

# Aggregation Kinetics of Colloidal Nanoparticles in a Circulating Microfluidic Cavity

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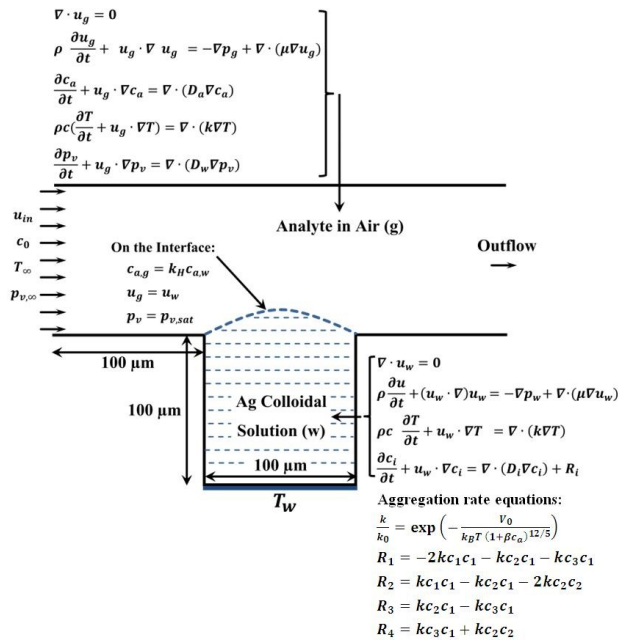
## Abstract

COMSOL Multiphysics V4.3 is used to simulate the kinetics of colloidal nanoparticles in a circulating microfluidic cavity. Pressure-driven air flow is directed over the microfluidic cavity, which induces circulating fluid motion in the cavity, as shown in Figure 1. Analyte contained in the air stream is absorbed into the cavity, mixes as a result of the circulating cavity flow, and interacts with the nanoparticles. As a result, the nanoparticles sequentially aggregate into clusters of higher orders. This process is highly non-linear and described by the system of equations shown in Figure 1. Our numerical model captures the following physical phenomena: fluid dynamics of the air flow, fluid dynamics of the microfluidic cavity, and second order aggregation kinetics. In addition, at the interface we account for momentum transport, heat transfer, mass transport through evaporation-driven phase change, and mass transport through analyte adsorption. To control the evaporation rate from the interface, the temperature of the cavity and relative humidity of the air are specified. Heat transfer equation and diffusion-convection of water vapor into air are added to the model to calculate the evaporation rate. The final result for concentration of the aggregates in ambient condition  $T_{\infty} = 20^{\circ}\text{C}$  and  $\text{RH} = 90\%$ , inlet velocity  $u_{\text{in}} = 1 \text{ mm/s}$ , analyte concentration  $c_a = 1 \text{ mM}$  is shown in Figure 2 and 3. We will consider the effect of analyte concentration, ambient conditions and air velocity to find the optimum condition to get the highest number of the dimers in the cavity. For these conditions, dimer concentration (green curve, Fig. 3) peaks at around  $t \sim 100\text{s}$ . At larger times, the number of dimers decreases as higher order aggregates form, and the available monomers decreases.

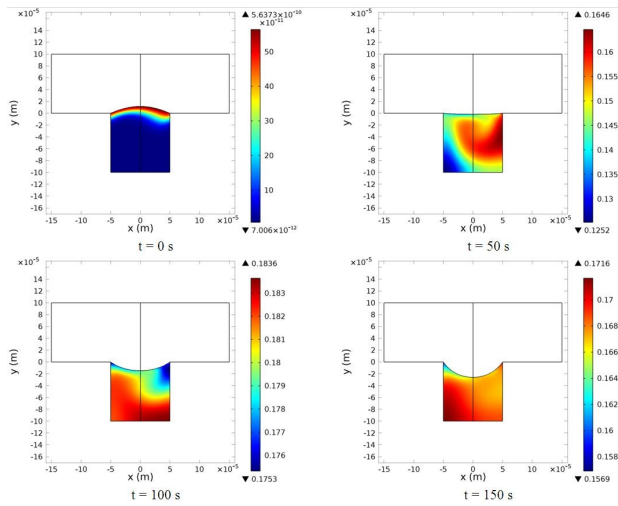
## Reference

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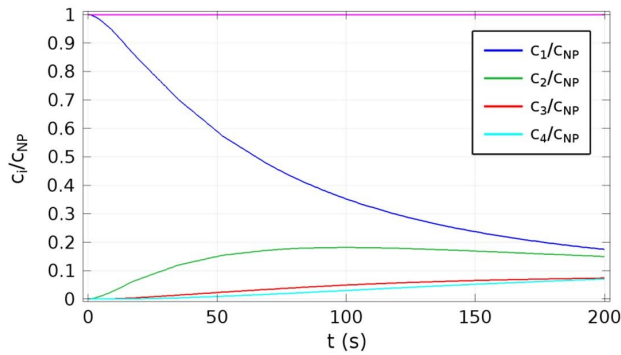
## Figures used in the abstract



**Figure 1:** Computational Domain and governing equations. Air flow containing airborne analyte flows over the Ag colloidal solution in the cavity. The absorbed analyte stimulates the aggregation process between silver nanoparticles. The position of the interface is controlled by evaporation rate based on temperature, relative humidity and air velocity.



**Figure 2:** Formation of dimers in the cavity and movement of the interface due to evaporation in the ambient condition  $T_\infty = 20\text{oC}$  and  $\text{RH} = 90\%$ , inlet velocity  $u_{in} = 1 \text{ mm/s}$  and analyte concentration  $c_a = 1 \text{ mM}$ .



**Figure 3:** Average concentration of formed aggregates in the cavity in time in the ambient condition  $T_\infty = 20\text{oC}$  and  $\text{RH} = 90\%$ , inlet velocity  $u_{in} = 1 \text{ mm/s}$  and analyte concentration  $c_a = 1 \text{ mM}$ . There is an optimum point that the dimer concentration is maxima which depends on analyte concentration, ambient conditions and air velocity.