

Nanoparticle transport in heterogeneous column experiments: the use of magnetic techniques

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Publication:

Riley, M. S., Suttie, N., Stevenson, C. T., Tellam, J. H. (2019) in *Colloids and Surfaces A*

Masters projects:

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Engineered nanoparticles (ENPs) in groundwater

- ENPs present in many everyday products
- certain to transfer to groundwater
- concerns over potential toxicity

The challenge

Identification and quantification of processes governing ENP migration

Engineered nanoparticle transport in rock

Processes might include:

- Advection
- Dispersion
- Physical Straining
- Attachment (irreversible)
- Attachment (reversible)

Potential model parameters:

- Effective porosity
- Dispersivity
- Straining coefficients
- Attachment rates
- Detachment rates
- Attachment capacities

Column experiments



Problems

- Non-unique parameter sets for a mathematical model (model equivalence)
- Many alternative mathematical models
- Heterogeneity of attachment processes

Magnetic Susceptibility Monitoring and Modelling (MSMM)

- Non-invasive system for monitoring and modelling column experiments
 - Multiple “breakthrough curves” within the column
- Magnetic particles
- A model fitting technique
- Imaging potential

Magnetic susceptibility

$$\text{Volume susceptibility } (\chi_v \text{ or } \kappa) = \frac{\text{Magnetisation}}{\text{Strength of applied field}} \quad [\text{Dimensionless}]$$

Sufficiently small magnetite NPs are *superparamagnetic*

In randomly arranged groups of identical superparamagnetic NPs, the net susceptibility is proportional to the number of NPs present

BUT

The susceptibility of NPs in suspension is greater than that of NPs that are not free to rotate

Experimental Rig



Bartington
MS2C core logger

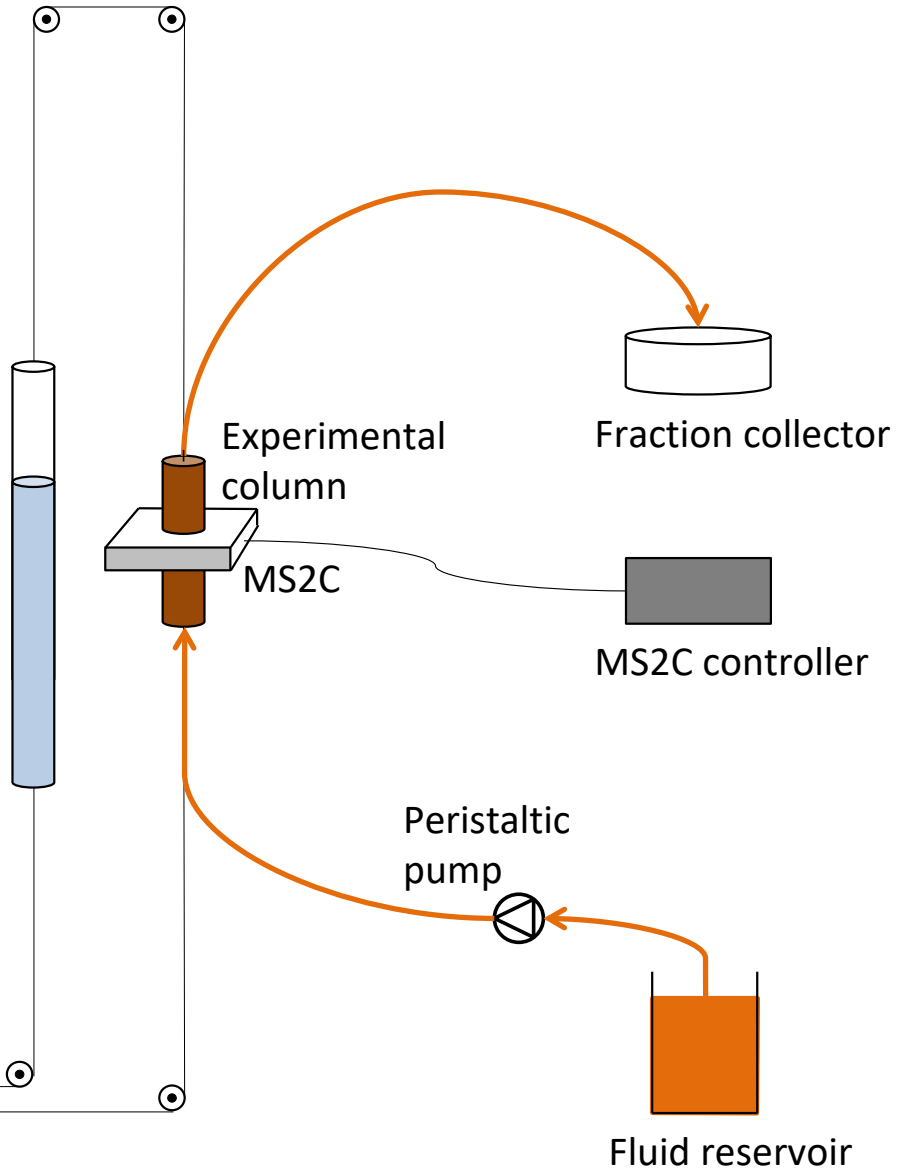


Bartington MS2B dual
frequency sensor

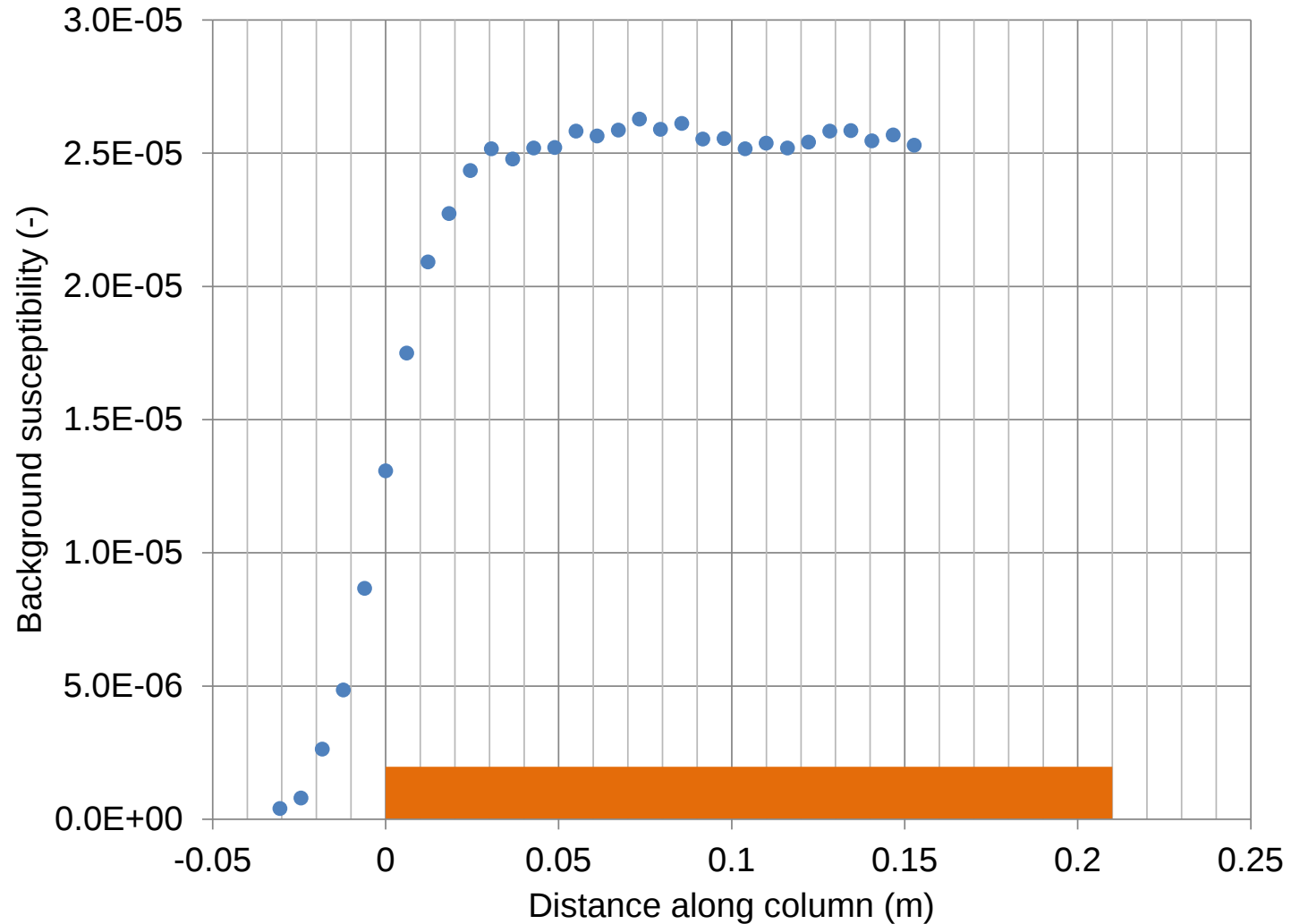


Stepping motor

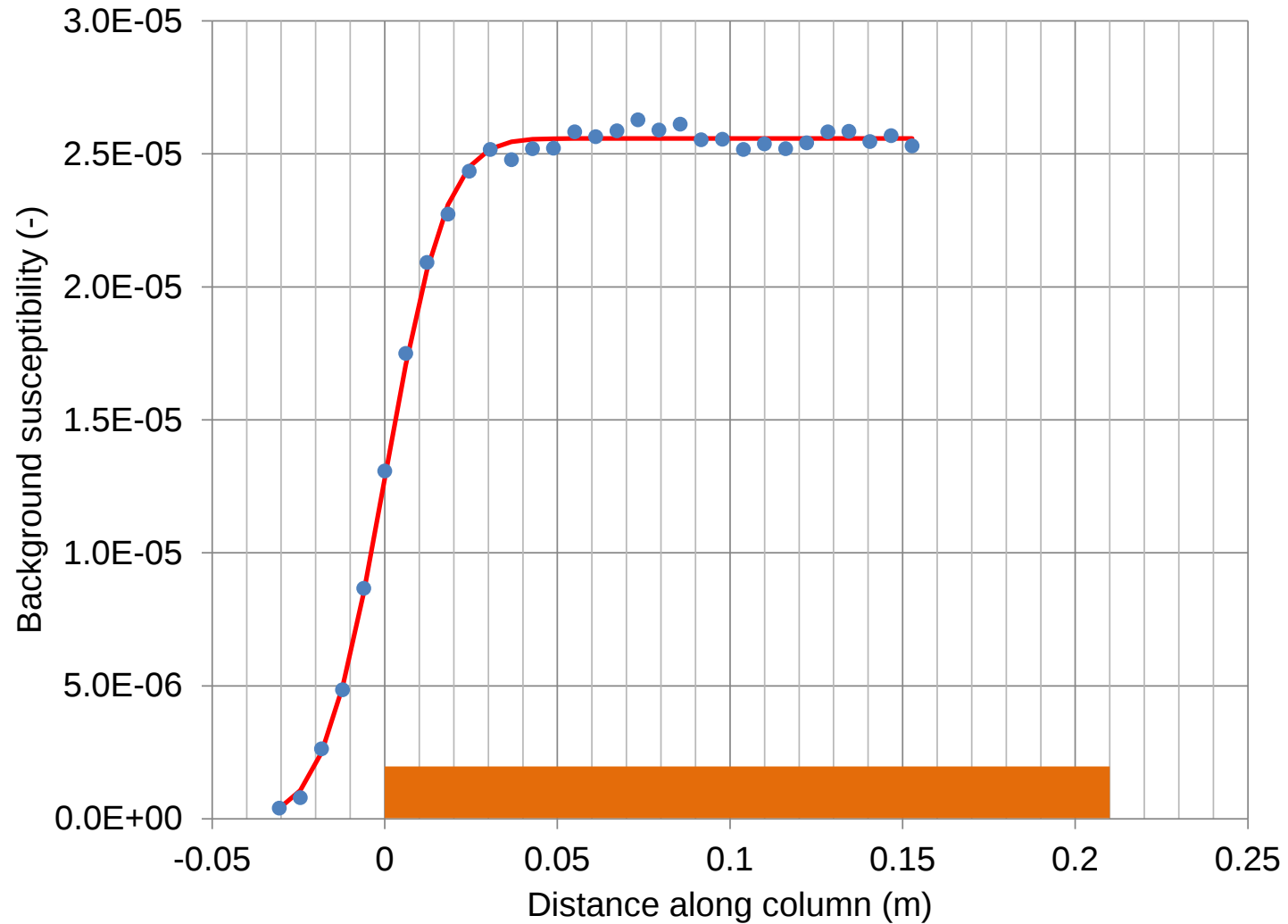
Water-filled
counterweight



Instrument Response Function



Instrument Response Function

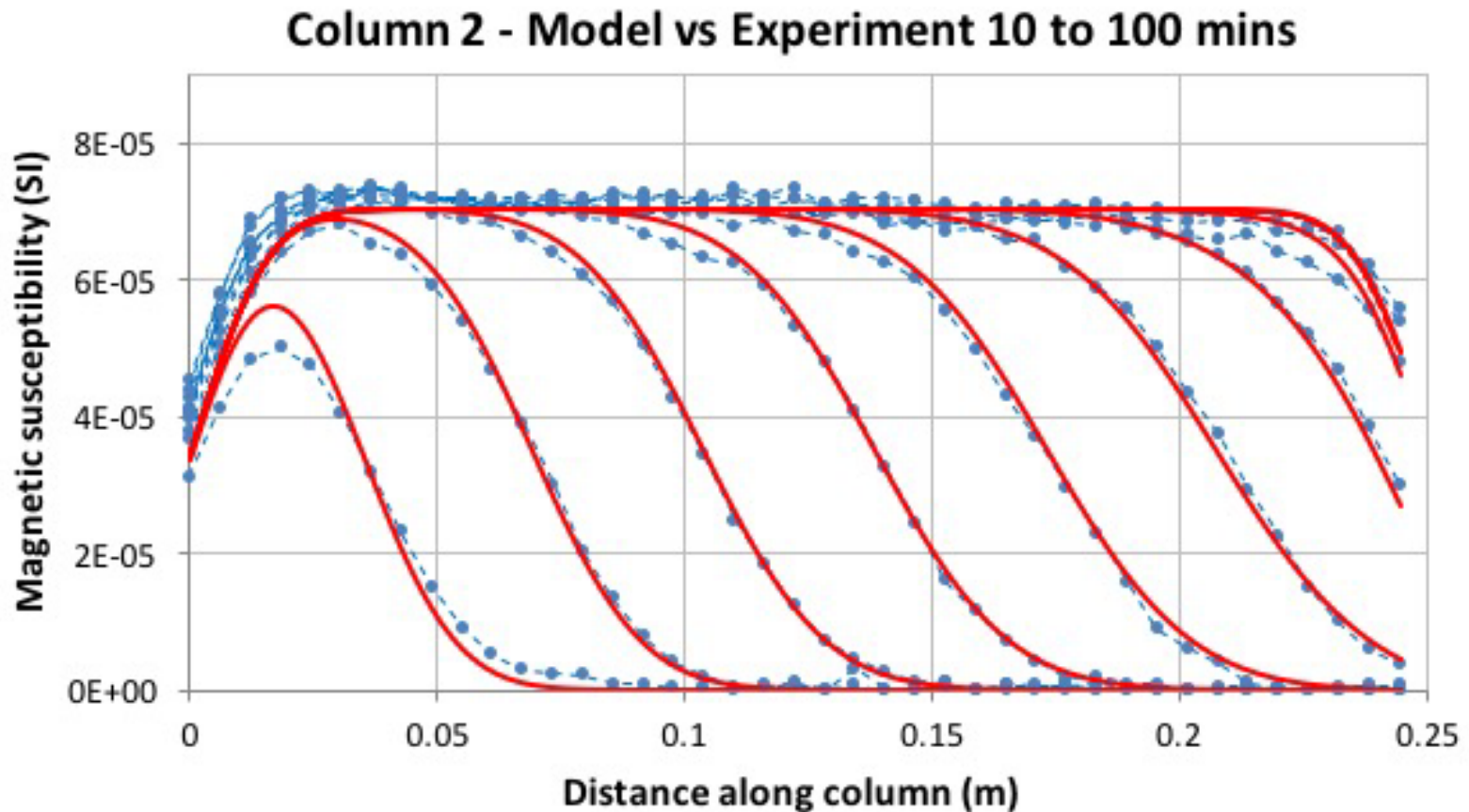


Modelling Strategy

- Select the mathematical model to be tested
- Simulate the transport experiment using the model
- Simulate the measurement process based upon the modelled concentrations
- Compare the results with the experimental data

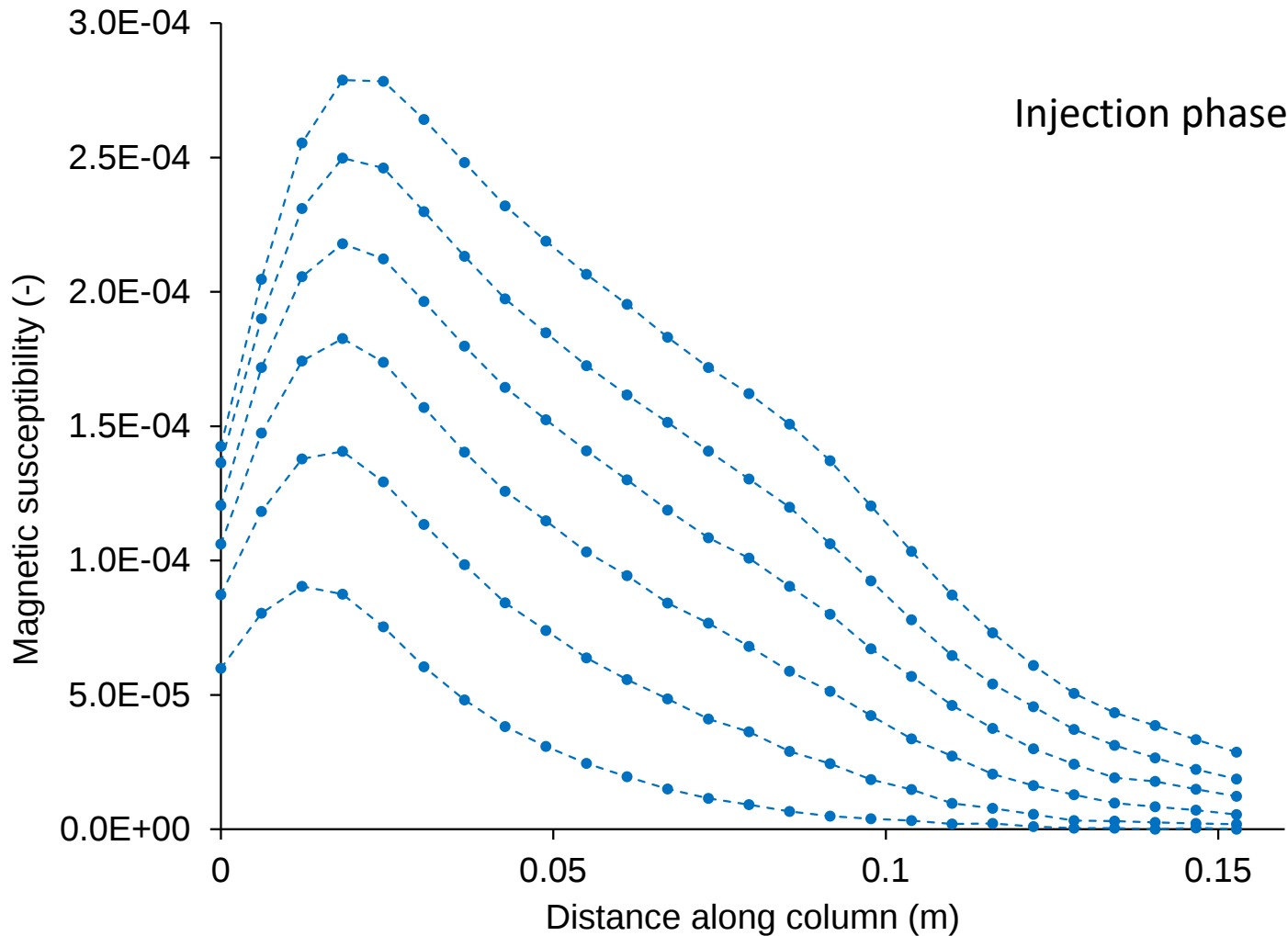
Homogeneous column – no particle retention

Injection phase (10 nm diameter magnetite ENPs)

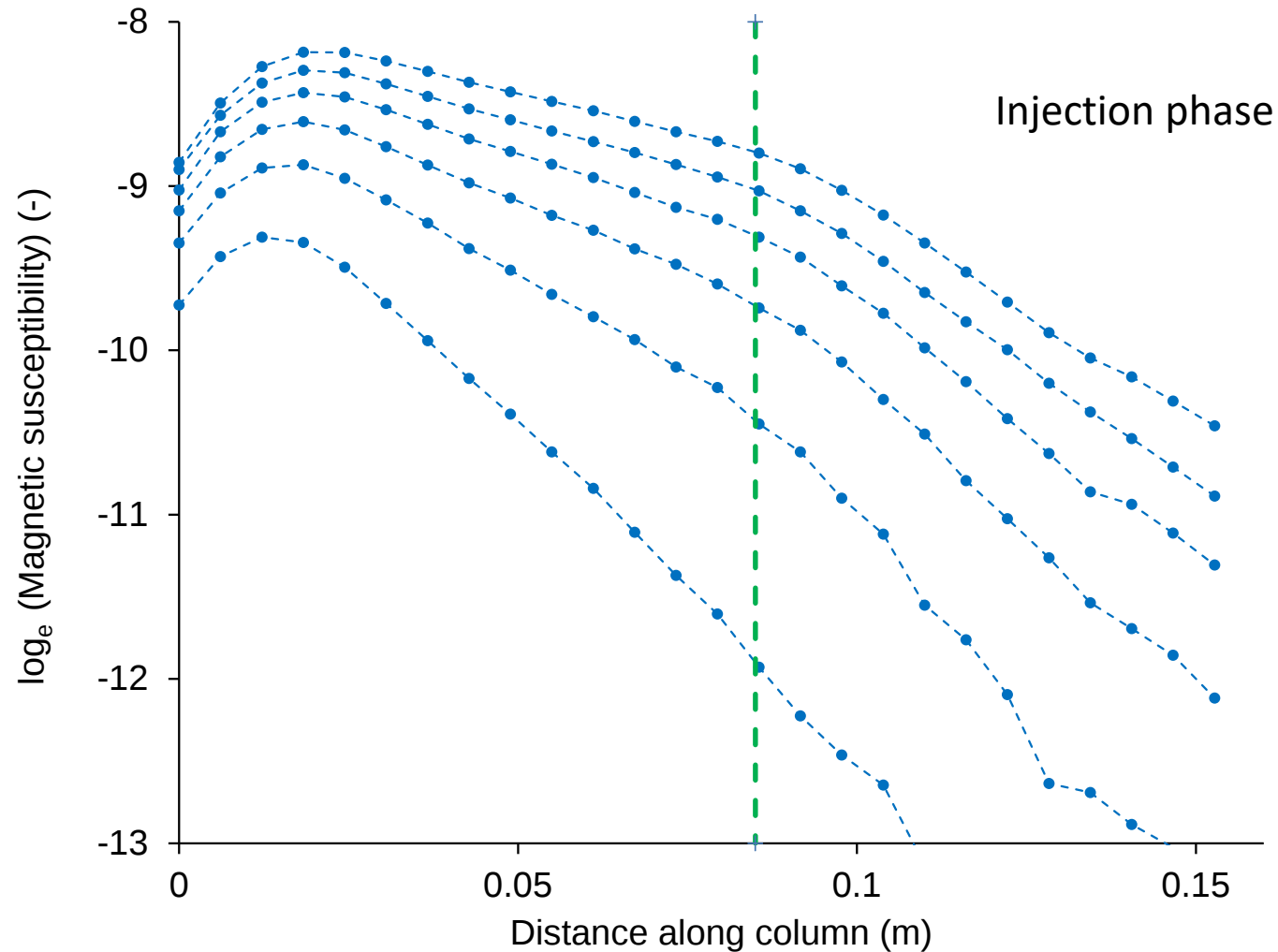


Measurements: Solid blue circles
Model: Red lines

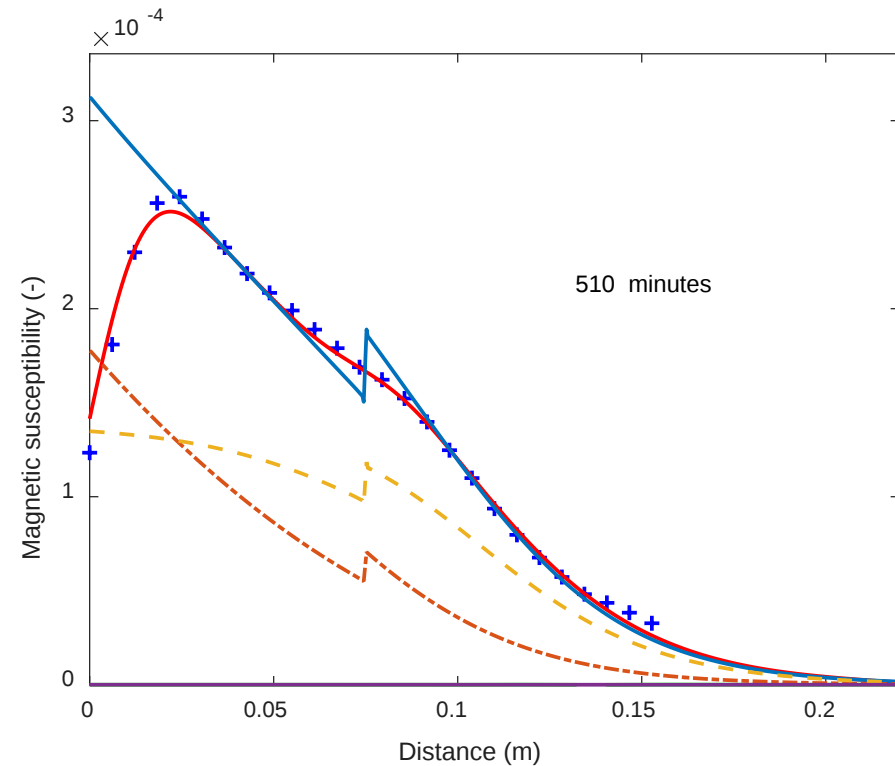
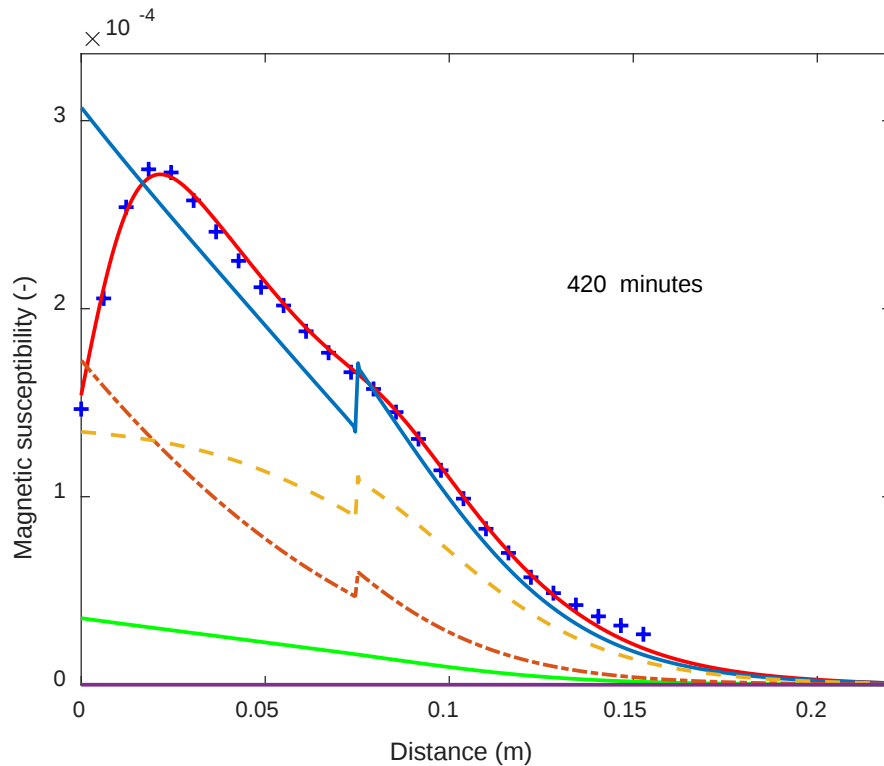
Complex column with strong particle retention



Complex column with strong particle retention



Complex column – strong particle retention



Measurements

+ + + + +

Modelled measurements

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Fluid phase

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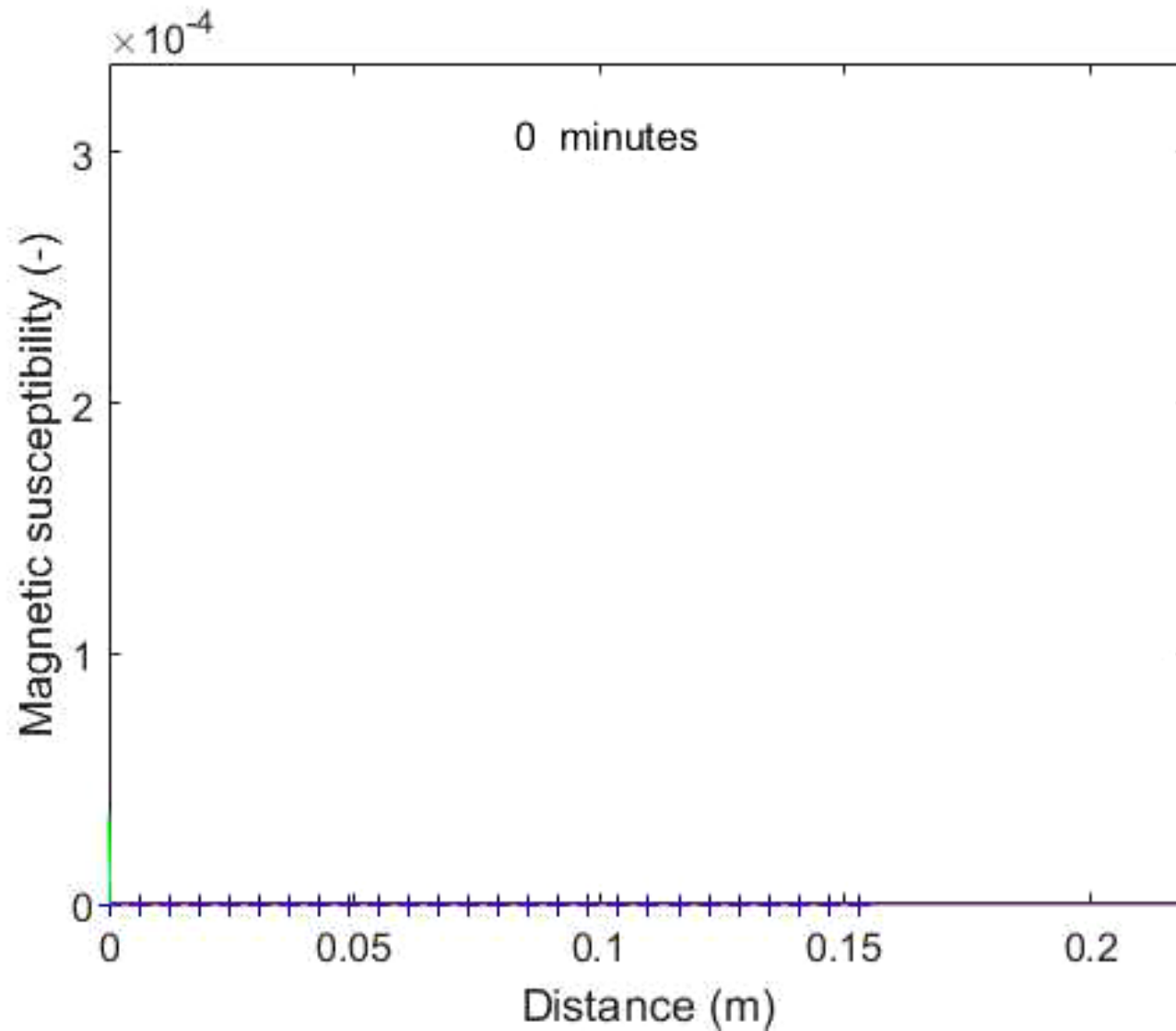
Strained phase

Irreversibly attached phase

Total of retained phases

—

Complex column – strong particle retention



Summary

Magnetic susceptibility monitoring and modelling allows us to “look inside” an experimental column, which

- produces exceptionally large data sets

and has the potential to:

- reduce the problem of model equivalence
- identify column heterogeneity
- quantify processes in heterogeneous columns

