Aggregation Kinetics of Colloidal Nanoparticles in a Circulating Microfluidic Cavity

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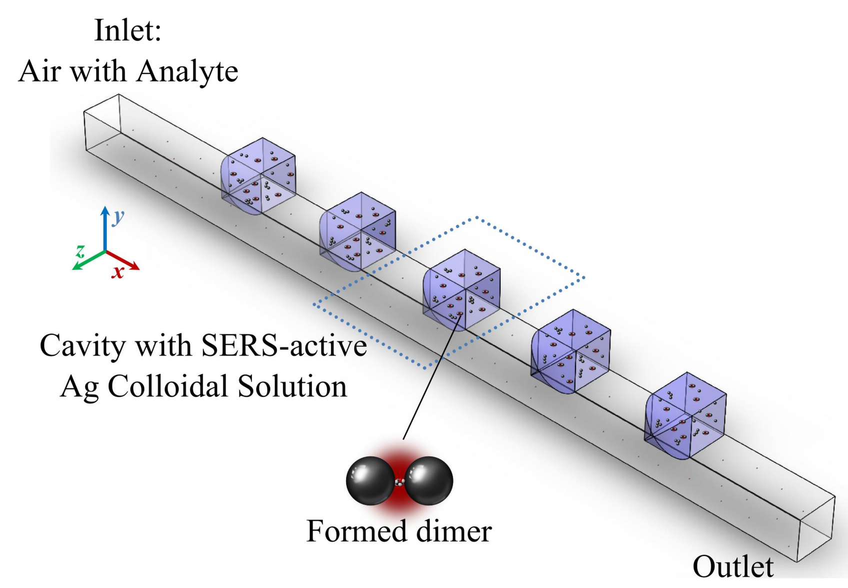
Introduction: Analyte contained in the air stream is absorbed into the cavity, mixes with the nanoparticles as a result of the circulating cavity flow. Therefore, the nanoparticles sequentially aggregate into clusters of higher orders which enables analyte detection using Raman spectroscopy.



Physical phenomena:

- Fluid dynamics of the air flow
- Fluid dynamics of the microfluidic cavity
- Evaporation from air/liquid interface
- Absorption of the analyte from the interface
- Second order aggregation kinetics of nanoparticles

Goal:

- Optimum condition to get the highest number of the dimers in the cavity for efficient chemical detection

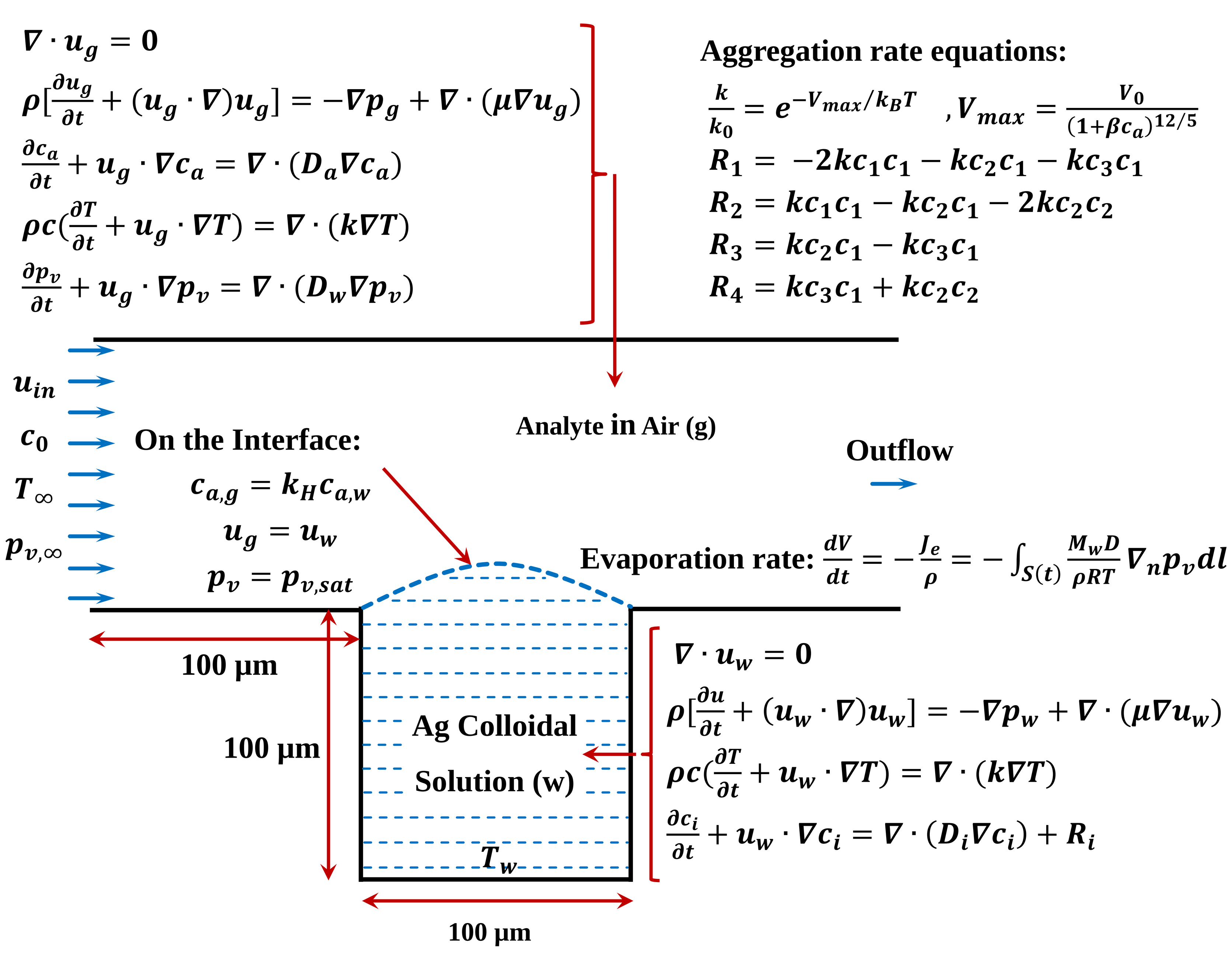


Figure 1. Computational Domain and governing equations

Table 1. Multiphysics model

Physics	D	Variables	Domain
Weak form PDE: Initial curvature of the interface	1D	F	Interface
Deformed Geometry: Moving interface	2D	X, Y	Entire
Laminar Flow 1: Air flow in the microchannel	2D	u_g, v_g, p_g	Air
Laminar Flow 2: Liquid flow in the cavity	2D	u_w, v_w, p_w	Liquid
Heat Transfer: Temperature in the domain	2D	T	Entire
Transport of Diluted Species: Vapor pressure of water	2D	p_v	Air
Weak form PDE: Concentration of analyte at the interface	1D	c_{BC}	Interface
Transport of Diluted Species: Analyte concentration in air	2D	c_a	Air
Transport of Diluted Species: Aggregation kinetics	2D	c_a, c_1, c_2, c_3, c_4	Liquid

Results: The dimer concentration is maximize to have an optimum analyte detection. The optimum point happens at:

$$\max\left(\frac{c_2}{c_{NP}}\right) \ at\ kc_{NP}t \approx 0.7$$

Conditions for numerical simulations:

- Ambient condition: $T_\infty = 20^oC$, $T_w = 10^oC$, $RH = 50\%$
- Inlet velocity: $u_{in} = 10\ mm/s$,
- Analyte concentration: $c_a = 1\ mM$
- Initial concentration of nanoparticles: $c_{NP} = 100\ pM$
- Aggregation kinetics: $k_0 = 10^8\ [M^{-1}s^{-1}]$, $V_0 = 3k_BT$ and $\beta = 10^4\ [M^{-1}]$

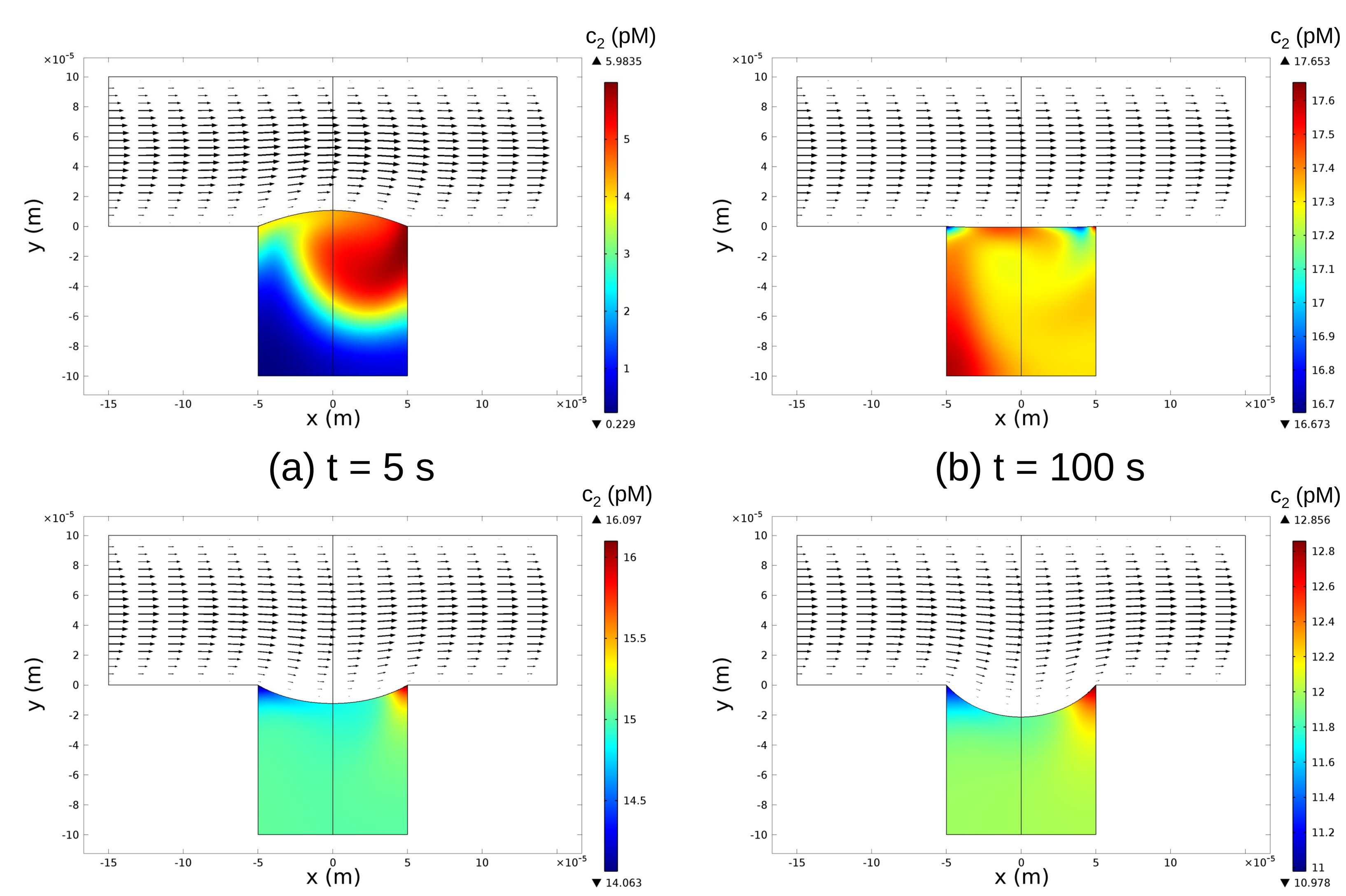


Figure 2. Formation of dimers in the cavity for c_{NP} = 100 pM

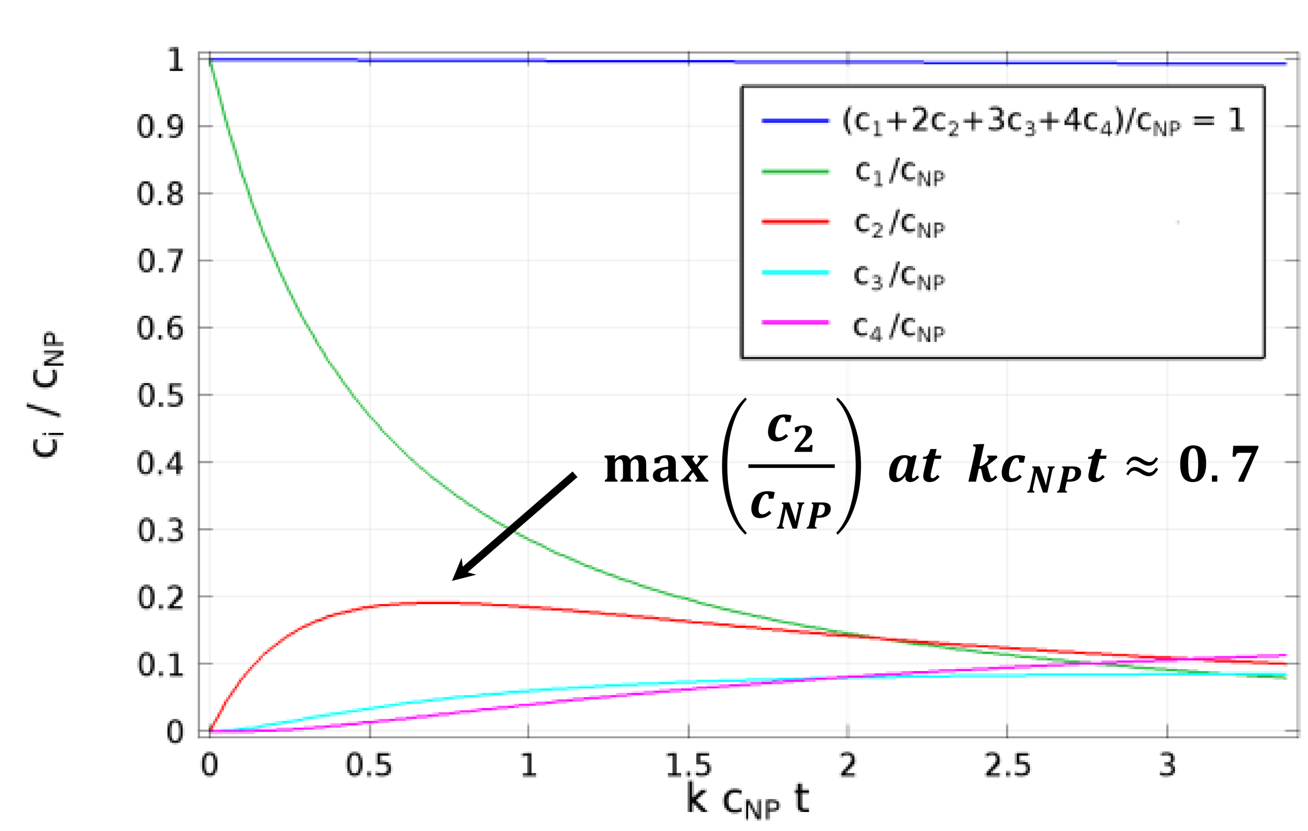


Figure 3. Formation of dimers in the cavity and air velocity vectors

Conclusions: We investigate the flow field, mass transport and aggregation kinetics to find the number of formed dimers according to the concentration of the analyte. There is an optimum point at $kc_{NP}t \approx 0.7$ where the number of formed dimers is maxima for optimal chemical detection.

References:

1. Piorek, B., Lee, S., Santiago, J., Moskovits, M., Banerjee, S., Meinhart, M., Free-surface microfluidic control of surface-enhanced Raman spectroscopy for the optimized detection of airborne molecules, *Proceedings of the National Academy of Sciences*, **104**, 18898 (2007).
2. Moskovits, M.; Vlcková, B., Adsorbate-induced silver nanoparticle aggregation kinetics, *The Journal of Physical Chemistry B*, **109**, 14755–14758 (2005).
3. Hu, H., Larson, R., Evaporation of a sessile droplet on a substrate, *The Journal of Physical Chemistry B*, **106**, 1334–1344 (2002).
4. Girard, F., Antoni, M., Sefiane, K., On the effect of Marangoni flow on evaporation rates of heated water drops, *Langmuir*, **24**, 9207–9210 (2008).

Excerpt from the Proceedings of the 2012 COMSOL Conference in Boston