPROXIMATION ERROR MODEL

- **Kaipio, J. and Somersalo, E.**, *Statistical and Computational Inverse Problems*, Applied Mathematical Sciences 160, Springer-Verlag, 2004
- **Kaipio, J., and Somersalo, E.,** Statistical Inverse Problems: Discretization, Model Reduction and Inverse Crimes, *Journal of Computational and Applied Mathematics*, vol. 198, pp. 493–504, 2007.

In the approximation error model (AEM) approach, the statistical model of the approximation error is constructed and then represented as additional noise in the measurement model [1,19-23]. With the hypotheses that the measurement errors are additive and independent of the parameters **P**, one can write

$$\mathbf{Y} = \mathbf{T}_c(\mathbf{P}) + \mathbf{e} \qquad (16)$$

where $\mathbf{T}_c(\mathbf{P})$ is the sufficiently accurate solution of the complete model given by equations (1.a-h). The vector of measurement errors, $\mathbf{e}$ are assumed here to be Gaussian, with zero mean and known covariance matrix **W**.

4. Solution of the Inverse Problem

APPROXIMATION ERROR MODEL

$$\mathbf{Y} = \mathbf{T}(\mathbf{P}) + [\mathbf{T}_c(\mathbf{P}) - \mathbf{T}(\mathbf{P})] + \mathbf{e}$$

By defining the error between the complete and the surrogate model solutions as

$$\boldsymbol{\varepsilon} = [\mathbf{T}_c(\mathbf{P}) - \mathbf{T}(\mathbf{P})]$$

equation (17) can be written as

$$\mathbf{Y} = \mathbf{T}(\mathbf{P}) + \boldsymbol{\eta}$$

where

$$\boldsymbol{\eta} = \boldsymbol{\varepsilon} + \mathbf{e}$$

4. Solution of the Inverse Problem

APPROXIMATION ERROR MODEL

η is modeled as a Gaussian variable

Enhanced error model:

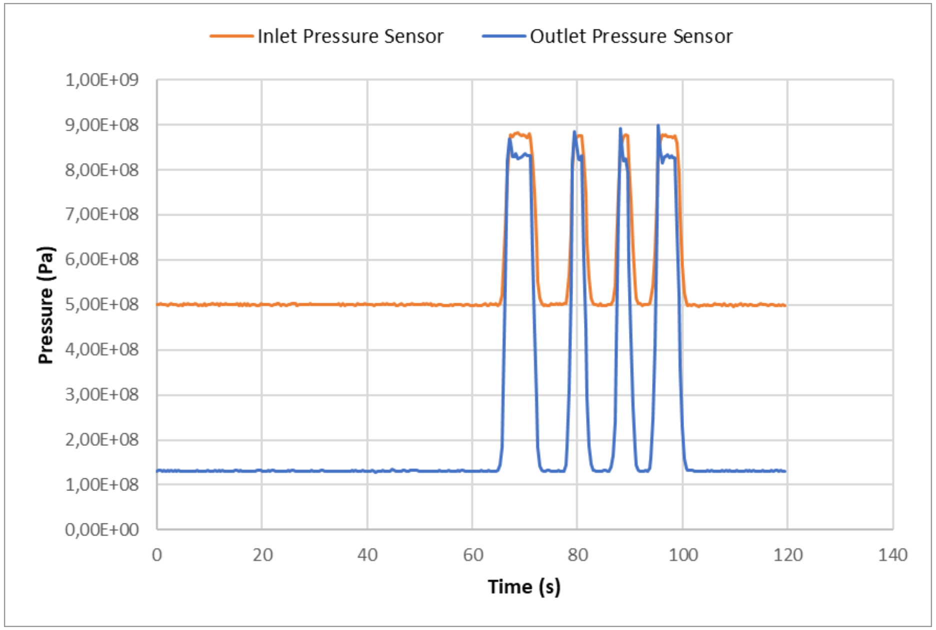
$$\begin{cases} \bar{\boldsymbol{\eta}} \approx \bar{\boldsymbol{\varepsilon}} \\ \tilde{\mathbf{W}} \approx \mathbf{W}_{\boldsymbol{\varepsilon}} + \mathbf{W} \end{cases}$$

Modified Likelihood

$$\tilde{\pi}(\mathbf{Y} \,|\, \mathbf{P}) \propto \exp\left\{ -\frac{1}{2} [\mathbf{Y} - \mathbf{T}(\mathbf{P}) - \bar{\boldsymbol{\eta}}]^T \, \tilde{\mathbf{W}}^{-1} [\mathbf{Y} - \mathbf{T}(\mathbf{P}) - \bar{\boldsymbol{\eta}}] \right\}$$

5. Results

- Transient flow of water.
- Hydraulic circuit with total length of 150 m.
- Measurements of pressure and flow rate at the inlet and outlet of the circuit.



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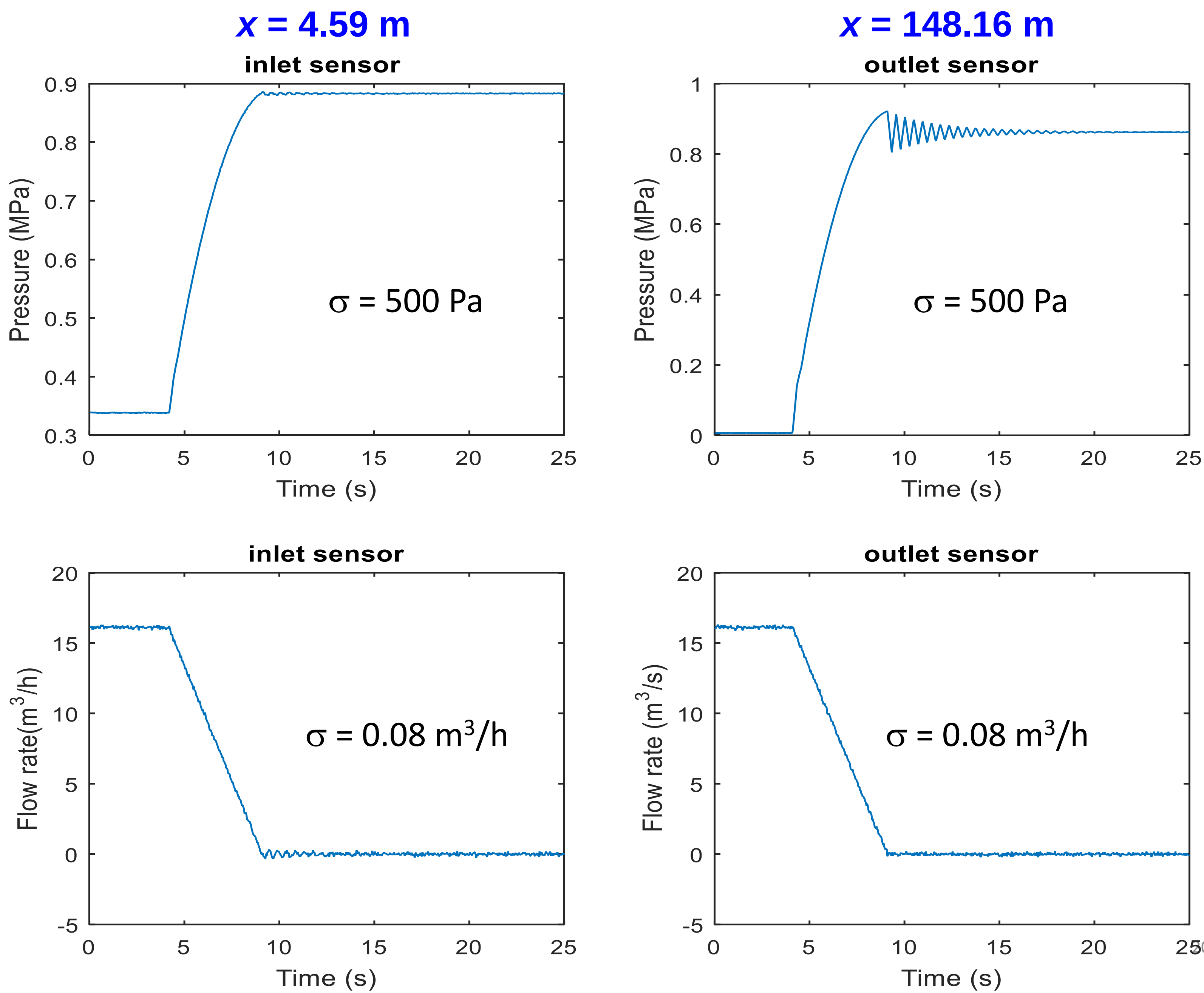
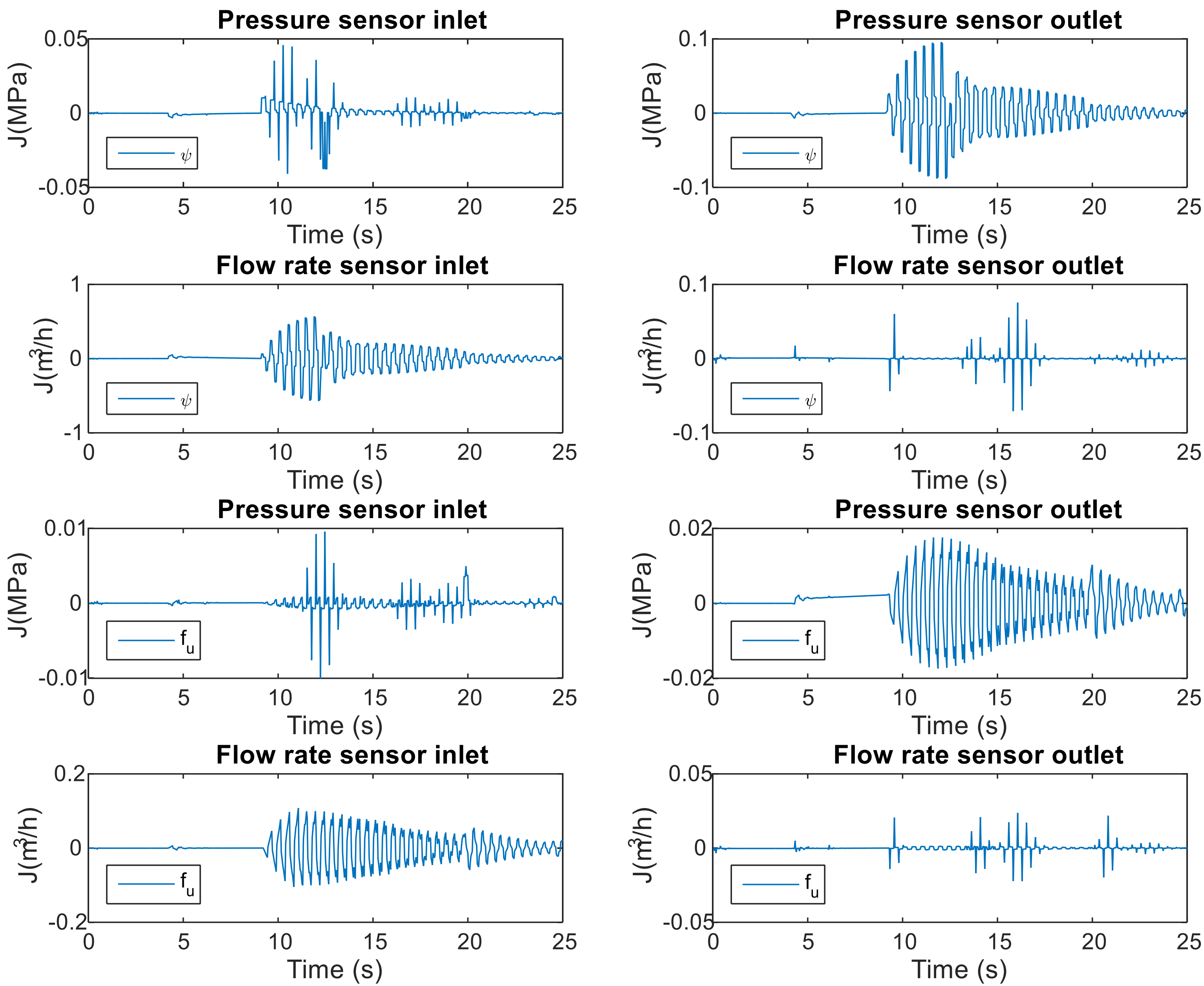
SIMULATED MEASUREMENTS

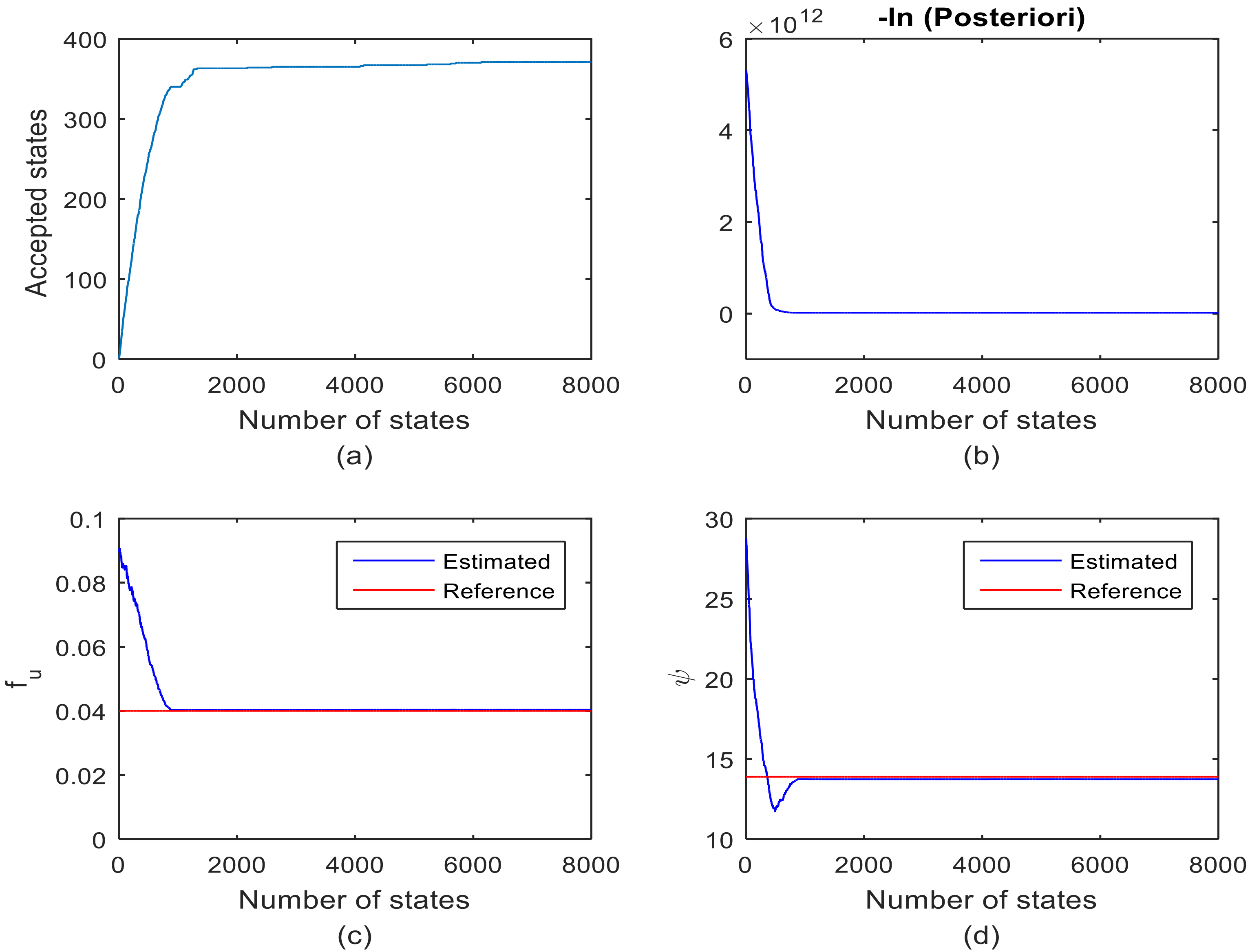


Reduced sensitivity coefficients: Parameters are linearly independent.



5. Results

WAF-TVD AND PARALLEL METROPOLIS-HASTINGS



5. Results

- High-fidelity WAF-TVD solution of the water hammer model took about 3 minutes with a compiled C computer code: Markov chains with 8000 states were generated in at least 70 hours by using the parallel computation version of the Metropolis-Hastings algorithm
- EvoNN metamodel took 0.001 s of computational time with a Python computer code: serial Metropolis-Hastings with the EvoNN metamodel took 12 minutes to generate a Markov chain with 10^6 states.
- The calculation of the 2000 solutions of the high-fidelity model (1500 required for training the EvoNN and 500 for calculating the approximation error) took 101.7 hours.
- The training of the EvoNN and the calculation of the statistics of the approximation error took 128 minutes and 20 minutes, respectively.

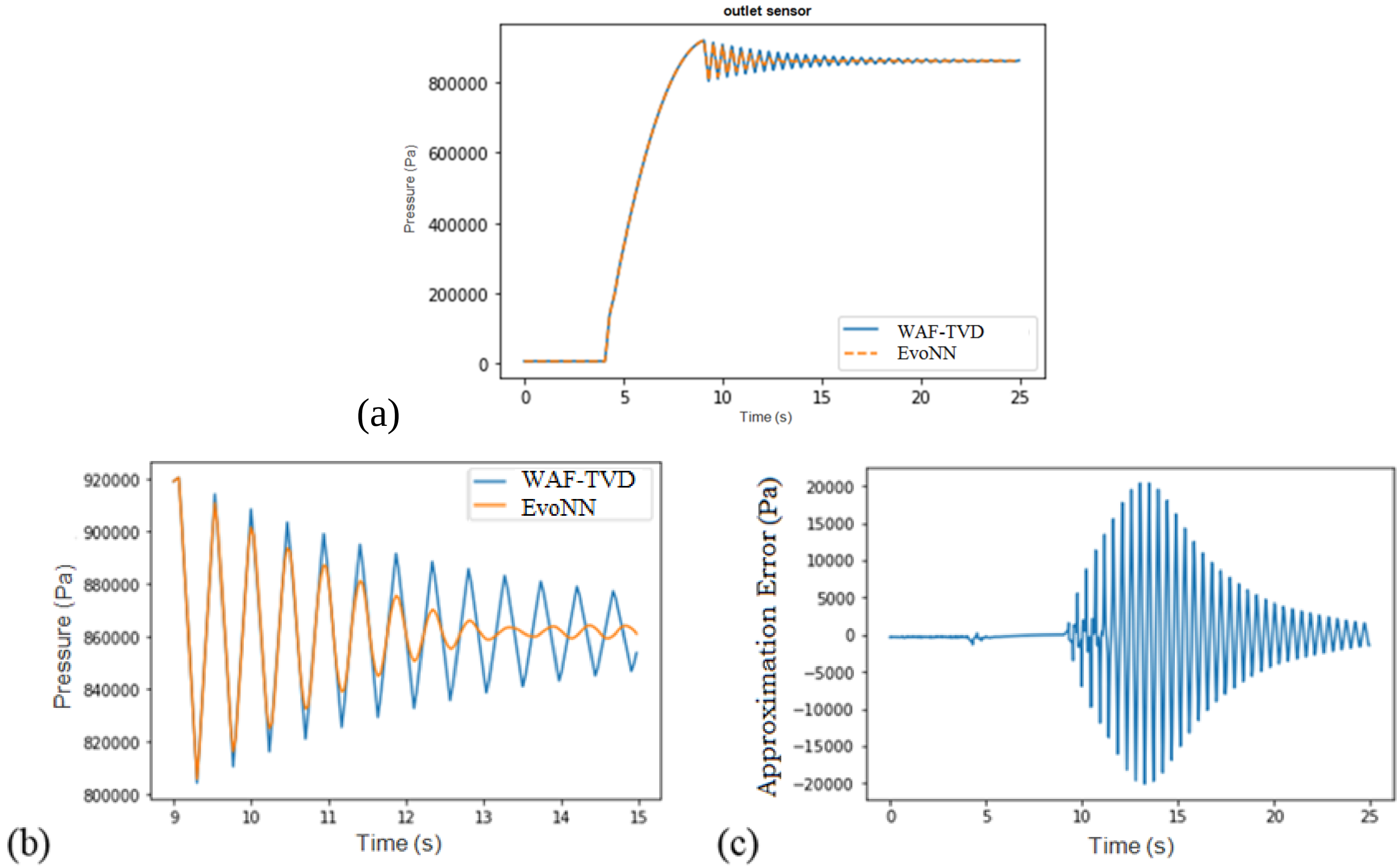
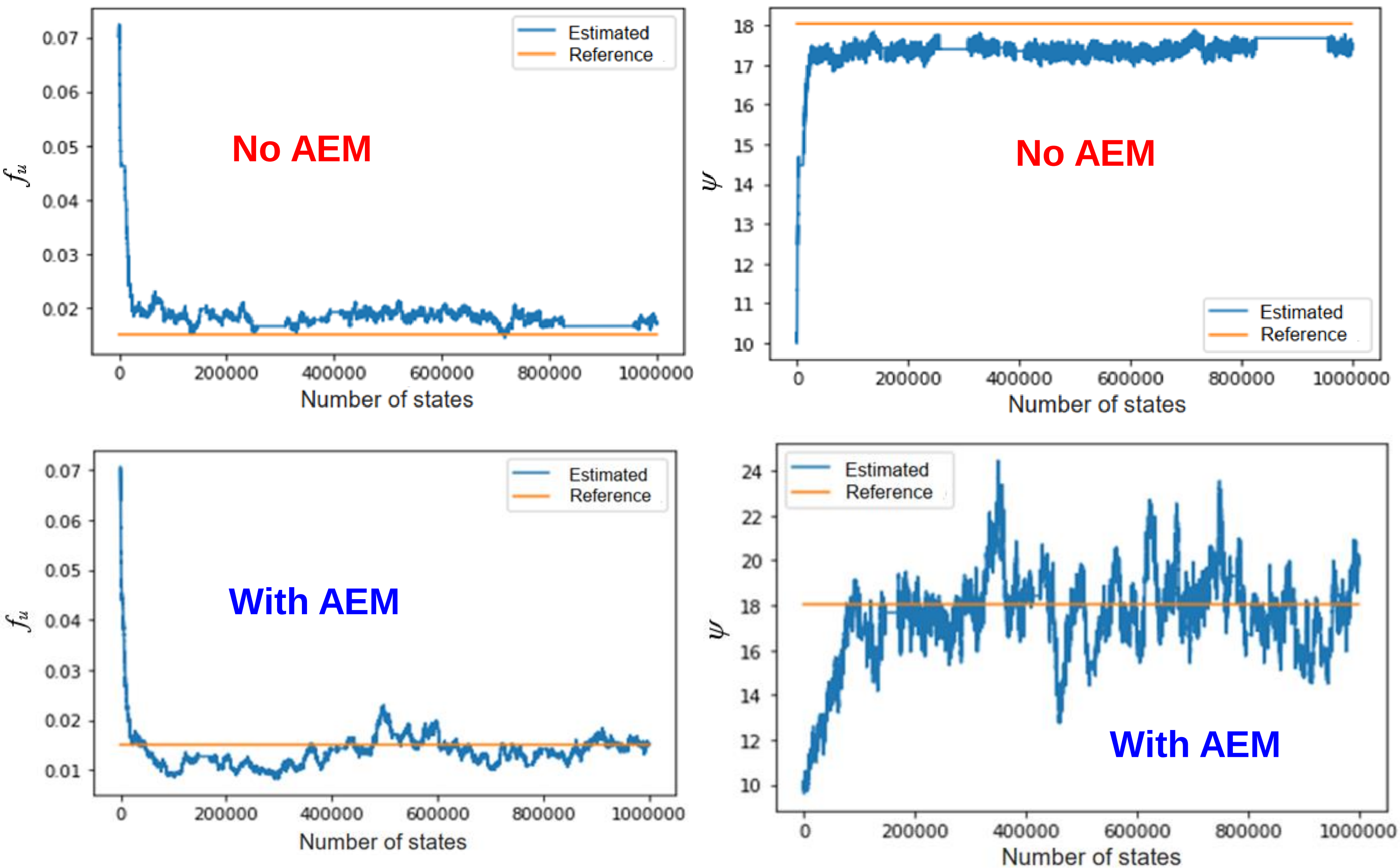


Figure 7. Comparison of the high-fidelity and metamodel solutions for pressure at x = 148.16 m with the parameter set A: (a) Whole-time domain; (b) Time interval when the water hammer effects are significant (c) Mean of the approximation error.

5. Results

EVONN AND SERIAL METROPOLIS-HASTINGS



5. Conclusions

- A comparison of the high-fidelity solution and the output of the EvoNNs revealed that this metamodel was not capable of completely representing the most significant effects resulting from the water hammer phenomenon. **As a result, the solutions of the inverse problem by replacing the high-fidelity model with the metamodel were biased.**
- **The Approximation Error Model (AEM) approach was then implemented**, and the modeling errors were represented as Gaussian variables.
- **The samples of the parameters used for computing the approximation errors with Monte Carlo simulations were different from those used for the training of the EvoNNs.**
- With the EvoNN metamodel and the AEM approach used in this paper**, Markov chains with 10^6 states could be generated with small computational cost**, thus providing samples that could appropriately represent the posterior distributions of the model parameters.
- **Even accurate metamodels like EvoNNs, as a replacement of high-fidelity models, might require the modeling of the approximation errors for the unbiased solution of inverse problems related to the water hammer phenomenon.**

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