Solutocapillary for Self-Control Precipitation in Enclosed Geometries by Using Microcavities

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In this work the possibility to endow enclosed geometries with a passive feedback mechanism to prevent precipitation when their walls are deliberately lined with air-filled hydrophobic microcavities is discussed.

Keywords. *Capillary convection; Marangoni stress; Sedimentation*

I. INTRODUCTION

The object of this work was a first assessment for the deliberated use of walls lined with hydrophobic air-filled microcavities in enclosed geometries to prevent the gravitational settling of particles at the bottom of small containers which ultimately would result in irreversible agglomerations. The use of hydrophobic microcavities in channels may be traced back to the early work of Baier at al (2010), [1], and experimental results in practical application for microfluidic pumping was recently reported (2018), [2]. The core idea behind the use of such microcavities lies in the introduction of fluid-air interfaces which by applying a thermal gradient across a Marangoni thermocapillary stress results due to the thermal dependence of the surface tension with temperature. However, because the surface tension is also dependent of the concentration of species (solutocapillary), the use of hydrophobic microcavities open the possibility to prevent or at least to mitigate sedimentation in enclosed

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geometries. Indeed, the Marangoni stress will be passively activated by the vertical gradient of concentration resulting from the progressive gravitational settling of particles of solute at the bottom of the vessel.

II. MATERIALS AND METHODS

It must be considered that the gravitational settling of particles during the sedimentation process occurs when the gravitational field is comparatively larger that the thermal energy. Gravity constantly pulls an individual particle downward in the container while thermal agitation tends to keep the particle dispersed thorough the container. The importance of gravity in comparison with thermal motion can be assessed by comparison of the ratio between gravitational energy, E_g, and the thermal energy E_t

$$\frac{E_g}{E_t} = \frac{(\rho_p - \rho)V_p g L}{\kappa_B T} \tag{1}$$

where g is gravity, $\kappa_B$is the Boltzmann‘s constant, T is the absolute temperature, V_p is the volume of the particle, ρ_p and ρ the density of the particle and the fluid, respectively., and L is the elevation in the gravitational field (the characteristic length of the container). For spherical particles $V_p = \frac{\pi d_p^3}{6}$ being d_p the diameter of the particle and thus Eq.(1) becomes

$$\frac{E_g}{E_t} = \frac{(\rho_p - \rho_f)\pi g d_p^3 L}{6\kappa_B T} \tag{2}$$

Thus for containers with lengths around 0.05 m, particles with diameters around a few micrometer their gravitational energy could be comparative with thermal energy. As regard of the momentum generated by the capillary, the maximum capillary velocity at the interface may be approximately assessed with the expression, [3] by,

$$v_{max} \approx \frac{h}{\mu}\frac{d\sigma}{dz} \tag{3}$$

where h is the width of the container; μ is the dynamic viscosity of the fluid; σ the surface tension; and z the vertical coordinate (parallel to the air-fluid interface). If the surface tension gradient comes from a concentration gradient, then Eq.(3) becomes

$$v_{max} \approx \frac{h\sigma_c}{\mu}\frac{dc}{dz} \tag{4}$$

where σ_c is the surface tension of concentration coefficient and $\frac{dc}{dz}$ the concentration gradient across the interface. On the other hand, the terminal velocity of gravitational settling is given by

$$v_t = \sqrt{\frac{4gd}{3c_d}\left(\frac{\rho_p - \rho}{\rho}\right)} \tag{5}$$

where c_d is the drag coefficient.

- **Discussion**

In order to obtain some idea of the potential to prevent gravitational settling we assume as an illustrative example some typical values for a NaCl solution with a fluid density $\rho \approx 10^3$ kg/m^3 and $\mu \approx 10^{-3}$ Pas; with a particle density $\rho_p \approx 2.17 \times 10^3$ kg/m^3 and $\sigma_c = 1.2 \times 10^{-3}$N/(m)(Molarity), [4], and for a width of the container $h = 1$ cm and a drag coefficient $c_d = 0.9$. The resulting curves for the ratio between the maximum capillary velocity (Eq.(4)) and the terminal velocity (Eq.(5)) are shown in Fig. 2 as function of the concentration gradient.

A. Computational Simulation

In order to asses the capability for the proposed self-sustained control mechanism, hydrodynamic computational simulations in unsteady state conditions were performed using Ansys Fluent CFD software version 14.

- **Problem description**

The problem to be considered is shown schematically in Fig. 3. NaCl solution was considered inside a rectangular box of sides $l = 5$ mm and $b = 5$mm. The boundary conditions were as follows: at the bottom and top a wall zero slip condition, left and right sides as walls but instead of zero condition it was activated the Marangoni stress shear condition. However, because Ansys Fluent CFD Marangoni stress option is only directly available for thermocapillary flow, i.e., considering thermal coefficient of surface tension, then it was necessary to define a User-defined function (UDF) which allows to customize FLUENT. The UDF function read the local concentration gradient at the wall and then defined a ”fictitious” thermal gradient associated at this place using the following expression

$$\nabla_z T = \frac{\sigma_c}{\sigma_T} \nabla_z c \tag{6}$$

which allows to reproduce the Marangoni effect. In order to avoid any undesired collateral effect for the use of a fictitious thermal gradient, the thermal expansion coefficient of the fluid was set to zero. Finally, in order to reproduce a free surface at the bottom of the container, a gap of air with a thickens 0.1 mm was introduced. The Analysis was carried out with simple algorithm and Presto for pressure discretization, second order upwind scheme for momentum and energy. Relaxation factors were taken to be default values. Convergence criterion set for 10^{-3} for continuity, z-momentum and x-momentum and 10^{-6} for energy. Constant properties of water was considered, with $\rho = 10^3$ kg/m^3; $\mu = 10^{-3}$ Pas. For the thermal coefficient of surface tension $\sigma_T = -0.073$ mN/(mK) and for the concentration coefficient of the surface tension for supersaturated solution of NaCl with particles sizes near nanometric size, it was taken as $\sigma_c = 100$ mN/(m)(mass fraction of NaCl),

III. RESULTS

Fig. 4 and Fig. 5 show, for the sake of illustration, some sequence of the computational simulation for the concentration profile without and with Marangoni effect, respectively.

IV. CONCLUSIONS

The possibility to endow enclosed geometries with a passive feedback mechanism able to prevent or at least mitigate precipitation when their walls are deliberately lined with air-filled hydrophobic microcavities and inducing convective Marangoni currents was investigated. It was shown that providing that the solute particles have surfactant properties, i.e, the capability to affect surface tension, the resulting vertical concentration of particles developed during gravitational settling may trigger the apparition of Marangoni convection current which could oppose gravitational settling.

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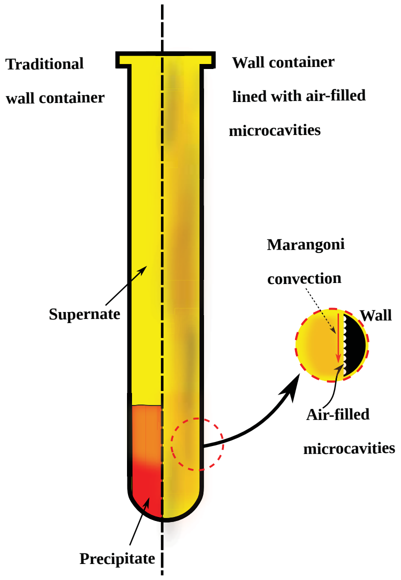

FIG. 1: Marangoni Passive Precipitation Control. **Left:** a common container. **Right:** the same container but lined with air-filled microcavities which owing to the concentration gradient resulting from the precipitation process a Marangoni feedback flow counteracts the precipitation.

V. REFERENCES

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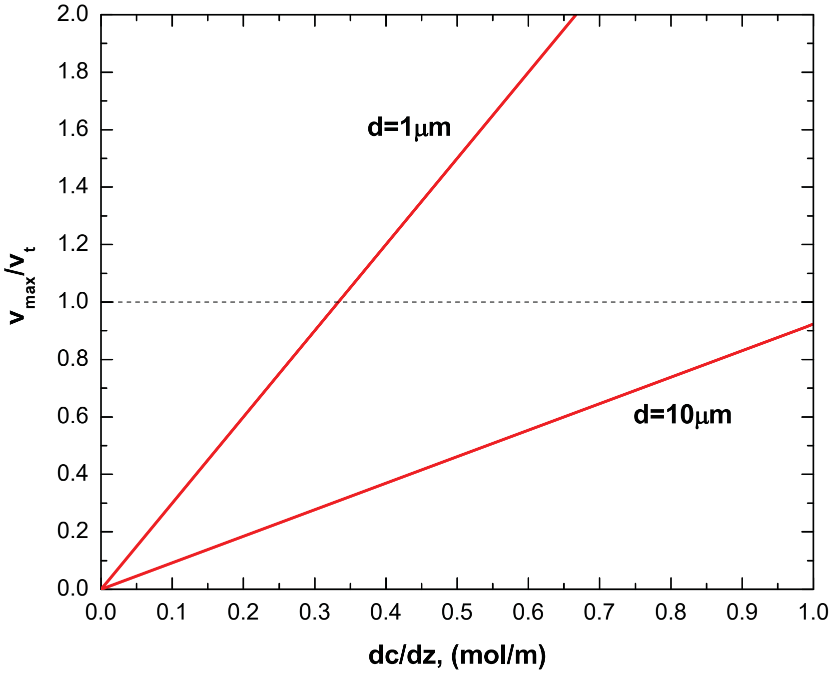

FIG. 2: The ratio between maximum capillary velocity and terminal velocity as a function of the concentration gradient for particles between 1μm to 10μm.

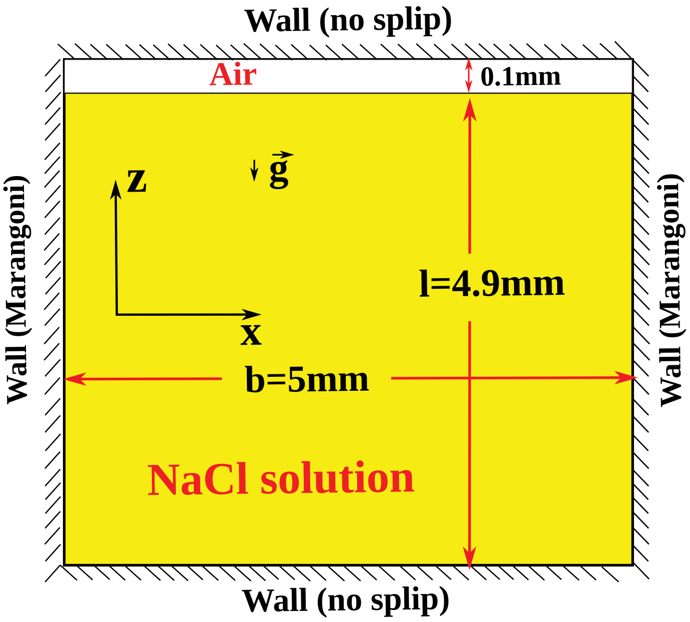

FIG. 3: Geometry for numerical simulation. Schematic depicting the geometry and the boundary conditions used in FLUENT Ansys ® Software.

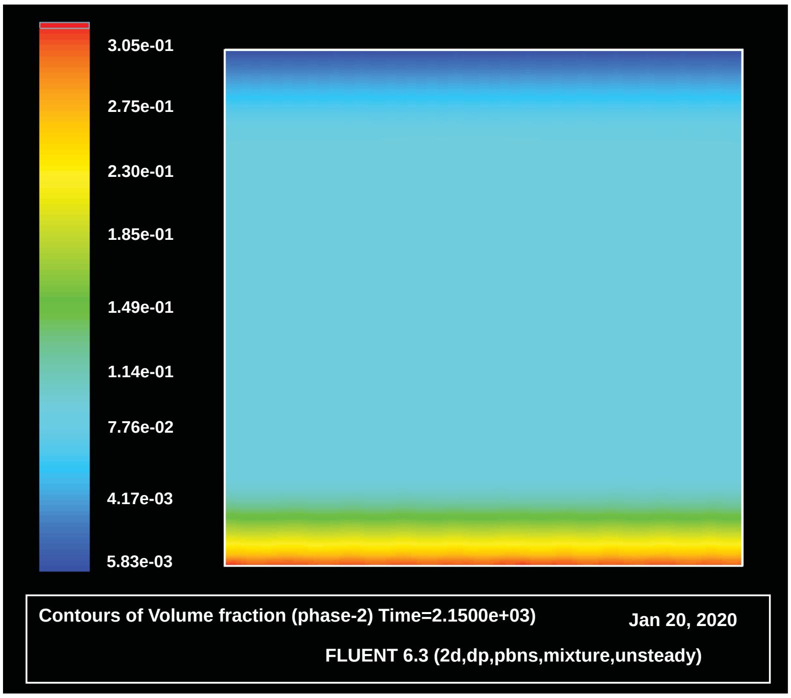

FIG. 4: CFD concentration profile for the gravitational settling of particles of 1 μm diameter without Marangoni stress.

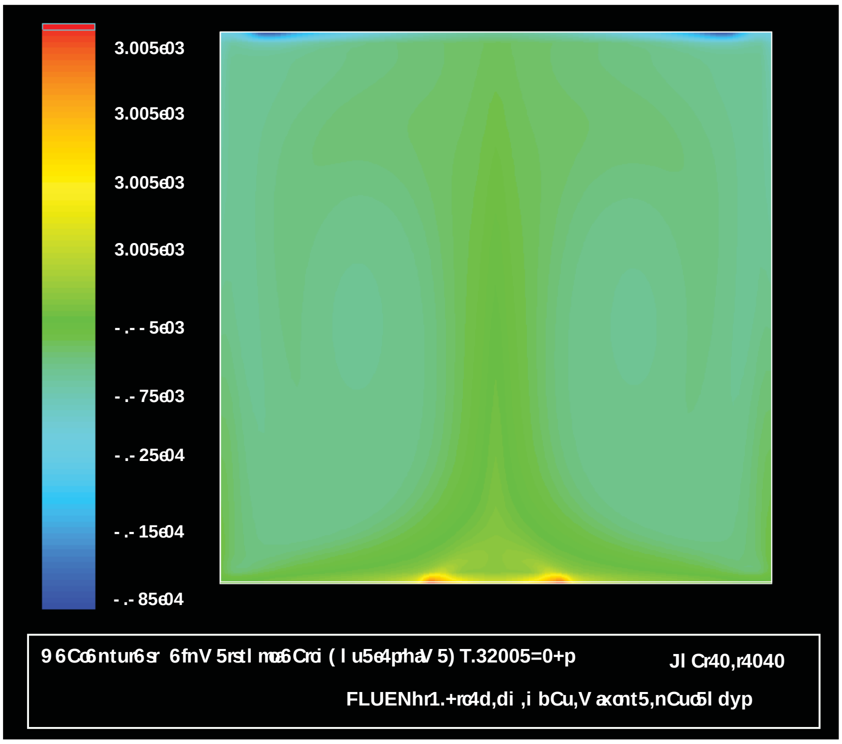

FIG. 5: CFD concentration profile for the gravitational settling of particles of 1 μm diameter with Marangoni stress.