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# Modeling Mass Transfer in Small Scale Reactors using Computational Fluid Dynamics

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## BACKGROUND

Sufficient mass transfer in chemical reactor systems is very important in order to achieve good and effective processes. In heterogeneously catalyzed reactor systems it is for example important to contact the reacting species with the reactive sites, and in aerobic fermentation systems it is important to avoid badly mixed zones and to provide sufficient oxygen in order to avoid growth limitations of the microorganisms.

Computational fluid dynamics (CFD) is a valuable tool for studying mixing and flow phenomena in chemical reactors. Mixing times can be simulated by modeling the spatial distribution of an additional variable (A.V.) over time and furthermore can chemical reactions involving the A.V. be implemented with help of kinetic reaction models. The oxygen transfer coefficient ' $k_L a$ ' can be simulated as the product of the simulated specific interfacial area ' $a$ ' and mass transfer coefficient ' $k_L$ '. The mass transfer coefficient ' $k_L$ ' is often modeled as a function of the diffusion coefficient of oxygen in water ( $D_L$ ), the viscosity ( $\nu$ ), the energy dissipation rate ( $\epsilon$ ) and a proportionality constant  $C_p$  according to the eddy cell model [1] shown in the following equation:

$$k_L = C_p \left( \frac{D_L}{\nu} \right)^{0.5} (\epsilon \nu)^{0.25}$$

## METHOD

The CFD software Ansys CFX 15.0 was used for all simulations. Experimental  $k_L a$  and mixing times values [2] for the 1 ml impeller driven microbioreactor shown in Figure 1 were simulated using a free-surface two-phase model (water and air) and the k- $\epsilon$  turbulence model.

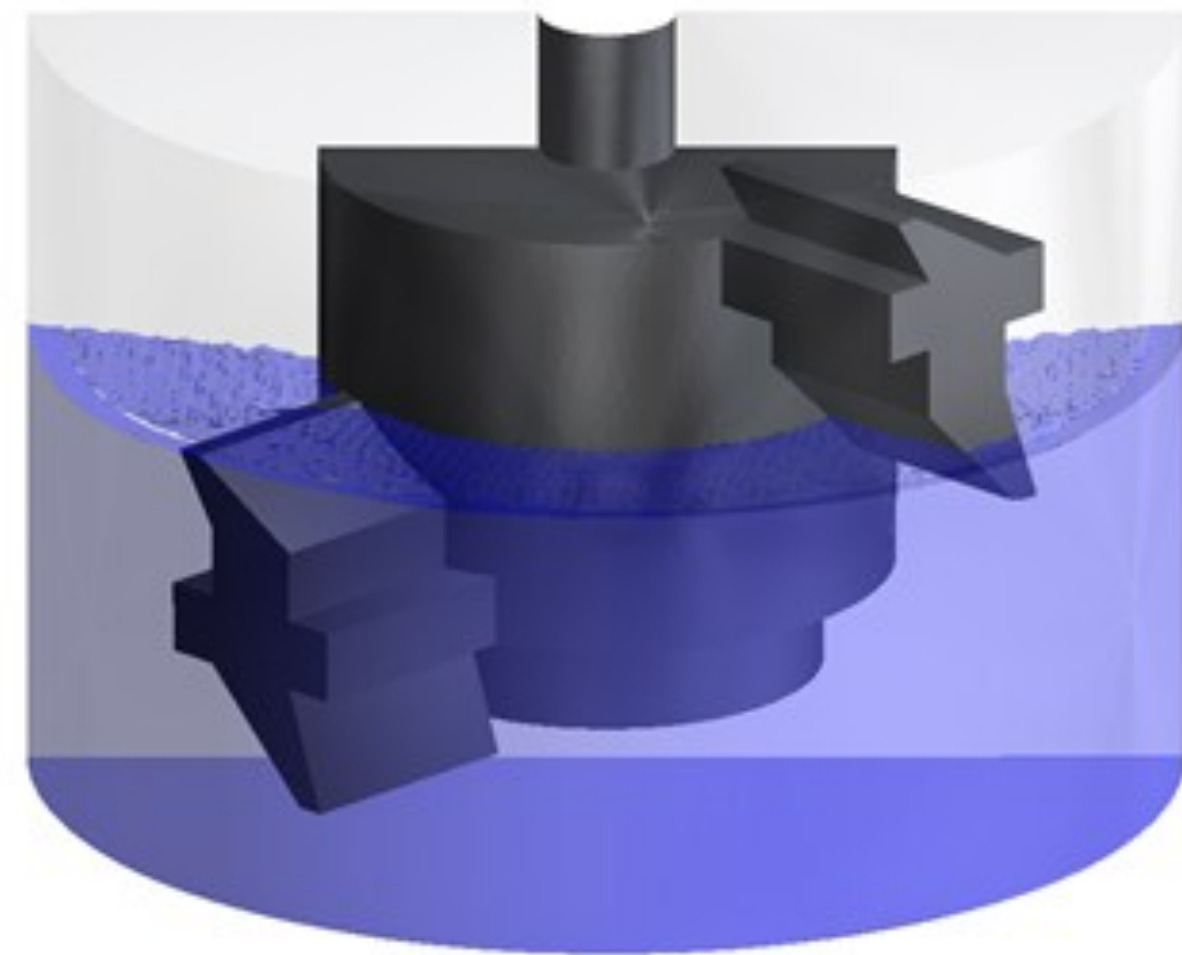


Figure 1. The two-phase system (water and air) and the geometry of half of the microbioreactor.

The SpinChem<sup>®</sup> is a rotating flow reactor that can be filled with porous solid material, e.g. catalysts or ion-exchange resins. The fluid dynamic conditions created by a SpinChem placed in a 160 ml baffled reactor were simulated using a one-phase model (water), the k- $\epsilon$  turbulence model and a pressure loss model for the porous material.

Figure 2. The modeled SpinChem placed in a baffled reactor. The green material inside of the SpinChem is the catalytic porous material.

## RESULTS AND DISCUSSION

### MASS TRANSFER IN THE SPINCHEM

The total simulated flow through the SpinChem for different rotational speeds can be seen in Figure 3, and it is clear that the rotational speed has a significant impact on the mass transfer through the porous material. Another important parameter affecting the flow is the pressure loss coefficient in the porous material (data now shown).

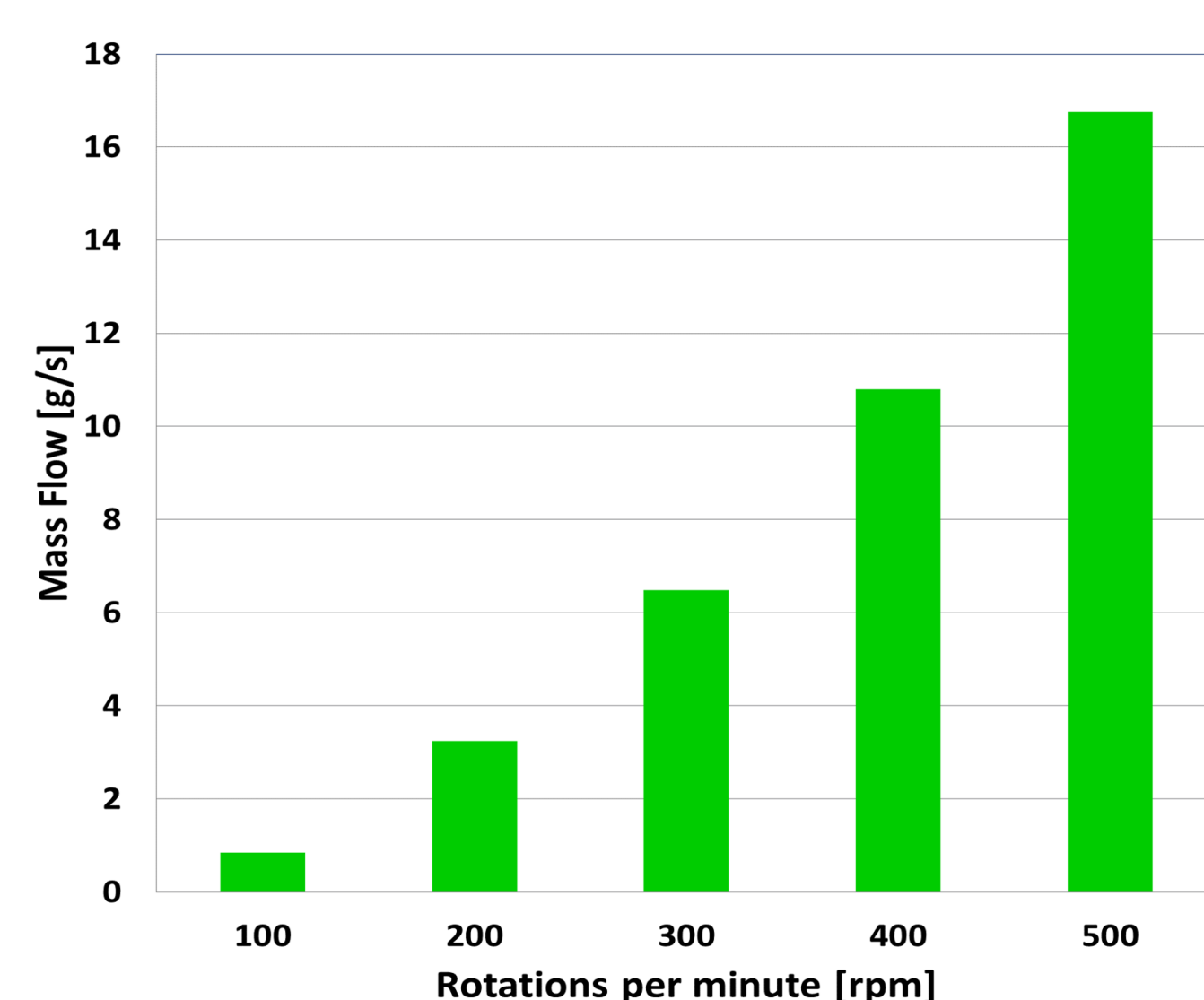


Figure 3. The flow through the porous material in the SpinChem for different rotational speeds.

### CATALYSIS IN THE SPINCHEM

The liquid was initialized with unity concentration of an A.V. that was allowed to spread in the liquid by the induced flow fields and (mainly turbulent) diffusion. Furthermore was a zero-order reaction consuming the A.V. implemented in the porous material. The velocity vectors for the 500 rpm simulation as well as the distribution of A.V. after 3.7 s on two cut-planes can be seen in Figure 4.

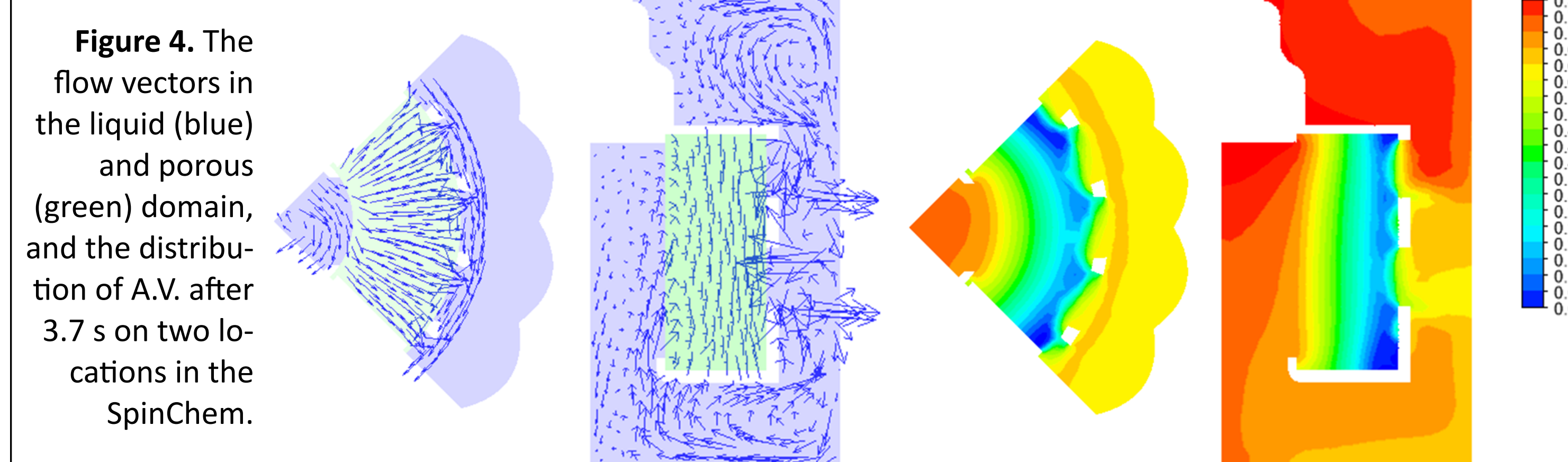


Figure 4. The flow vectors in the liquid (blue) and porous (green) domain, and the distribution of A.V. after 3.7 s on two locations in the SpinChem.

## RESULTS AND DISCUSSION

### MIXING IN THE MICROBIOREACTOR

Mixing time simulations were performed in the microbioreactor by the introduction of an A.V. from a source point during transient simulations. The maximal value of the A.V. in the reactor as well as its value in a virtual measuring point (M.P.) was monitored over time, and mixing time was defined as the time when the fluid entered within the  $\pm 5, 10$  or 15% interval of its final value.

The simulated and experimental mixing times are shown in Figure 5, where it can be seen that the 1000 rpm simulation deviates from the general trend with shorter mixing times for higher rotational speeds. This behaviour is caused by a poorly mixed zone in the 1000 rpm liquid, which is suggested in Figure 6 and shown in Figure 7.

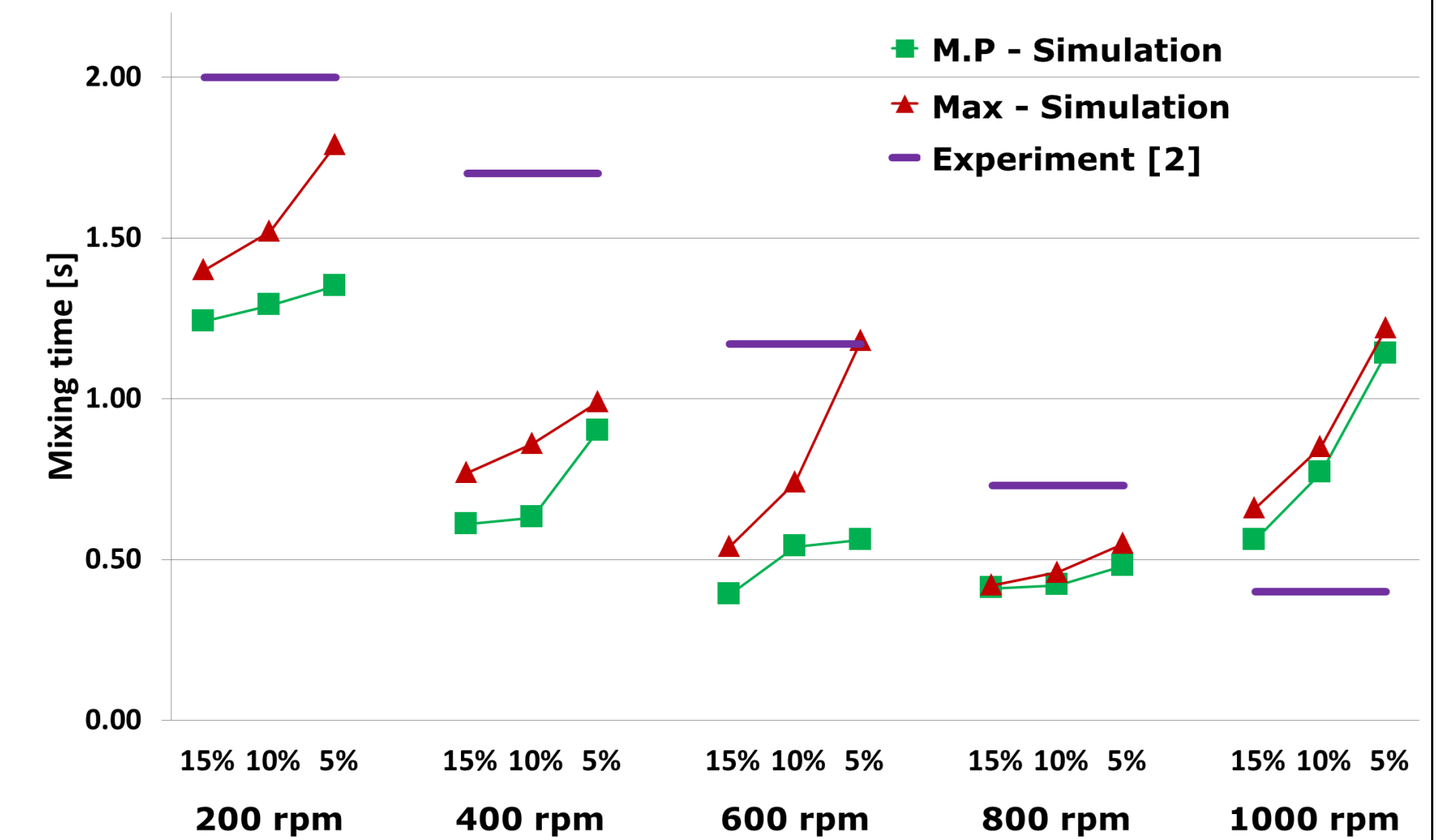
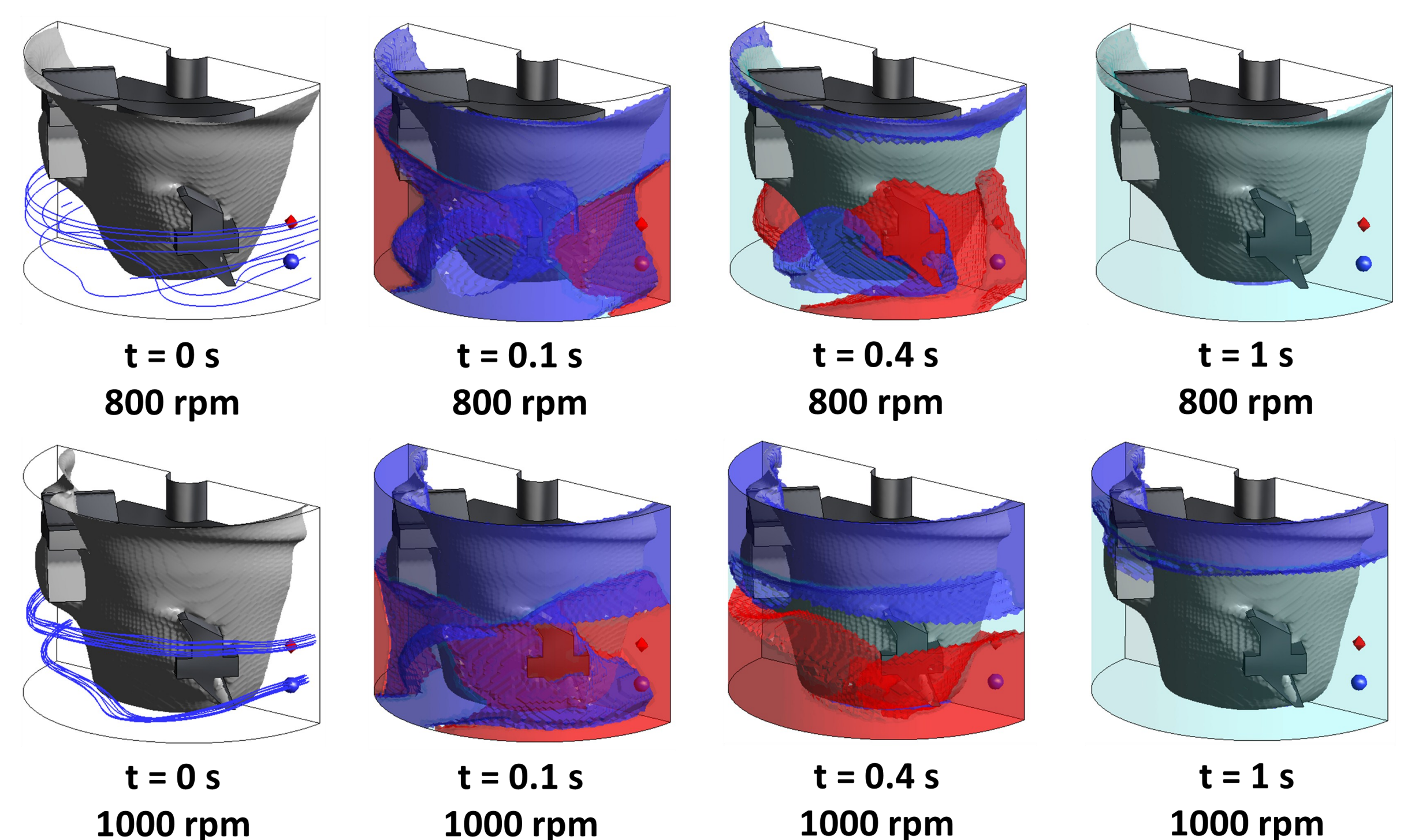
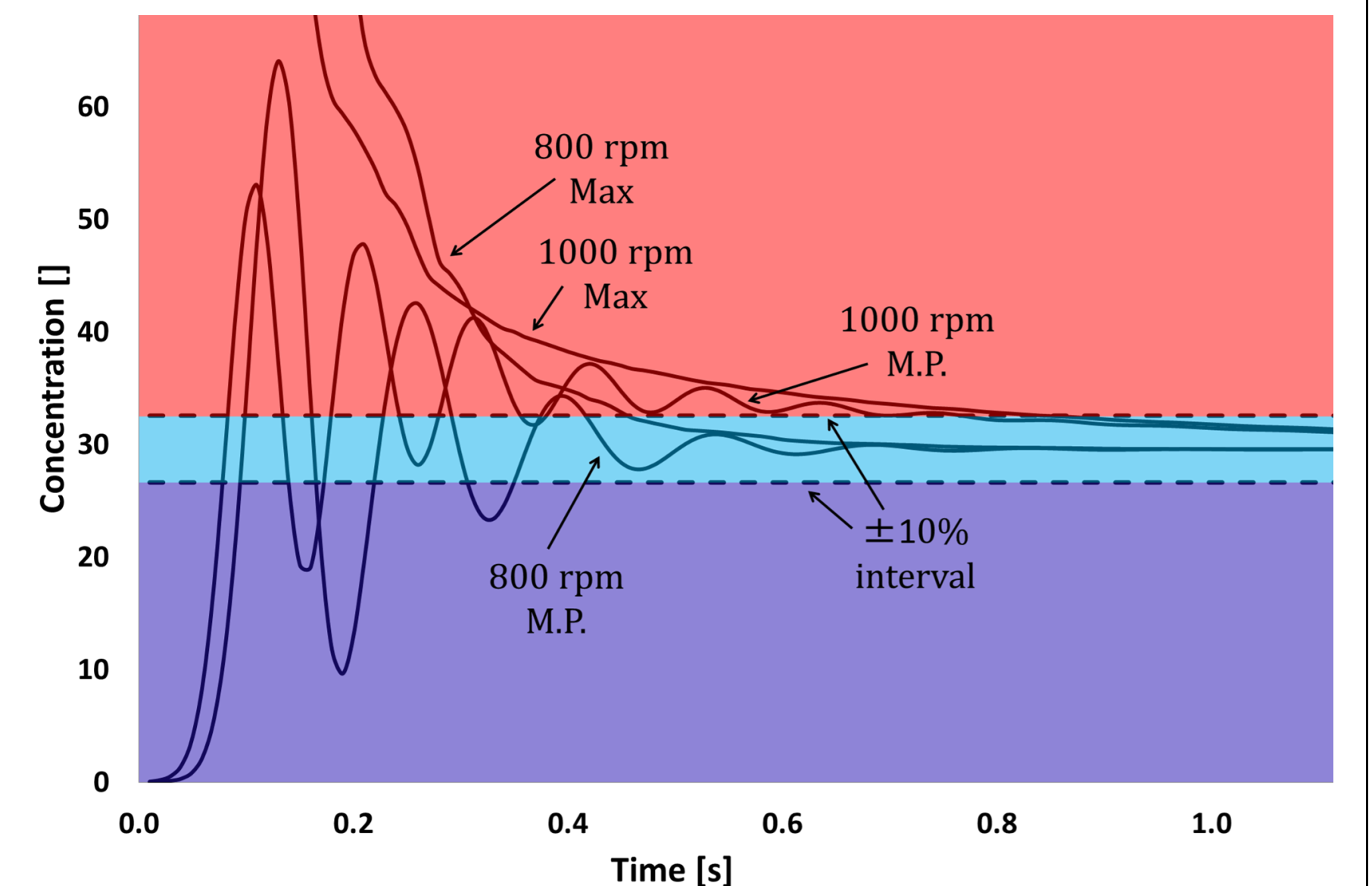


Figure 5. Simulated and experimental mixing times for the microbioreactor.

Figure 6. The maximal values of the A.V. in the microbioreactor and its values at the M.P. plotted over time. The  $\pm 10\%$  interval, defining the 10% mixing time, is the turquoise shaded area.

Figure 7. Visualization of the mixing simulations following the coloring in Figure 6, i.e. the A.V. concentrations within the  $\pm 10\%$  interval are shown as turquoise etc. The streamlines start from the source point (red octahedron) and the M.P. (blue sphere).

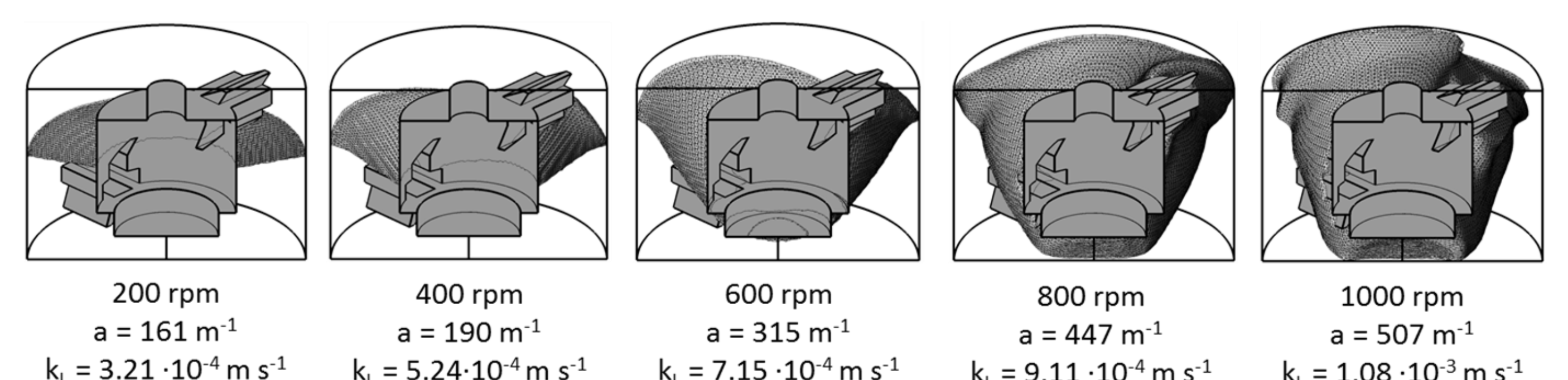
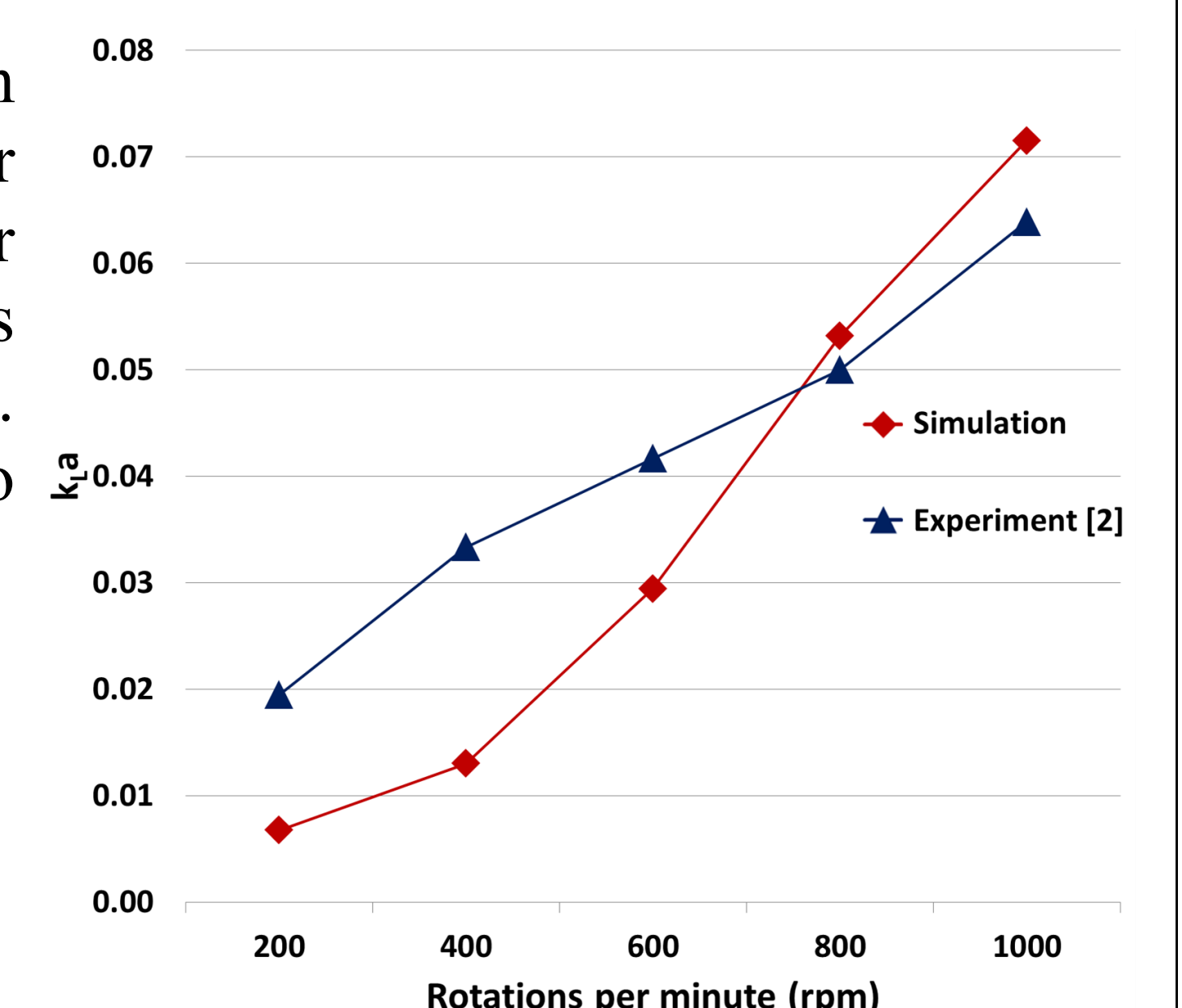


### OXYGEN TRANSFER IN THE MICROBIOREACTOR

The appearance of the gas-liquid interfaces in the microbioreactor for different rotations per minute (rpm) can be seen in Figure 8 together with the simulated specific interfacial areas and the simulated mass transfer coefficients. The simulated ' $k_L a$ ' values are compared to experimental data in Figure 9.

Figure 8. The gas-liquid interfaces and  $k_L$ -values (for  $C_p=1$ ) for the different stirring speeds.

Figure 9. The simulated  $k_L a$  values (for  $C_p=0.13$ ) compared to experimental values.



SpinChem<sup>®</sup> is a registered trademark owned by Nordic ChemQuest AB

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[2] Bolić, A., Krühne, U., Prior, R. A., Vilby, T., Hugelier, S., Lantz, A. E., Gernaey, K. V., 2012. One-Millilitre Microbioreactor with Impeller for Improved Mixing, Poster session presented at 12<sup>th</sup> International Conference on Microreaction Technology (IMRET12), Lyon, France.