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Inverse model of single-fracture hydraulic and tracer experiments including a laser scanning data correction

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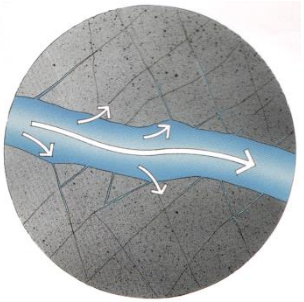
Introduction

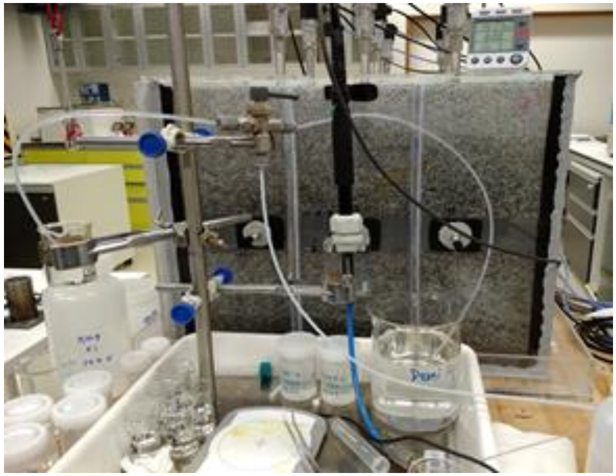
- Aim:
  - "Evaluate experiment" (**common project lead by UJV – EGU display D356**)
  - Understanding phenomena related to fracture heterogeneity
  - Developing/testing experimental and modelling methods



- Application:
  - Spent nuclear fuel repository safety
  - Other contaminants (heavy metals, nanomaterials)
  - Hard rock environment (fractures)
- State of the art
  - Laser-scan data used recently for similar experiments but without full evaluation of hydraulic and transport spatial data
  - Problems: raw data x model input, resolution x computational demands
  - Fracture solute transport: extensively studied, heterogeneous models based on significant abstraction (stochastic, channel network), qualitative fit

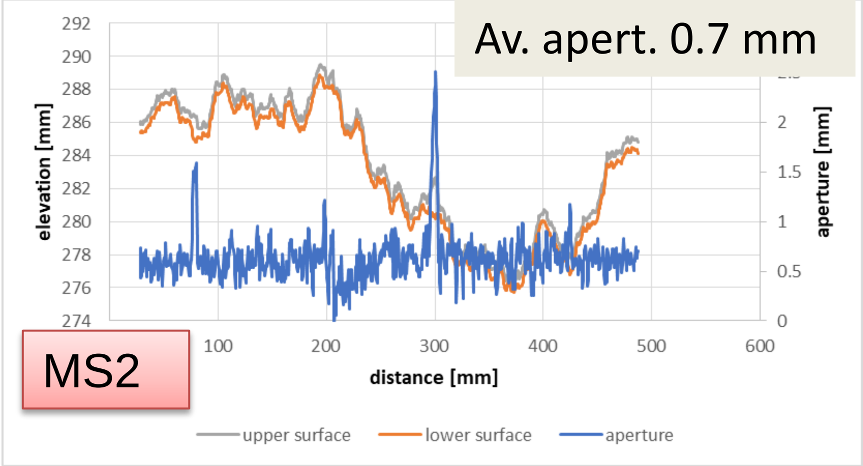
Experiment

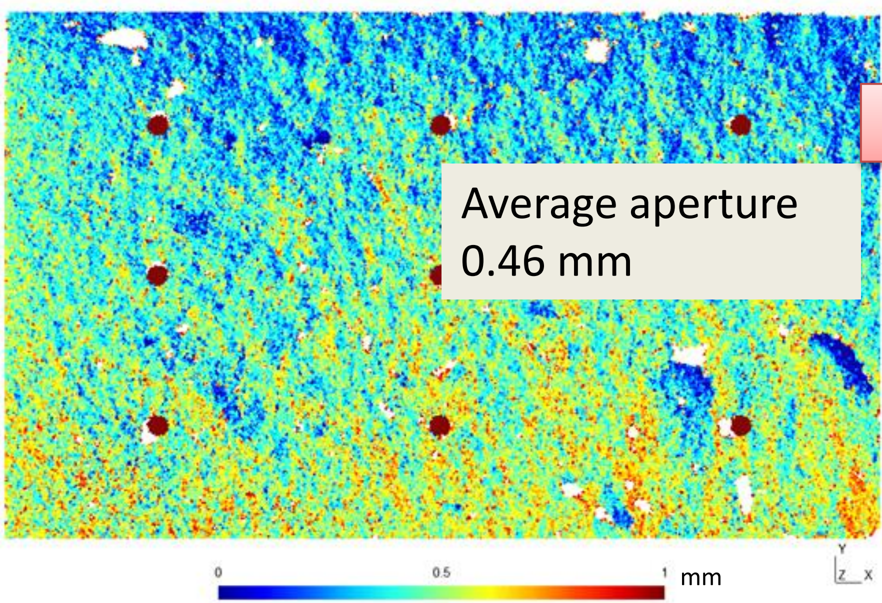
- Block of granite, artificially split to get a fracture
  - 2 samples MS1 and MS2, approx. 800 x 500 mm
- 8 in/out holes (various combinations), 9 micro-boreholes through the upper piece
- Flow-rate controlled (various cases)
- Tracers NaCl, KCl, KI (detection by electric conductivity, ion-selective)
- Variable instrumentation: pressure sensors / tracer sensors
  - Data p_1…p_9, c_in(t), c_out(t), c_1(t)…c_9(t)

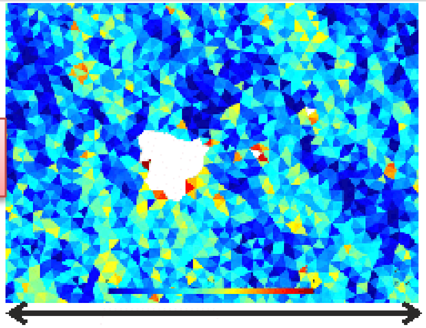


Laser-scanning data

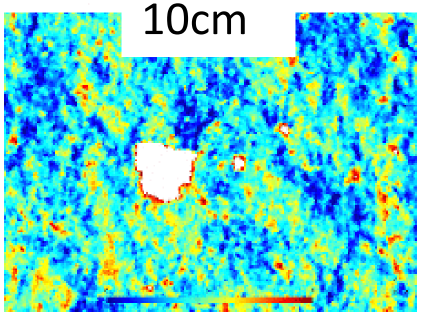
- Two surfaces (lower, upper) separately + whole block … coordinate fitting
- μm resolution, 15M (x,y,z) points
- Point cloud converted to regular grid (Kriging) and projected to computational mesh (3mm / 1mm triangular unstructured)
- Fracture opening (aperture) by surface subtraction …b(x,y)







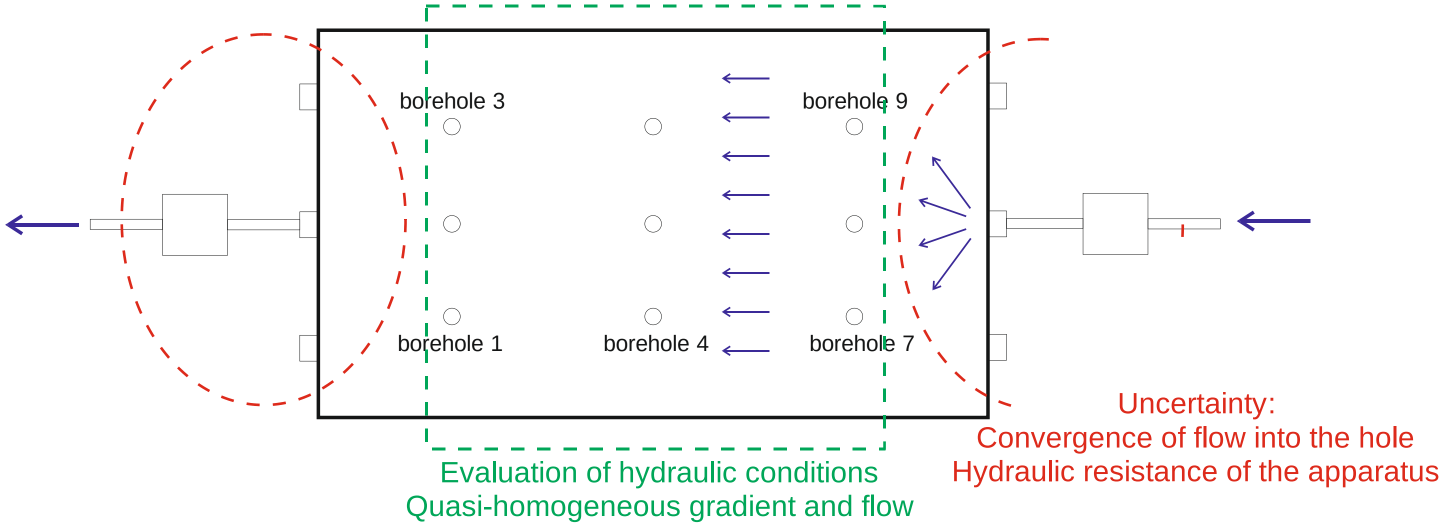
3 mm mesh



1 mm mesh

Model setting

- 2D rectangle domain, element-wise data b(x,y), T(x,y)
- boundary: pressure / flow rate / concentration in inlet/outlet segments (5 mm = approx. diameter of tubes)
- Steady-state flow, transient transport



Model equations and parameters

- Water flow (hydraulics):
  - Planar fracture of variable aperture
  - Equiv. 2D Darcy's law, unit thickness
    with transmissivity T given by Hagen-Poiseuille (cubic law)

$$\vec{q} = T\nabla\left(\frac{p}{\varrho g}\right) \qquad \nabla \cdot \vec{q} = 0 \qquad T = \frac{\varrho g}{12\mu} b^3$$

$\vec{q}$

- Solute transport (tracer):
  - Advection and hydrodynamic dispersion
  - b equivalent of porosity

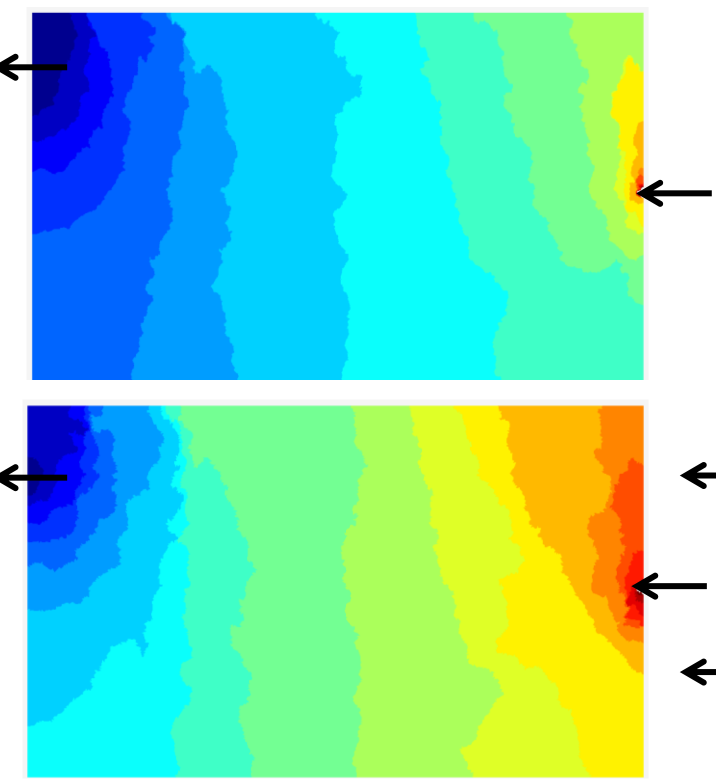
$$\frac{\partial c}{\partial t} + \nabla \cdot (\vec{v} c) - \nabla \cdot (D_h \nabla c) = 0 \qquad D_h(D_m, \alpha_L, \alpha_T)$$

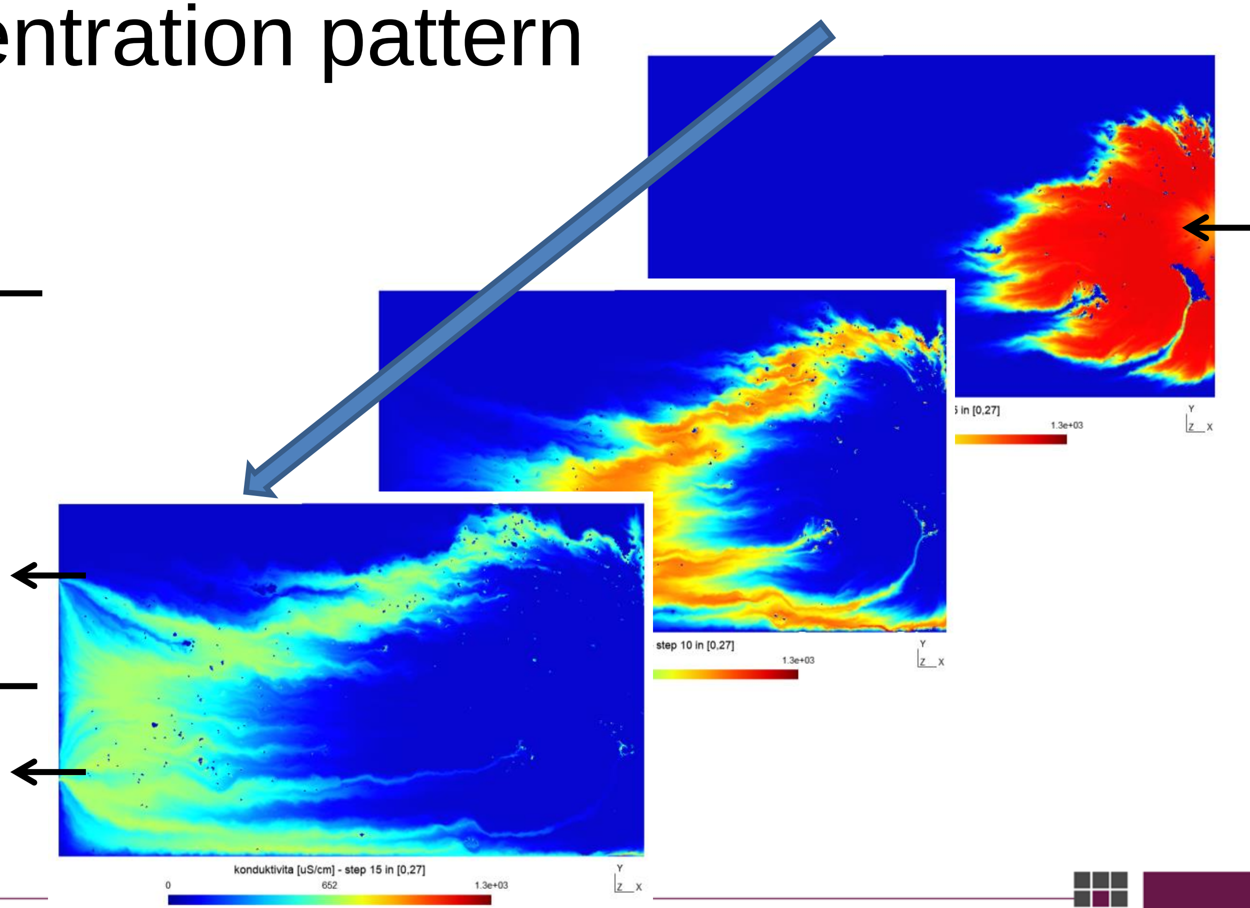
$$\vec{v} = \frac{\vec{q}}{b}$$

- *q* flux density [m²/s] vs. *v* real velocity [m/s]

Examples (model)

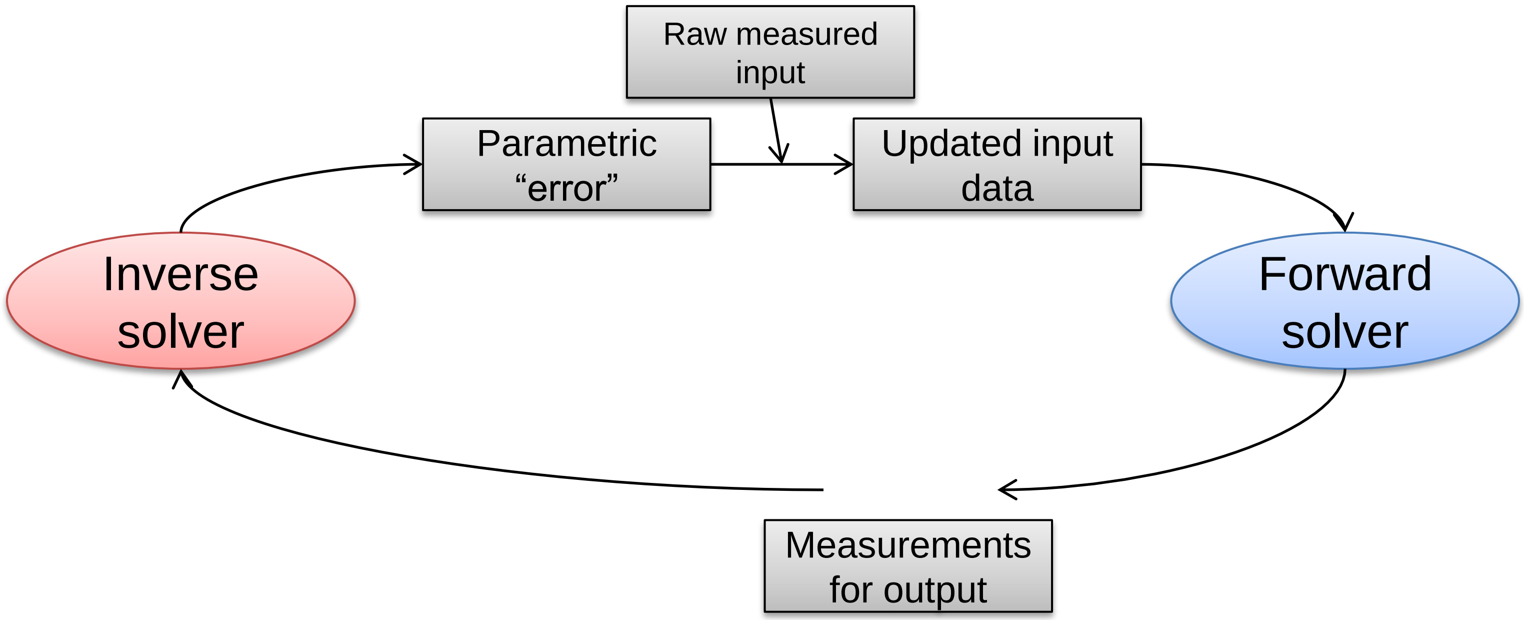
- Pressure distribution
- Tracer concentration pattern





Why inverse model

- Both inputs and outputs are given
- But better fit of model and experiment desired
- Ideas:
  - Input data are subject to systematic error (fitting of two surfaces)
  - Geometric data are not those controlling the phenomena (eqn / constitutive law validity)



Numerical solution

- Flow problem:
  - Mixed-hybrid finite elements (velocity linear approximation, discrete mass balance)
- Transport problem:
  - Discontinuous Galerkin
- In-house code Flow123d – open source (Březina et al., http://flow123d.github.io/)

- Inverse solver
  - Gradient methods
  - Differences by model input perturbation
- UCODE freeware (Poeter and Hill, USGS)

- **Project partners solutions:**
  - **MODFLOW+MT3D**
  - **FEFLOW**

Numerical features

- Problem containing singularities (surface contact/penetration)
- Avoided by thresholding b(x,y) by a minimum value with negligible effect globally (0.001 mm)
- Still $>10^9$ factor in the transmissivity coefficient T(x,y) … poorly conditioned
- Direct algebraic solver more successful than iterative

- Typical problem size and simulation time (1CPU)
  - 3mm hydraulic …100k elements (700k DoFs), <1min
  - 3mm transport (1000s, dt=5s…100s = coarse!) … 15min
  - 1mm hydraulic … 900k elements, 8min
  - 1mm transport … 4.5 hours

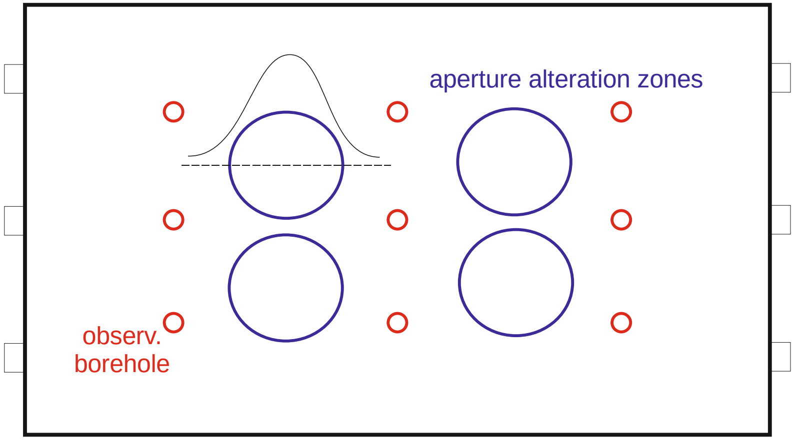
Parameterization

- Aperture correction
  - $b(x,y) = f\,(b_{raw}(x,y), p_1,\ldots, p_n)$
  - Uniform shift

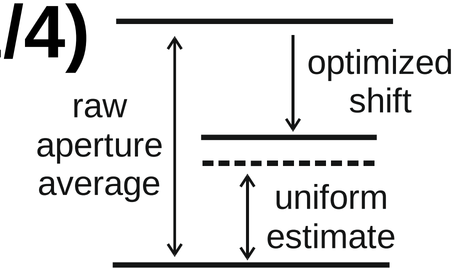
    $b_{raw}(x,y)-b_s$
  - Rotation around x and y

    $\ldots +k_x(y-y_c)+k_y(x-x_c)$
  - Zones of local deviation

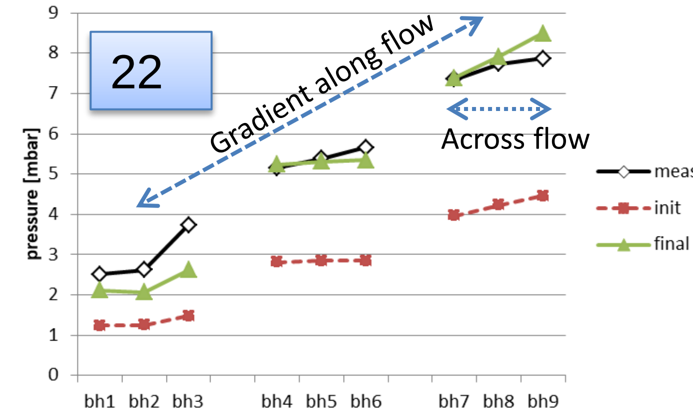
    $\ldots +b_z \exp(|\mathbf{x}-\mathbf{x}_c|^2/r^2)$
- Transport problem
  - Longitudinal dispersivity (i.e. “diffusion”)

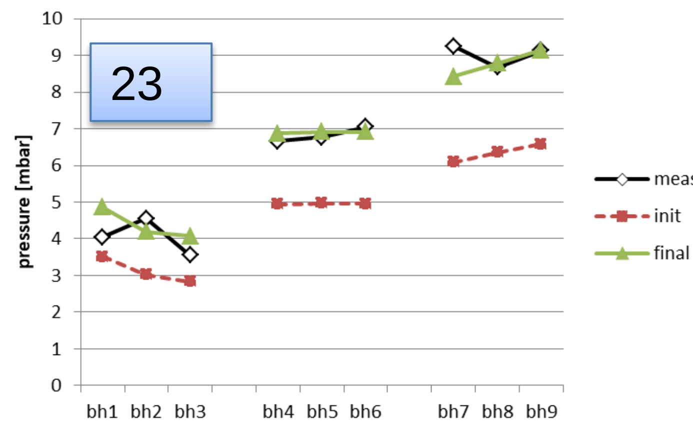


Results for 9 pressures and one breakthrough curve – group 1 (1/4)



- Single-parameter hydraulic model optimization
  - vertical shift of blocks b_s (positive value = closing fracture)
- Test with various in/out holes
  - Optimal cases partly consistent
- Significant mesh effect
  - Systematic
  - Better fit for finer case
- Consistent with uniform fracture estimation (aperture of 0.15 - 0.2 mm)



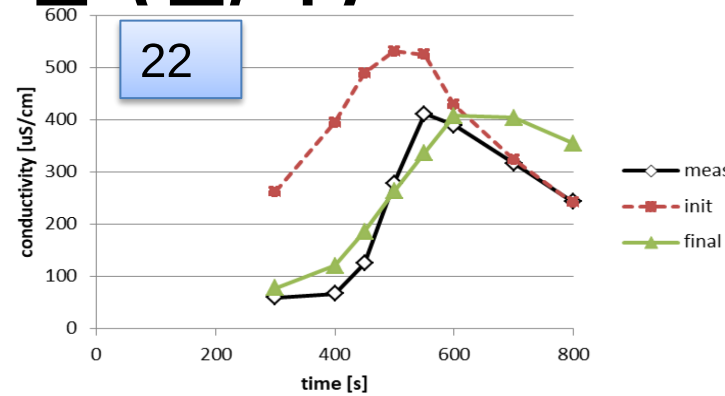


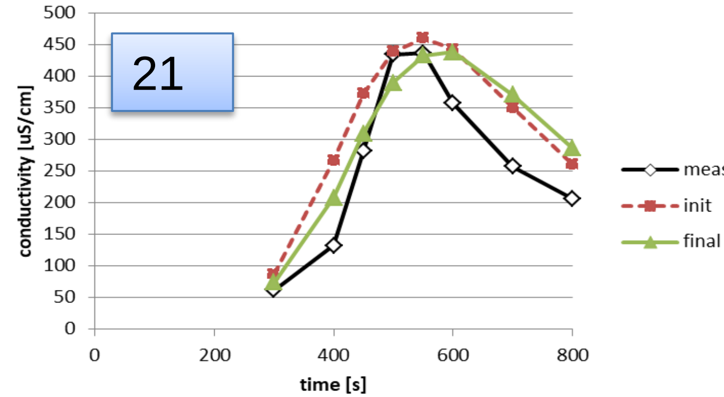
test code	optimal shift		fit criterion	
	3mm mesh	1mm mesh	3mm mesh	1mm mesh
MS1 21 G-C	0.201	0.2242	5.5526	4.2192
MS1 22 G-A	0.2247	0.2438	2.0463	2.2371
MS1 23 G-C	0.199	0.2215	2.6895	1.8427
MS1 30 G-C	0.1888	0.2109	2.9857	2.5706
MS2 G-ABC		0.3261		0.56694
MS2 G-B		0.4305		0.37934

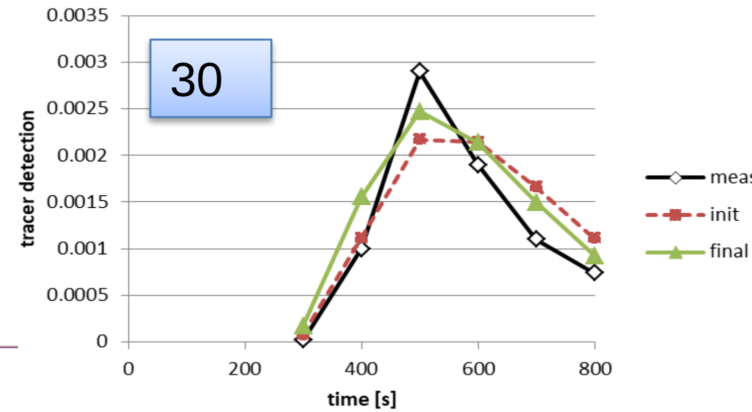
Results group 1 (2/4)

- Single-parameter transport model optimization
  - vertical shift of blocks b_s (positive value = closing fracture)
- Different from hydraulic optimization
- Optimal fit criterion does not correspond to the “optimal” peak position (i.e. correct transport velocity)
- Correct peak position consistent with hydraulic optimal value

test code	optimal shift		fit criterion	
	3mm mesh	1mm mesh	3mm mesh	1mm mesh
MS1 21 G-C	0.1845	0.194	34511	32364
MS1 22 G-A	0.1001		32948	
MS1 22a G-A	0.1408		24840	
MS1 23 G-C	0.1422		56378	
MS1 30 G-C	0.1975		7630	







Results group 1 (3/4)

- Multiparameter optimization of aperture field (hydraulic)
  - Block rotation
  - 4 local zones connecting/isolating sensor places
- Optimum more difficult to find, often not reasonable, rather small improvement of fit criterion
- Intuitive choice of initial estimate helps

test code	mesh	uniform shift [mm]	local shift [mm]				fit criterion
			zone1	zone2	zone3	zone4	
MS1 21 G-C	3mm	0.1997	-1.79E-04	-3.88E-05	-6.53E-03	6.68E-03	5.6123
MS1 21 G-C	3mm	0.1711	0.00E+00	-1.29E-01	-1.30E-01	0.00E+00	2.8429
MS1 21 G-C	1mm	0.2011	-1.32E-03	-9.18E-02	-1.07E-01	4.83E-02	1.7374
MS1 21 G-C	1mm	0.1976	-2.58E-04	**-1.14E-01**	**-1.07E-01**	4.00E-02	1.782
MS1 23 G-C	1mm	0.2198	1.12E-03	-3.22E-05	-1.56E-03	-3.84E-03	2.0939

	uniform shift [mm]	rotation x	rotation y	fit criterion
MS1 21 G-C	0.2232	1.64E-04	4.92E-06	2.1974
MS2 G-ABC	0.33	-4.17E-07	-7.21E-09	0.60702
MS2 G-ABC	0.33	7.77E-07	-5.98E-08	0.60687

Results group 1 (4/4)

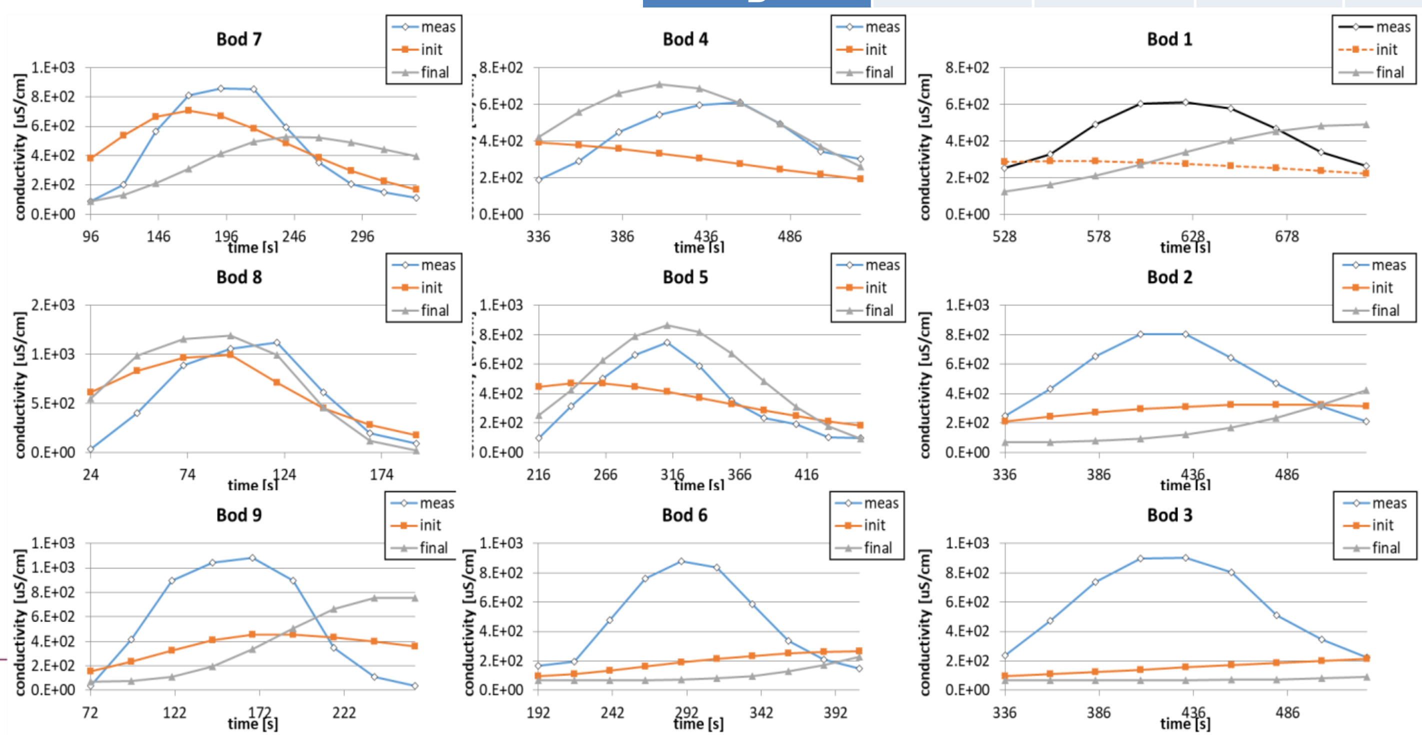
- Optimization of transport problem with dispersion
  - Uniform shift + longitudinal dispersivity [mm]
- Fit improvement but questionable physical meaning
  - Dispersivity values not consistent among tests
- Needs time step refinement to avoid numerical diffusion

test code	shift	dispersivity	fit criterion
MS1 21 G-C	0.1792	24.01	32041
MS1 22 G-A	0.1096	0.1	10138
MS1 22 G-A	0.1284	20.78	25124
MS1 23 G-C	0.1412	11.44	50822
MS1 30 G-C	0.2002	0.7868	6480

Results for 9 concentration observations (breakthough curves) - group 2

- Optimization of transport problem only
  - Uniform shift + longitudinal dispersivity [mm]
- Too large dispersivity ("fit with a constant")

Experimentu code	Mesh	No. observati ons	Shift [mm]	Dispersiv ity [mm]	Fit criteriu m
MS2 5.6.19 G-B	3 mm	87	0,3579	35,34	94824
MS2 5.6.19 G-B	1 mm	87	0,3506	35,24	94445
MS2 23.7.19 G-B	3 mm	81	0,3587	156,2	60251
MS2 5.9.19 G-B	3 mm	87	0,3952	62,5	95732

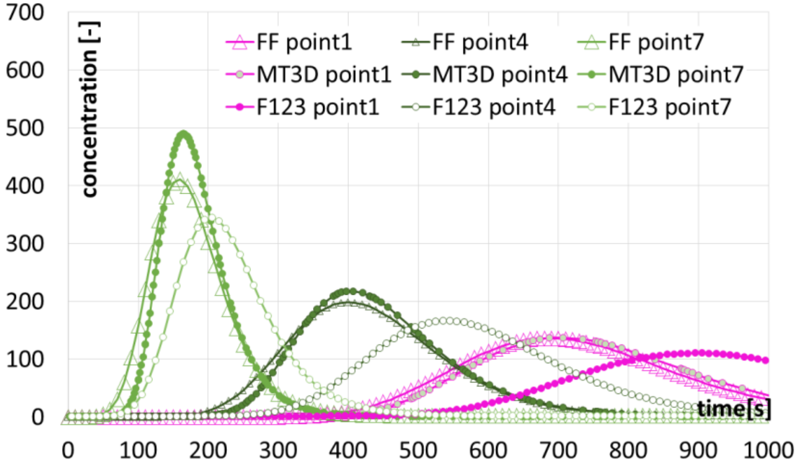


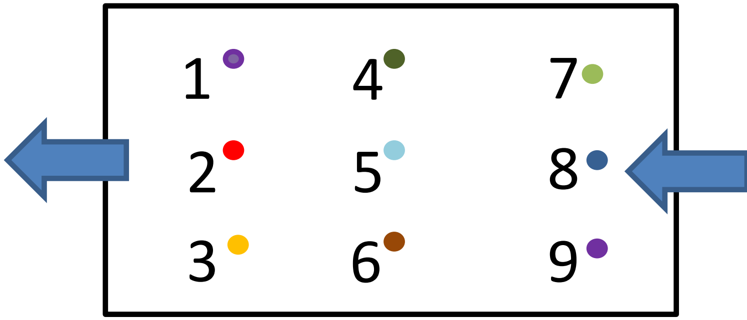
Model comparison

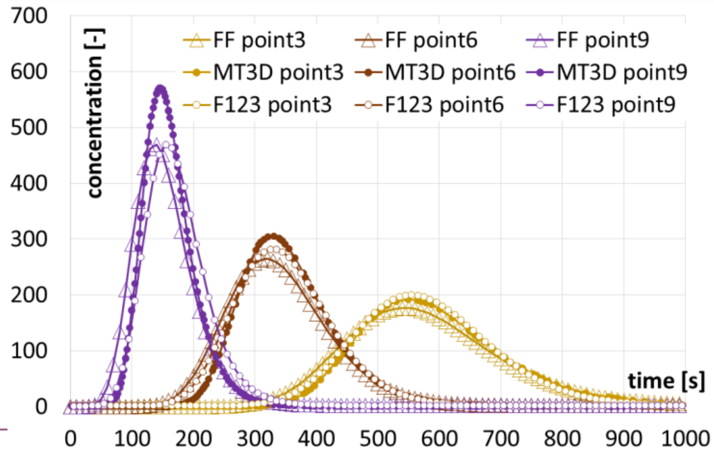
- Joint input parameter setting
  - Choice in/out points, flow rate, injection history
  - Median of aperture
- Three softwares
  - MT3D
  - FEFLOW
  - Flow123d

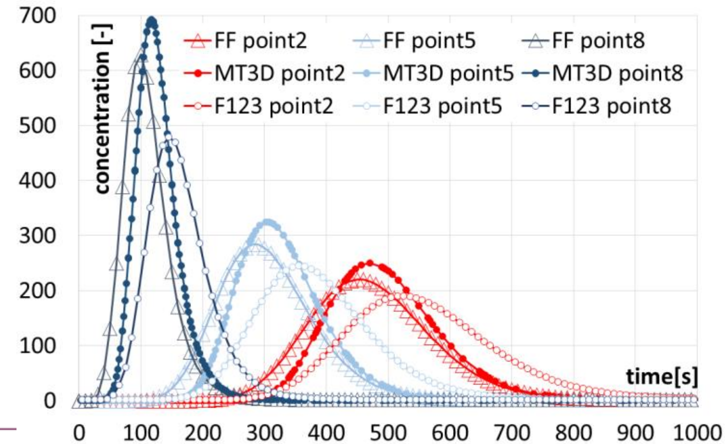
Model comparison

- Breakthrough curves in borehole grid
- Some of them fit well, but retardation of Flow123d results along the upper line … laser scan problems at the boundary (next slide figures)



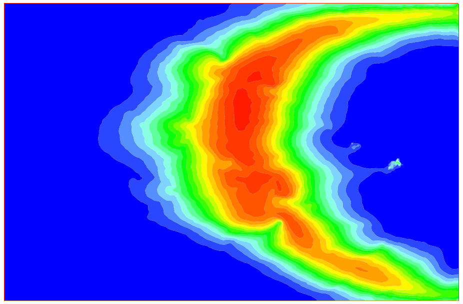




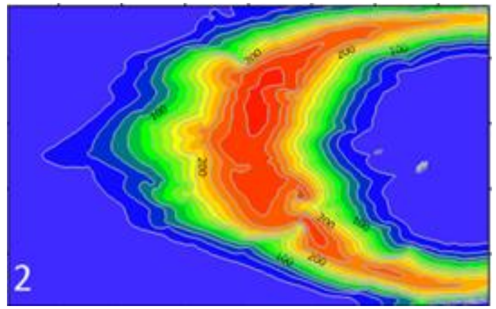


Model comparison

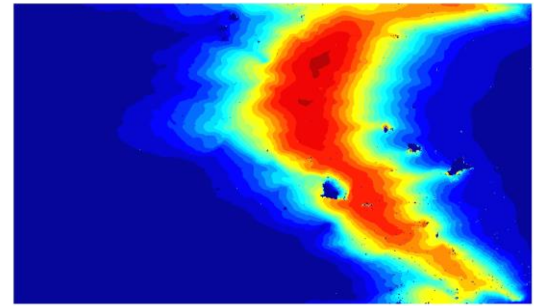
MT3D



FEFLOW



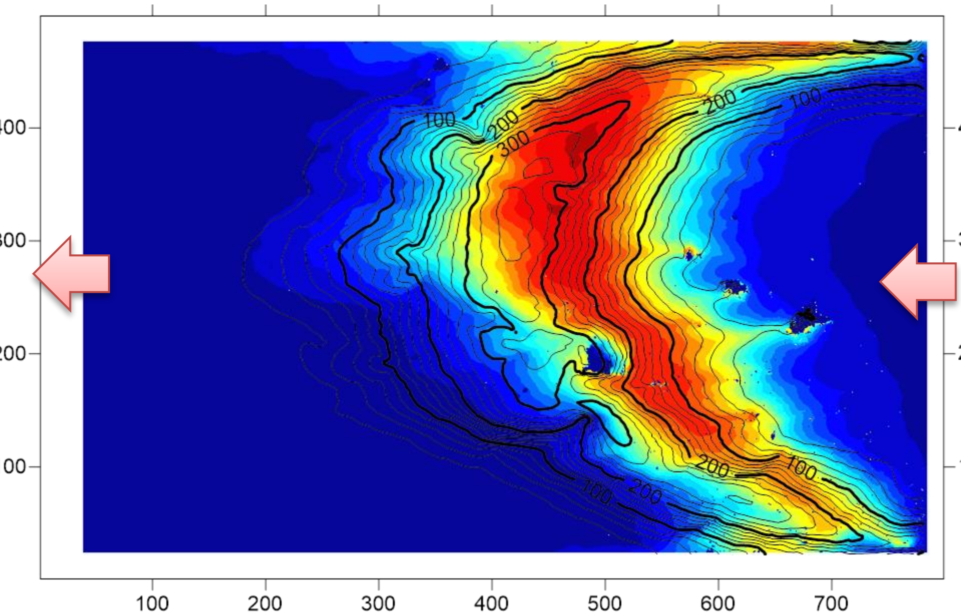
Flow123d

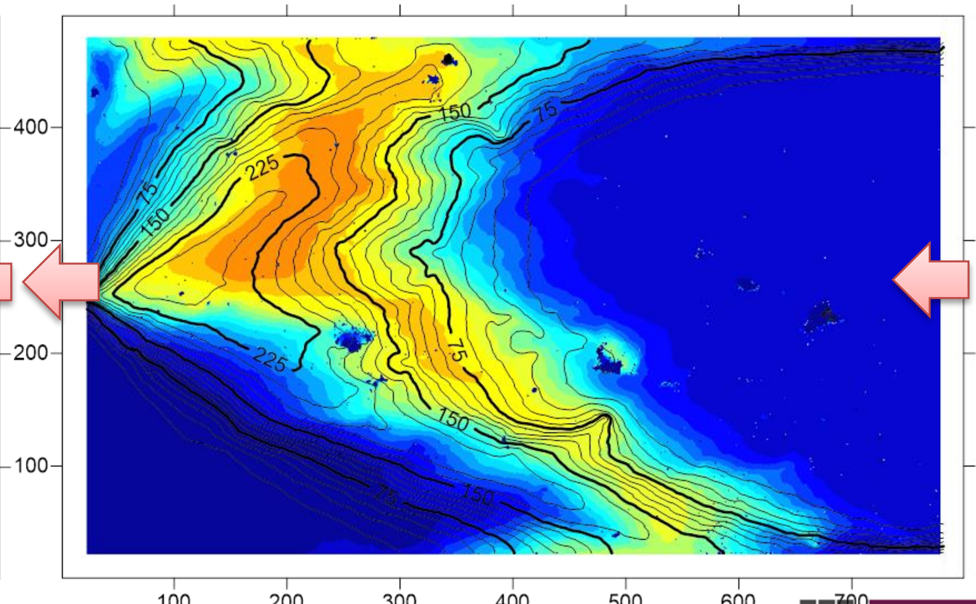


T=150s

MT3D lines over Flow123d contours

T=600s





Conclusion

- Introducing a correction to laser-scan input data of fracture aperture necessary to fit the experiment
- Inverse model successful to find the block shift (single parameter)
  - Physically consistent but some variation across realizations
  - Correctly captures the differences of the two blocks
- Capturing spatial inhomogeneity less successful
- Limited possibility to use the coarse problem for initial estimate (speed-up) of the fine problem optimization (systematic difference)
- Calibration of transport parameters (dispersion) mostly not successful

- Comparison of <u>transport</u> models (software+modellers) showed strong sensitivity on small deviations in data processing

- Thank you for your attention

- Acknowledgement
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  - Partners (experiment design, operation and joint evaluation): ÚJV Řež a.s., Research Centre Řež, PROGEO Ltd.