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Numerical simulation of bench-scale tank experiments to quantify transverse dispersion

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Abstract Transverse mixing has been studied within the context of contaminant transport in aquifers, as it represents an important mixing process and is an essential prerequisite for geochemical and biodegradation reactions. In this work, the effects of different hydraulic parameters on plume development in homogeneous and heterogeneous porous media were investigated. A series of detailed and well controlled 2D bench-scale tank experiments, where one or more conservative tracers are injected, was performed in a homogeneous porous medium consisting of a fine matrix (0.25–0.3 mm) and in a heterogeneous medium that has the same matrix grain size but includes a more permeable lens (grain size 1.0–1.5 mm). The experiments were evaluated by numerical simulation. Results of a sensitivity analysis show that contrary to the homogeneous experiments, the tracer distribution is not very sensitive to variations in transverse dispersivity. In fact, only the order of magnitude of this parameter can be estimated by fitting the numerical results to the laboratory measurements. The plume shape and position in the heterogeneous set-up is mainly controlled by the contrast in the hydraulic conductivities between the matrix and the more permeable inclusion. A unique parameter set could be calibrated to closely fit the measured concentration data. For porous media with a grain size of 0.2–0.3 mm and 1.0–1.5 mm (i.e. permeable inclusion in the heterogeneous set-up) and a porosity of 0.42 and 0.43, the fitted longitudinal dispersivities are 3.49×10^{-4} m and 7.6×10^{-4} m, while the transverse dispersivities are 1.48×10^{-5} m and 7.1×10^{-5} m, respectively.

Key words transverse mixing; heterogeneity; bench-scale experiments; conservative tracers

INTRODUCTION

Between 2004 and 2009 a series of tracer experiments was performed at the University of Tübingen in order to study in detail how hydrodynamic dispersion affects the transport and mixing behaviour of dissolved compounds in saturated porous media (Olsson & Grathwohl, 2007; Rolle *et al.*, 2009; Chiogna *et al.*, 2010). The dispersion behaviour of different compounds and the influence on reactions were studied in a series of detailed and well controlled 2-D bench-scale tank experiments, that mimic a transect of an aquifer, where one or more pollutants, as conservative tracers, are injected (Rolle *et al.*, 2009).

Previous numerical evaluation of those experiments and the results of a sensitivity analysis (Ballarini *et al.*, 2010) led to the development of an improved experimental tank set-up. A set of new experiments was performed utilizing glass beads of uniform grain size in order to reproduce a homogeneous porous medium, while two different grain sizes were used to construct an inclusion of high permeability in a matrix of smaller beads as a heterogeneous porous medium. Uranine, bromide and oxygen were injected as tracers. This paper reports the results of the numerical evaluation of these experiments.

MATERIALS AND METHODS

All tracer experiments described in this work were carried out in quasi-2D vertical glass tanks, with inner dimensions of 77.3 cm length, 14.0 cm height and 1.1 cm width. The tank was equipped at the inlet and outlet ends with nine ports, spaced at 1.1 cm intervals. Steady-state flow through the tank was established by employing multi-channel peristaltic pumps operating at the same rate at the inlet and at the outlet side, as shown in Fig. 1. The pumps were connected to the tank through tygon and stainless steel tubing with an inner diameter of 1.0 mm. A granular medium, which consists of silica glass beads of uniform grain diameters of 0.25–0.30 mm, was filled into the tank using a funnel and during the filling the water level was always kept above the grains to achieve a uniform packing and to avoid the entrapment of air bubbles. The same procedure was used to create the heterogeneous set-up, which additionally included a 20 cm long and 1 cm high lens of higher permeability (grain size 1.0–1.5 mm) placed at 20 cm from the left border of the tank.

Uranine or bromide, together with oxygen depleted water were injected as tracers through the central port 5 (from the bottom, see Fig. 1), forming a plume in the tank. Measurements include oxygen concentrations, measured non-invasively at seven oxygen sensitive strips (PreSens, Germany) during the homogeneous experiments, while the heterogeneous set-up includes two additional strips (B1 and B2 in Fig. 1). Also the concentrations of the three tracers are measured by sampling at the outlet ports. In total six experiments were performed. Four were conducted in a homogeneous set-up at two different advective velocities, while two were performed in the heterogeneous set-up at only one advective velocity.

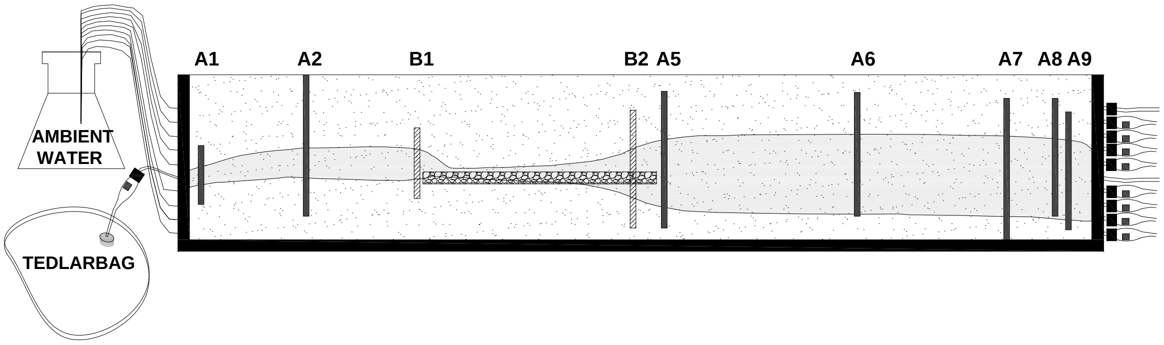

Fig. 1 Experimental set-up showing the steady-state plume in the heterogeneous experiments. On the left side the injection ports are connected to oxygen saturated water. The tedlarbag containing the tracer solution is connected to Port 5 through a vial that includes 1 cm^2 oxygen sensitive strip used to measure the concentration of the oxygen depleted solution. Nine oxygen sensitive strips positioned along the tank are used to delineate the oxygen depleted plume, but strips B1 and B2 are used only for the heterogeneous experiments. On the right side, the outlet ports (except Port 5) are equipped with similar vials as the one on the left side, in order to measure the oxygen distribution.

SENSITIVITY ANALYSIS

The revised experimental set-up used for the six new tracer tank experiments was developed on the basis of the main outcomes of synthetic tank experiments and a successive sensitivity analysis. These synthetic tank experiments, performed by high resolution numerical simulation, allow for a full sensitivity analysis of the variations in experimental observations on parameter uncertainty, and allowed the development of a consistent method for the determination of dispersivities from the experiments (Ballarini *et al.*, 2010).

The results of the sensitivity analysis performed for the heterogeneous experiments (for the matrix and the lens the values of the hydraulic parameters were changed separately) were compared to those for the homogeneous case (Ballarini *et al.*, 2010) and are exemplarily shown in Fig. 2 (breakthrough curves) and Fig. 3 (depth profiles at outlet ports). In contrast to the homogeneous case, where transverse dispersivity α_T strongly influences all the measurements (Figs 2(a) and 3(a)) its effect on the tracer concentration in the heterogeneous case is mostly evident in the measurements taken at the outlet ports and only when variations of orders of magnitude are considered (Figs 2(b),(c), 3(b),(c)). While in the homogeneous case the effect of hydraulic conductivity K on the plume can only be inferred from the plume position at the oxygen sensitive strips, in the heterogeneous set-up K (for the matrix (K_1), as well as for the lens (K_2)) appears to be the main parameter influencing the tracer distribution at the outlet ports (Fig. 3(e),(f)) and the slope and maximum concentration of the breakthrough curve BTC (Fig. 2(e),(f). More important than the K values themselves is the ratio of the matrix K_1 and the permeable inclusion K_2. While the model simulations for the heterogeneous case show that it is only possible

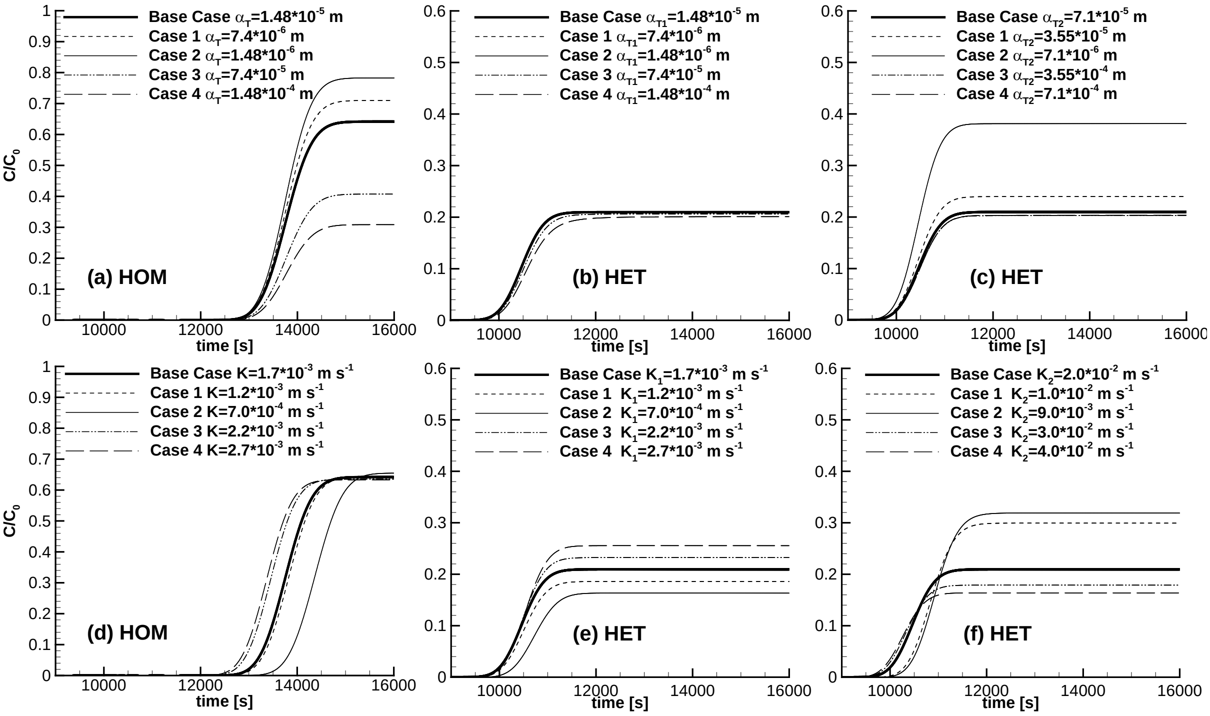

Fig. 2 Simulated breakthrough curve of the conservative tracer (uranine) measured at the outlet port 5. (a) and (d) represent the homogeneous case, where first αT and then K were varied. (b) and (c) show the effects of changes of αT of the matrix and of the lens, and (e) and (f) the influence of different K for the matrix and the lens in the heterogeneous experiments.

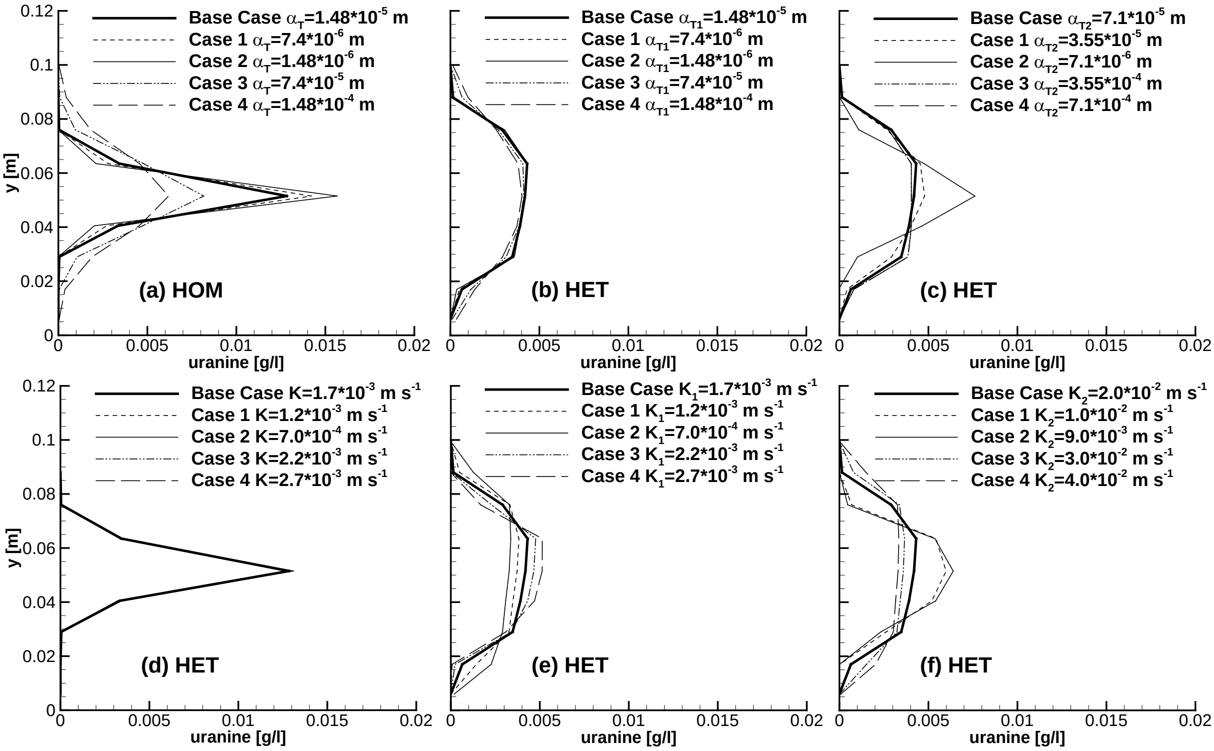

Fig. 3 Influence of α_T and K on the tracer depth profiles at the outlet ports. (a) and (d) represent the homogeneous case, where α_T and simulated K were varied. (b) and (c) show the effects of changes of α_T of the matrix and of the lens, and (e) and (f) the influence of different K for the matrix and the lens in the heterogeneous experiments.

to determine the order of magnitude of α_T from the measurements, the ratio K_2/K_1 can be evaluated with good accuracy as even small variations significantly affect the tracer distribution at all measurement locations. Therefore, if the value of K_1 for the matrix is known from previous homogeneous experiments, it is possible to obtain K_2 of the more permeable inclusion.

Results also show that variations in the aqueous diffusion coefficient D_{aq} of the tracer influence the maximum concentration of the breakthrough curve (BTC), at the strips and at the outlet ports in the homogeneous and heterogeneous set-up (not shown). The porosity n was changed separately for the two materials in the heterogeneous case. This parameter influences the arrival time of the tracer in the BTC (not shown). As pointed out in Ham *et al.* (2004), longitudinal dispersivity α_L does not influence the plume shape at steady-state, therefore it only affects the slope of the BTC (not shown).

RESULTS

Experiments with revised tank set-up

A set of six new tracer experiments was performed at the University of Tübingen in order to test the revised experimental set-up developed on the basis of the main outcomes of the synthetic experiments and sensitivity analysis. Four were carried out in a homogeneous porous medium and tracer distributions were compared at two different advective velocities v_a of 4.9 and 10.5 m d^{-1}. The other two experiments were run with a heterogeneous porous medium at v_a of 5.0 m d^{-1}. The heterogeneous set-up consists of a fine matrix with the same grain size as the homogeneous experiments, but it also includes a more permeable inclusion of coarser grains (1.0–1.5 mm).

Nine oxygen sensitive strips (A1, A2, B1, B2, A5–A9 in Fig. 1) were used in the new set-up. The strips are positioned at 0.01, 0.10, 0.195, 0.38, 0.41, 0.57, 0.70, 0.74 and 0.75 m from the tank inlet (Fig. 1), respectively. Strip B1 is placed directly in front of the permeable lens where the plume converges towards the permeable medium and B2 a few cm in front of the end of the lens where the plume starts to diverge. Measurements of oxygen profiles along these strips can be used to estimate the ratio K_2/K_1, as the degree of plume focusing and spreading is controlled by the conductivity contrast.

The experimental set-up also includes oxygen measurements at the outlet ports in order to verify that these are consistent with the measurement data at the oxygen sensitive strip A9. Moreover, these measurements can be used to compare the oxygen distribution at the outlet ports to those of the other two tracers.

Numerical evaluation of the new tank experiments

The experiments were evaluated by trial-and-error calibration of a numerical model to the measurements, i.e. tracer breakthrough curves and concentration profiles across the outlet ports as

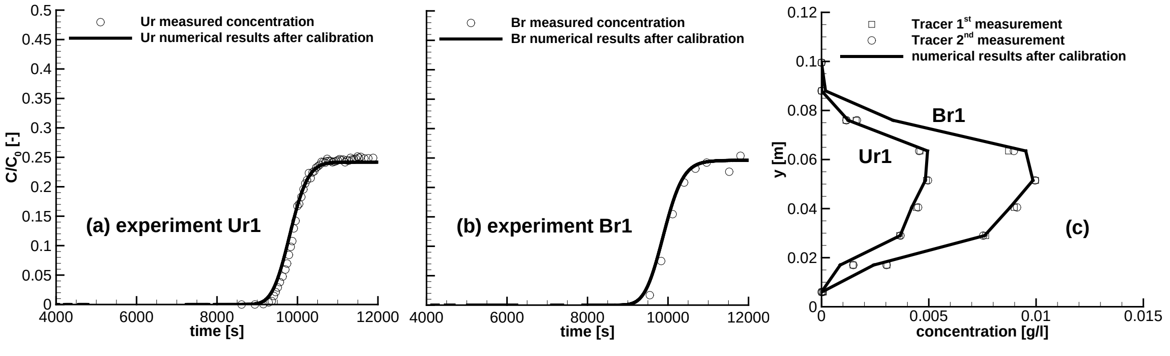

Fig. 4 Measured and simulated tracer concentrations at the BTC in the two heterogeneous experiments (Ur1 and Br1).

well as along the oxygen sensitive strips. A consistent parameter set, which produces an excellent fit of the numerical model output to the experimental observations, was found for all six experiments.

Based on the main outcomes of the sensitivity analysis, only the parameters found to influence the distribution and concentration of the tracers are included in the calibration procedure. For the heterogeneous experiments, only the ratio between the hydraulic conductivities can be determined from the measurements and either the hydraulic conductivity of the matrix or of the lens must be known in order to obtain a reliable fit. In this study, the hydraulic conductivity of the porous medium was first determined by numerical evaluation of the homogeneous experiments and then considered as a known parameter in the fitting procedure of the heterogeneous experiments, while K_2 is used as calibration value. All the homogeneous experiments could be reproduced very well by numerical modeling with a unique calibrated parameter set, including only a single value for transverse dispersivity α_T of 1.48×10^{-5} m.

The two heterogeneous experiments were performed using uranine and oxygen depleted water (experiment Ur1) and then substituting uranine with bromide in the second experiment (Br1). The hydrodynamic parameters determined for the homogeneous tank were fixed during the numerical evaluation of the heterogeneous experiments, while α_{L2}, α_{T2}, n_2 and K_2 of the high permeability inclusion were considered as calibration parameters. The hydraulic conductivity of the lens K_2 could be determined from fitting of oxygen profiles downgradient of the lens as well as oxygen, bromide or uranine measurements at the outlet ports. In fact, the amount of plume spreading due to transverse mixing within the high permeability lens is highly sensitive to the ratio K_2/K_1, but insensitive with respect to the transverse dispersivity of the lens material α_{T2}. Accordingly, the latter parameter could not be determined with certainty (cf. Sensitivity Analysis). Figure 4(a) and (b) present a comparison of measured BTCs and simulated data of both heterogeneous experiments, while (c) shows the distribution of uranine and bromide at the outlet ports. The simulated uranine and bromide BTCs and profiles match the measurements very well. A very good match was also obtained for the oxygen concentrations measured at the outlet ports (not shown). Note that the different maximum concentrations of uranine and bromide in Fig. 4(c) are due to distinct initial input concentrations.

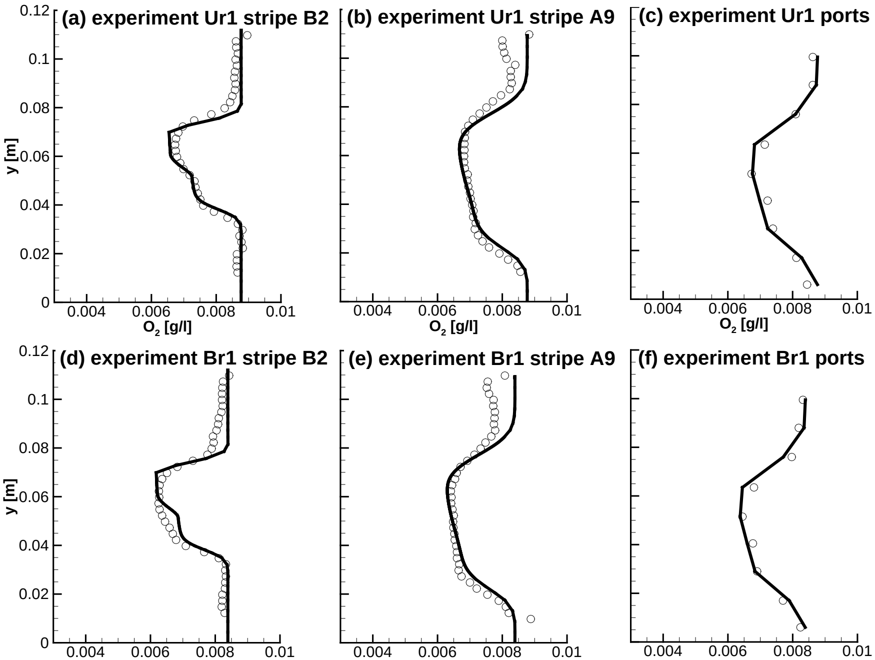

Fig. 5 Measured concentrations of oxygen at three sensitive strips represented by circles (A2 before entering the lens, B2 in the lens and A9 close to the extraction ports) plotted *versus* the numerical results (black line).

In Fig. 5 oxygen measurements at two sensitive strips (B2 and A9) and at the outlet ports for experiments Ur1 and Br2 are exemplarily reported. Fig. 5(a) and (d) show profiles of the oxygen depleted plume across the permeable lens, while Fig. 5(b) and (e) (strip A9) display the oxygen depleted plume influenced by pumping a few centimetres from the outlet ports. Finally, Fig. 5(c) and (f) show oxygen depth profiles at the outlet ports. It should be noted that the oxygen concentration at Port 5 could not be measured due to the need to constantly collect samples for the BTC of uranine or bromide, therefore its value was determined from mass balance calculation. In the homogeneous as well as in the heterogeneous experiments, the oxygen sensitive strips A1 and A2 (located within the first 10 cm of the tank), did not yield reliable measurements of oxygen profiles. The measurements appear to be not mass balanced, as the plume is not depleted enough in comparison to the more downgradient oxygen measurements. Despite that, the measurements at strips A1 and A2 still could be used for the determination of the vertical oxygen plume position, which was important for the calibration of individual injection port pumping rates.

For all six experiments, simulated breakthrough curves, concentration profiles of all three tracers at the outlet ports, as well as oxygen profiles at strips A5–A9 and B2 show a very good agreement with the measured data.

DISCUSSIONS AND CONCLUSIONS

In this paper numerical transport modelling was used to improve the experimental set-up and subsequently the evaluation of well controlled bench-scale tracer experiments in quasi-2D flow through tanks for the quantification of transverse dispersion in homogeneous and heterogeneous porous media. A sensitivity analysis was performed to evaluate which parameters can be derived uniquely and accurately from the used experimental set-up. An improved tank experimental set-up was derived and implemented in a new set of six tank experiments: four of them were performed at two different v_a in a homogeneous porous medium, while two were carried out in a heterogeneous porous medium, where a high permeable lens was imbedded in a fine grained matrix. The experiments were evaluated by calibration of a numerical model to the data measured during the experiment. Experiments conducted in the improved set-up yielded reliable and reproducible estimates of the hydraulic parameters. The hydraulic parameters derived by calibrating the model to the measurements available for the homogeneous experiments (porous medium with a grain size of 0.2–0.3 mm) are 3.49×10^{-4} m for the longitudinal and 1.48×10^{-5} m for the transverse dispersivities. As in the heterogeneous experiments a matrix with the same grain size (0.2–0.3 mm) was employed, the previously fitted values were used, while the fitted longitudinal and transverse dispersivities for the permeable inclusion (1.0–1.5 mm) are 7.6×10^{-4} m and 7.1×10^{-5} m, respectively. A unique value of α_T could be identified from the three tracers used. This paper thus shows that experimental set-ups should be evaluated prior to their implementation by conducting synthetic experiments by numerical simulation as this allows for an optimization of the experimental set-up and more reliable parameter estimates.

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