Assessing validity of the dead zone model to characterize transport of contaminants in the River Wkra

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Objective and research questions

Objective: To evaluate validity of the dead zone model to characterize transport of contaminants in the River Wkra

Research questions	Methods
Is a deterministic solution of the dead zone model unique?	Optimization methods combined with Monte Carlo simulations
What is the model output uncertainty and what are sources of the uncertainty?	Sensitivity analysis Uncertainty analysis
What is the significance of model parameters/processes?	Sensitivity analysis
Could the model be simplified?	Sensitivity analysis Uncertainty analysis

Dead zone model

Main channel

$$\frac{\partial C}{\partial t} = -\frac{Q}{A}\frac{\partial C}{\partial x} + \frac{1}{A}\frac{\partial}{A\partial x}\left(AK_x \frac{\partial C}{\partial x}\right) + \alpha\left(C_S - C\right)$$

Storage zones

$$\frac{\partial C_S}{\partial t} = \alpha \frac{A}{A_S}\left(C_S - C\right)$$

Advection

Dispersion

Transient storage

K_x longitudinal dispersion coefficient [m^2/s]
A main channel cross-sectional area [m^2]
A_s storage zones cross-sectional area [m^2]
α storage zones exchange coefficient [$1/s$]

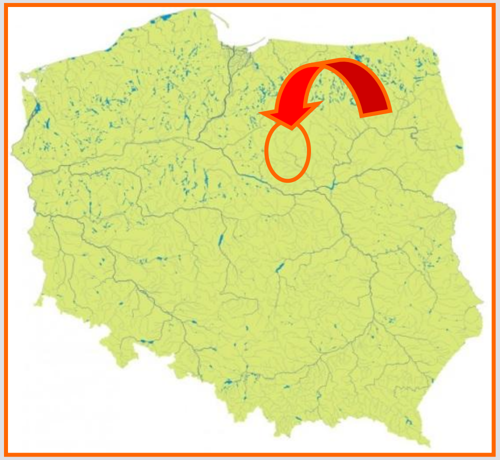
C, C_s main channel/storage zones solute concentration [kg/m^3]

Tracer test

- The tracer test conducted on the River Wkra in Central Poland by the Institute of Geophysics and Warsaw University of Life Sciences

- Instantaneous release of a passive and conservative tracer – rhodamine B in cross section P-0

- A tracer plume sampled at five cross sections below the injection point



Source: www.mapy.sej.pl

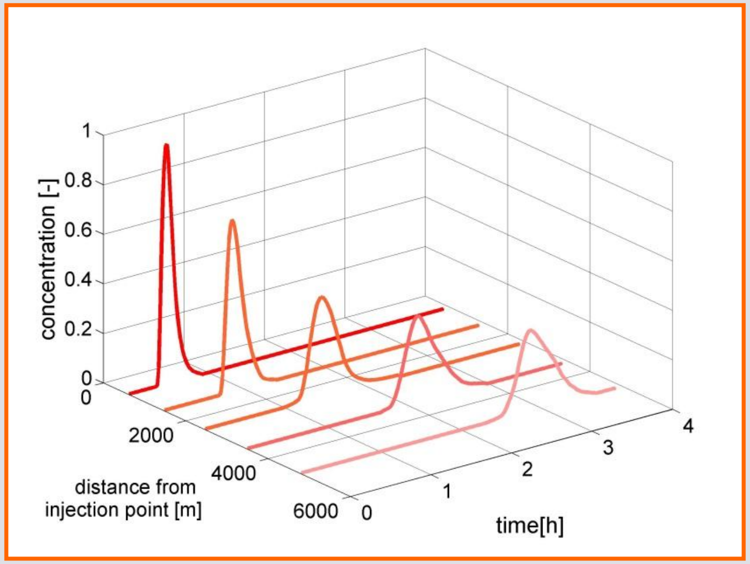
Field data

source: web.mit.edu/1.061/www/dream/home (07-09-08)

The tracer test was performed three times in steady flow conditions for the following flow rates:

Q1 = 4.18 m^3/s **Q2 = 3.97 m^3/s** **Q3 = 4.32 m^3/s**

Breakthrough curves



Deterministic calibration

- Calibration was performed for flow rates Q2 and Q3 for 4 sub-reaches separately.
- A breakthrough curve form an upstream cross-section of a sub-reach was a boundary condition. The output curve was computed in a downstream cross-section.

Least square objective function:

$$F = \sum_{t=1}^{t=n} \left(C_{o,t} - C_{s,t} \right)^2$$

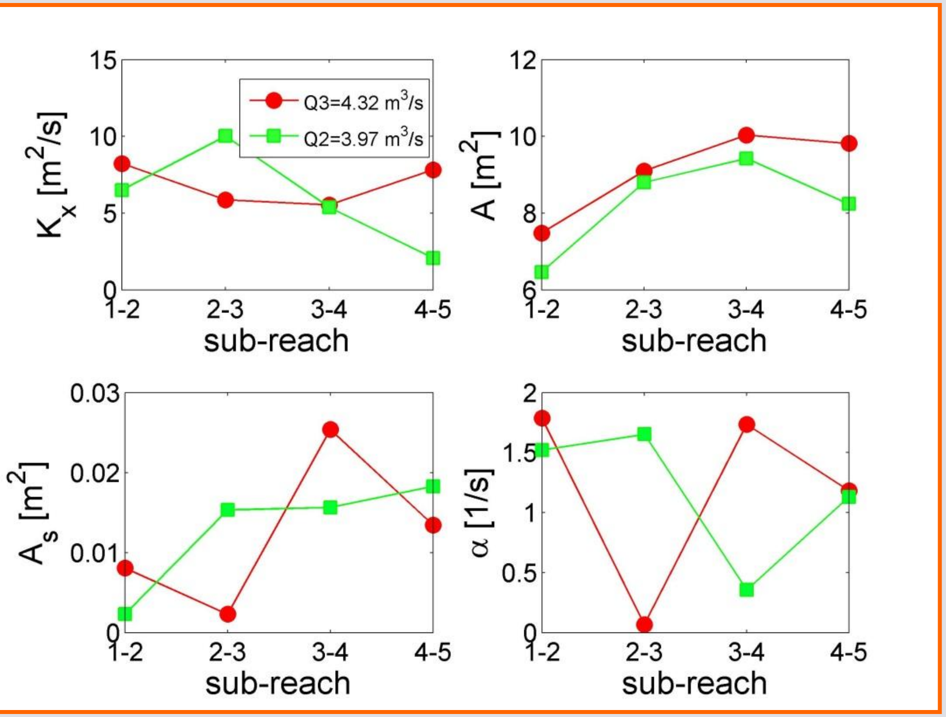
n – number of observations
$C_{o,t}$ - observed concentration at a time step *t*
$C_{s,t}$ - simulated concentration at a time step *t*

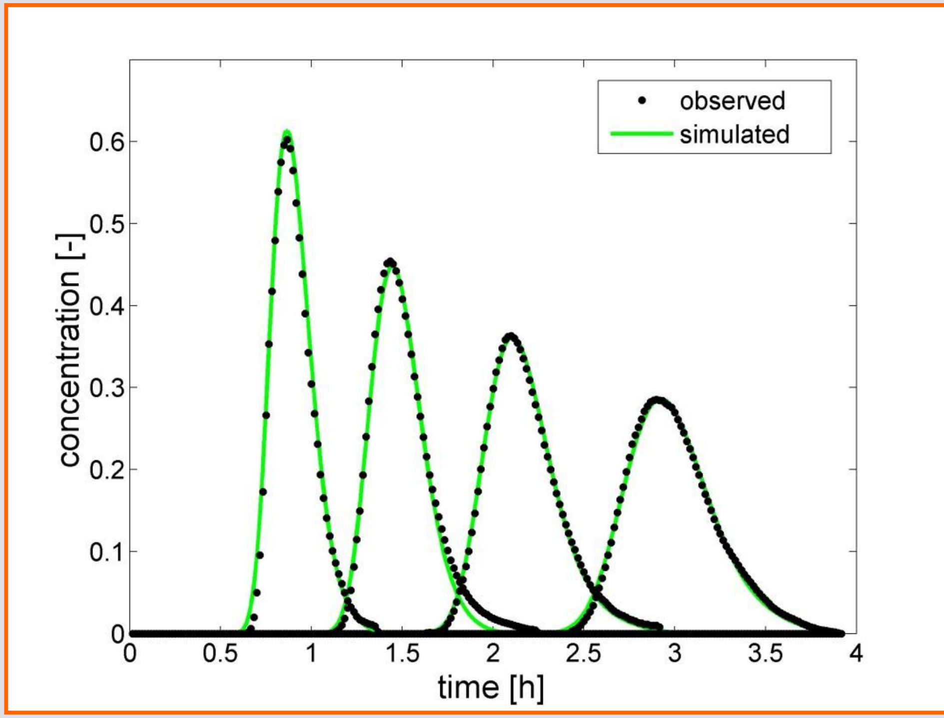
Optimization technique:

Differential Evolution (DE) - global optimization method

Ranges of parameter values:
(0,100) - A, K_x, A_s
(0,2) - α

Deterministic calibration results





Flow rate Q3

- Optimal parameter sets result in breakthrough curves that are in a good agreement with observations.
- Coefficient of determination R^2 is between 0.991 and 0.999.

Monte Carlo simulations – evaluation of response surfaces

1. 100 000 parameter sets composed of four parameters – K_x, A, A_s and α were created.

   Each parameter was drawn from a uniform distribution over the following intervals: K_x [1, 17], A [5, 12], A_s [0.01, 0.5], α [0.03, 3].

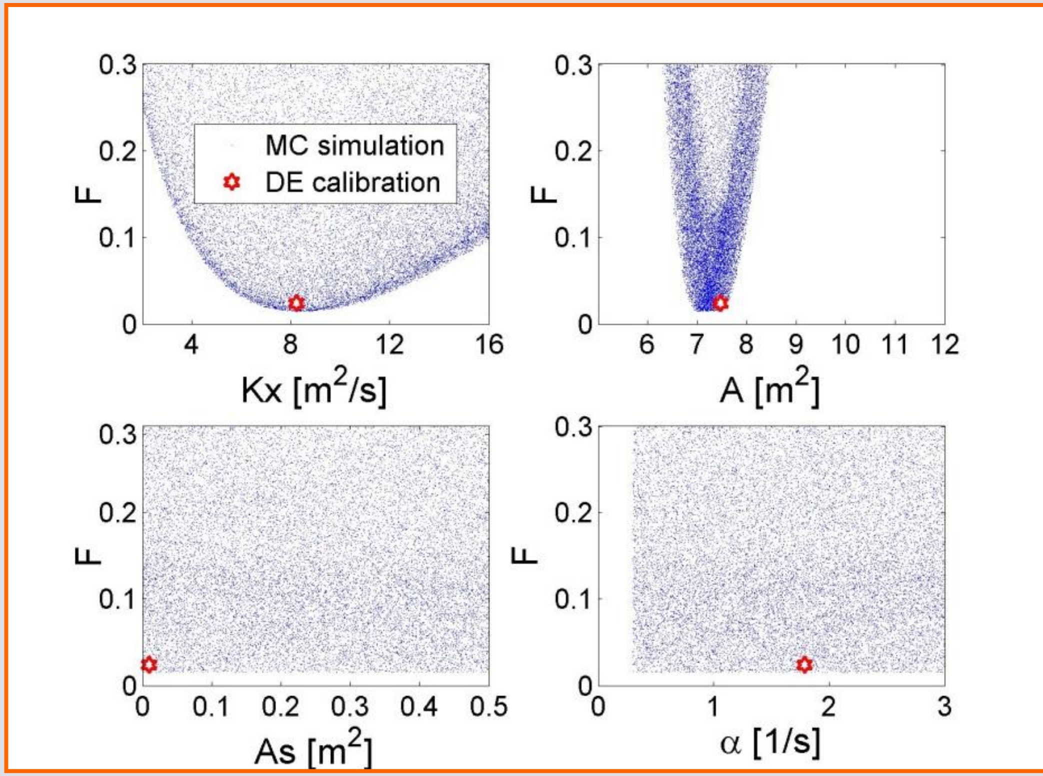
2. For each parameter set a simulation was computed, and a value of the least square objective function (the same as during calibration) was determined.

3. The response surfaces were created.

Monte Carlo simulations- evaluation of response surfaces

- Minimum values of the objective function exist for K_x and A within narrow ranges.

- Unique values of A_s and α do not exist for the objective function.



sub- reach 1-2, flow rate *Q3*

Conclusions:

- Unique choice of parameter set is not possible either by means of applied optimization method or by Monte Carlo simulations.

- The choice of optimal parameter set is very uncertain.

Uncertainty analysis

- The dead zone model is deterministic and it does not consider the uncertainty of results.
- To assess the parametric uncertainty of the model results **GLUE – Generalized Likelihood Uncertainty Estimation** was applied.

GLUE methodology:

1. Choosing prior parameters distributions basing on the knowledge of the modelled system - K_x and A - normal distribution, A_s and α - uniform distribution.

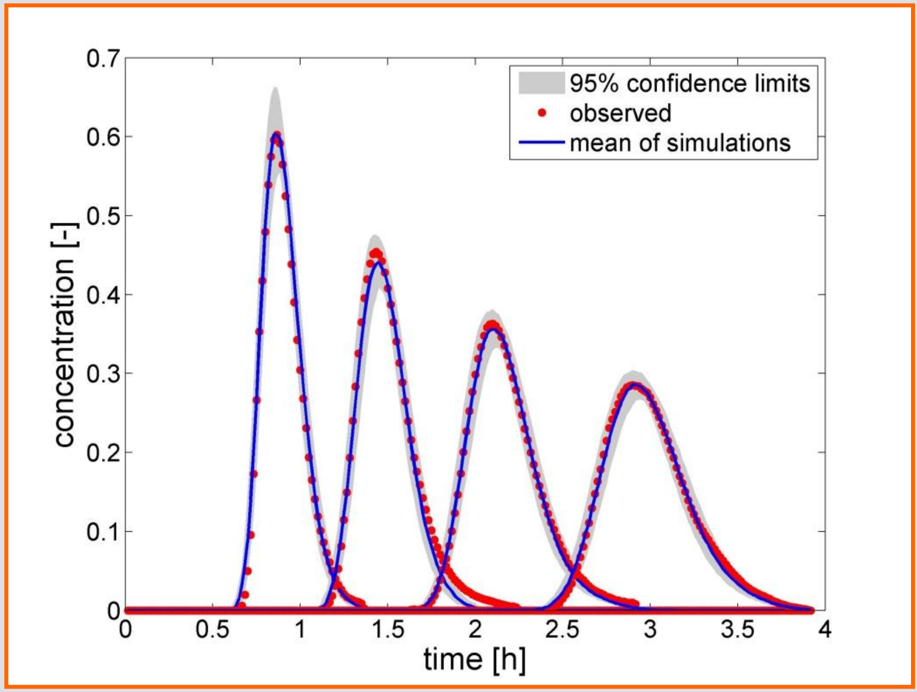
2. Sampling prior parameters distributions by the Monte Carlo method to create 100 000 parameter sets.

3. Choosing an informal likelihood measure, which evaluates acceptability of the parameter set according to the degree simulations fit to observations - measure proportional to the Gaussian distribution function.

4. Calculating the informal likelihood measure for each parameter set to obtain the posterior distribution.

5. Computing 95% confidence limits for simulations from posterior distribution.

Simulations with 95% confidence limits:



Sensitivity analysis (SA)

SA aims at establishing effect of model parameters on a model output.

The main objectives of the SA:

- identification of parameters that could be neglected to simplify a model
- identification of parameters/processes that affect the output to prioritize them in the research to reduce the uncertainty
- understand a model structure i.e. identify interactions between parameters

Sensitivity analysis - Sobol' decomposition method (variance-based SA)

Decomposition of model output (C_{max}) variance on the sum of conditional variances:

$$V(C_{\max}) = \underbrace{V_{K_x} + V_A + V_{A_s} + V_\alpha}_{\text{1st order conditional variances}} + \underbrace{V_{K_xA} + V_{K_xA_s} + V_{K_x\alpha} + V_{AA_s} + V_{A\alpha} + V_{A_s\alpha}}_{\text{2nd order conditional variances}} + \underbrace{V_{K_xAA_s} + V_{K_xA\alpha} + V_{K_xA_s\alpha} + V_{AA_s\alpha}}_{\text{3rd order conditional variances}} + \underbrace{V_{K_xAA_s\alpha}}_{\text{4th order conditional variance}}$$

Sensitivity indices:

First order sensitivity indices S_i:

$$S_{K_x} = \frac{V_{K_x}}{V(C_{\max})}$$

$$S_A = \frac{V_A}{V(C_{\max})}$$

$$S_{A_s} = \frac{V_{A_s}}{V(C_{\max})}$$

$$S_\alpha = \frac{V_\alpha}{V(C_{\max})}$$

- S_i quantifies sensitivity of C_{max} to the parameter i.
- Identification of a parameter with high S_i should be prioritized to reduce the uncertainty.

Total sensitivity indices S_{Ti}:

$$S_{TK_x} = \frac{V_{K_x} + V_{K_xA} + V_{K_xA_s} + V_{K_x\alpha} + V_{K_xAA_s} + V_{K_xA\alpha} + V_{K_xA_s\alpha} + V_{K_xAA_s\alpha}}{V(C_{\max})}$$

$$S_{TA}$$

$$S_{TA_s}$$

$$S_{T\alpha}$$

- S_{Ti} quantifies sensitivity of C_{max} to the parameter i and its interactions with the other parameters.
- A parameter with low S_{Ti} could be fixed to simplify a model and reduce the uncertainty.

If model is additive then no interactions occur and $S_{K_x} + S_A + S_{A_s} + S_\alpha = 1$ $S_{TK_x} + S_{TA} + S_{TA_s} + S_{T\alpha} = 1$

Sensitivity analysis (SA)

- To compute sensitivity indices Monte Carlo simulations of 100 000 parameter sets were performed.
- K_x and A were drawn from normal distributions. A_s and α were drawn from uniform distributions.

First order sensitivity index S_i

Q3	K_x	A	A_s	α
1 – 2	0.318	0.682	0.012	0.000
2 – 3	0.315	0.684	0.007	0.000
3 – 4	0.318	0.680	0.006	0.000
4 - 5	0.313	0.684	0.006	0.000

Flow rate Q3

Total sensitivity index S_{Ti}

Q3	K_x	A	A_s	α
1 – 2	0.320	0.682	0.012	0.000
2 – 3	0.318	0.684	0.008	0.000
3 – 4	0.323	0.681	0.007	0.000
4 - 5	0.319	0.685	0.007	0.000

Flow rate Q3

Conclusions:

- The dead zone model is additive - the sum of S_i and S_{Ti} is about 1.
- A and K_x affects C_{max} . The uncertainty of results depends mostly on these two parameters.
- α and A_s have no impact on results, as both sensitivity indices are near to zero. Transient storage process is not important in the studied case.
- The model could be simplified by neglecting α and A_s .

Fickian model

Omiting transient storage parameters result in reducing the dead zone model to the Fickian model:

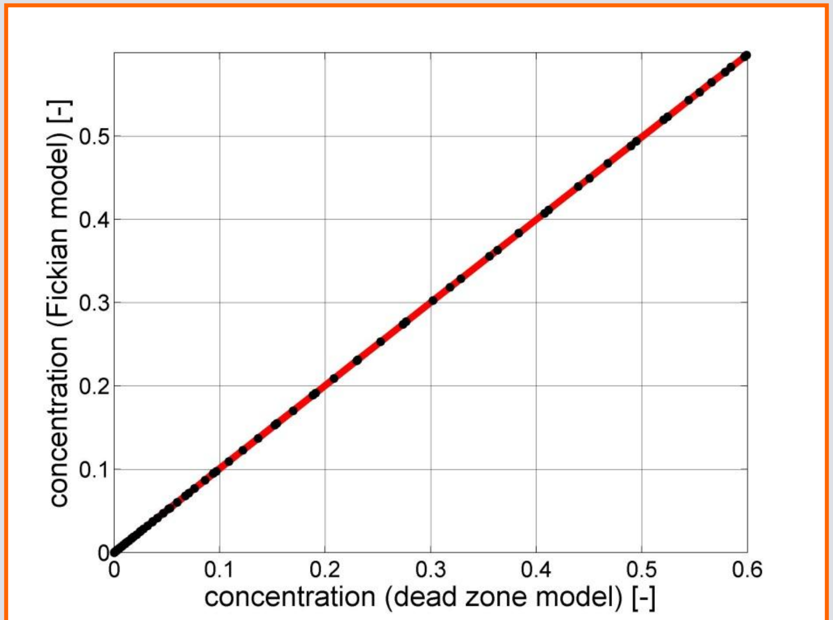
$$\frac{\partial C}{\partial t} = -\frac{Q}{A}\frac{\partial C}{\partial x} + \frac{1}{A}\frac{\partial}{A\partial x}\left(AK_x\frac{\partial C}{\partial x}\right)$$

Advection

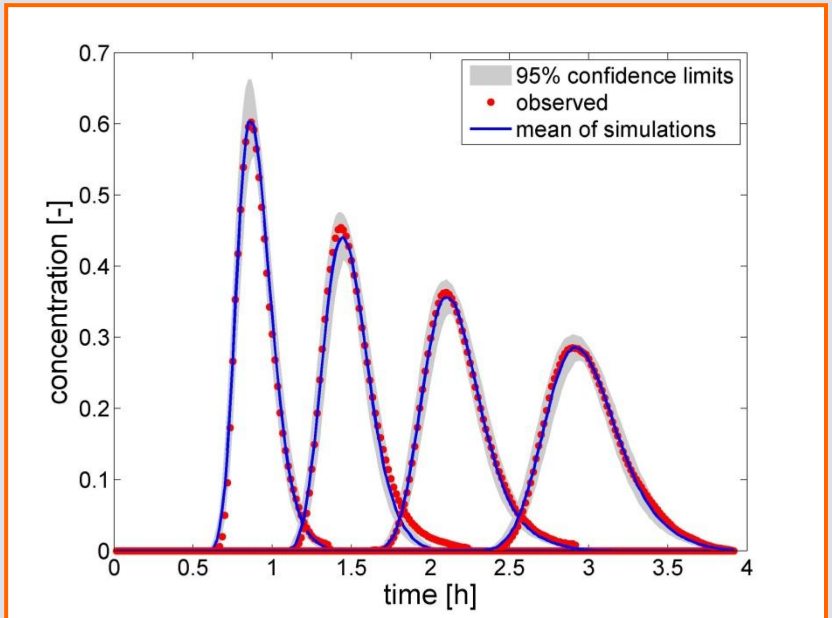
Dispersion

The Fickian model is sufficient to model contaminants transport in the studied case.

Comparision of the dead zone model and the Fickian model results (sub-reach 1-2 flow rate Q3):



Simulations with 95% confidence limits (flow rate Q3):



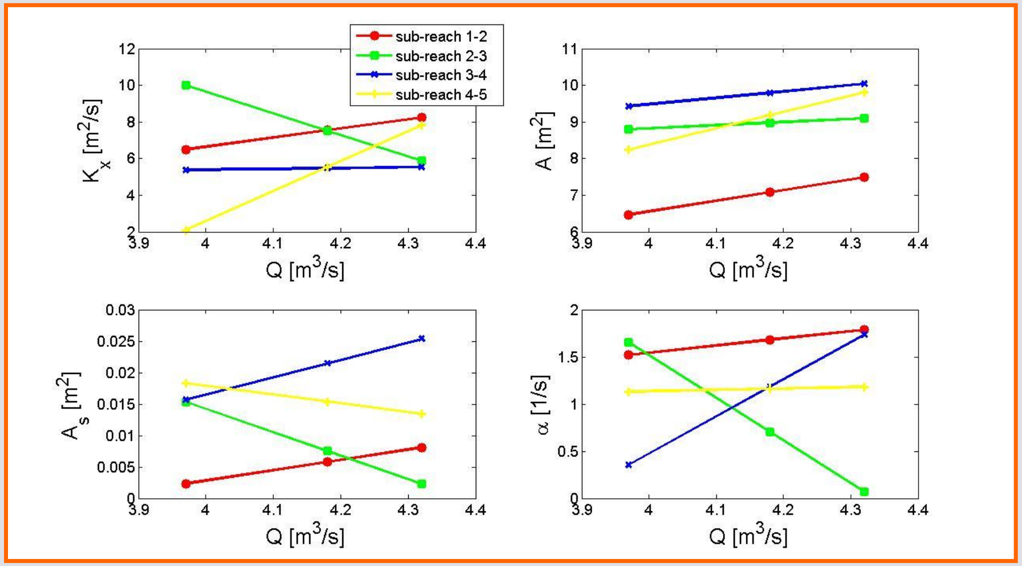
Conclusions

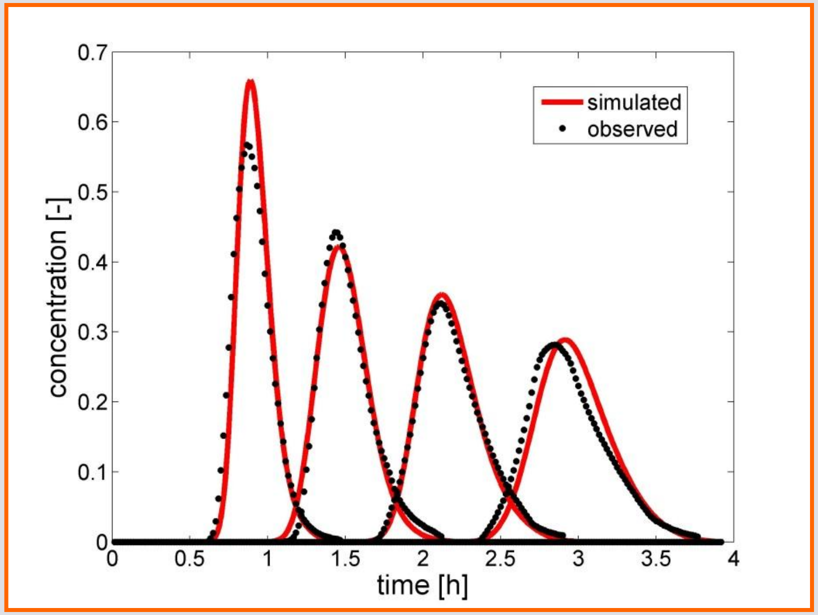
- A deterministic solution of the dead zone model is not unique (deterministic calibration and Monte Carlo simulations).
- The sensitivity analysis showed that:
  - The model output is most sensitive to parameters A and K_x.
  - Parameters α and A_s have no impact on the model output. Transient storage is irrelevant in the studied reach.
- **In the studied case, the dead zone model can be simplified to the Fickian model.**

Thank you for attention

Verification

- The dead zone model was verified for flow rate Q1.
- Values of parameters calculated by interpolation of optimal parameters values for flow rates Q2 and Q3.
- It was assumed that parameter values increase linearly with the flow rate.





Flow rate Q1