Modeling Hydrodynamic and Physicochemical Effects in Particles/Bacteria Deposition on Surfaces

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Introduction & Motivation

Particle and bacterium deposition on surfaces is not a fully understood phenomenon. A state-of-the-art model for deposition was presented by Smoluchowski-Levich (SL) [1], however recent experiments by Li et. al [2a,2b] have proven that the SL solution doesn't hold in some cases. The SL solution shows that the flux of bacteria decreases with the distance from the inlet (see Fig. 1(a)), in total contradiction to the experimental results of Li et. al (see Fig. 1(b)).

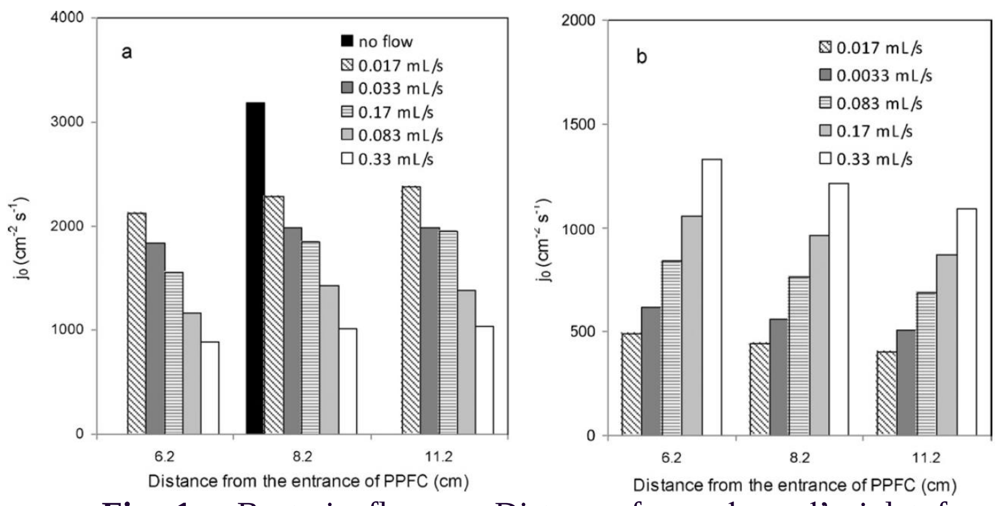


Fig. 1 - Bacteria flux vs. Distance from channel's inlet for different flow rates. (a) Simulation results (S-L approximation). (b) Experimental results (Li et. Al, 2011) .

It should be noted that our model is based on the behavior of particles, but it can also be used for the behavior of particle-like bacteria.

In contrast to previous models, this model regards the effects of forces such as gravity, lift and adhesion. Adhesion will be associated with a new parameter that considers particle interactions with the surface.

The purpose of our research is to develop a generic mathematical model that will cover a wider range of particle-surface systems.

Methods

The geometric framework of the system is the Parallel Plate Flow Chamber (PPFC), which is a well-known tool to measure and analyze deposition phenomena (see Fig.2). This effective experimental tool allows obtaining data regarding particle deposition on surfaces, using different variables such as: flow rate, solution concentration, viscosity etc.

COMSOL MULTYPHYSICS software was used to perform the numerical simulations, while we produced the optimization algorithms via MATLAB programming software.

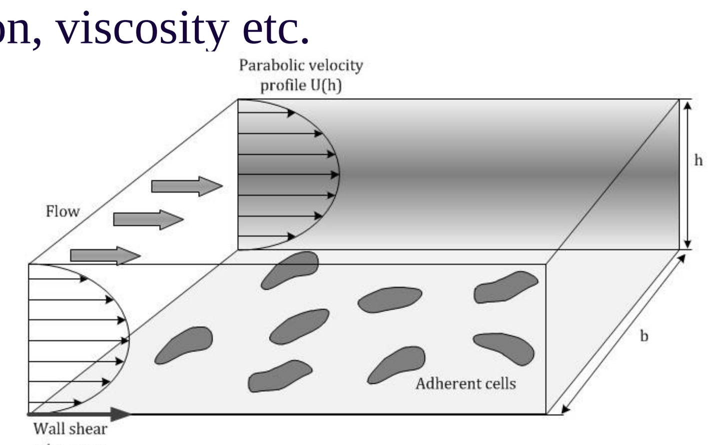


Fig. 2 - A 3-D model of a PPFC with a parabolic velocity profile.

Numerical Model

The model is based on a well-known diffusion convection equation with an additional migration flux:

$$\frac{\partial C}{\partial t}=-\vec{\nabla}\cdot\vec{J}=-\vec{\nabla}\cdot\left[-D\vec{\nabla}C+\frac{DC}{K_BT}\left(\vec{F_g}+\vec{F_l}\right)+\vec{U}C\right] \quad (1)$$

C is the particle concentration, J is the particle flux, D is the diffusion coefficient, K_B is the Boltzmann's constant, T is the temperature, F_g is the gravitational force, and F_l is the lift force and U is the medium velocity field.

The medium velocity field is presented by the Poiseuille flow:

$$U_{\hat{x}}=\frac{3}{2}U_m\left(1-\left(\frac{H-2y}{H}\right)^2\right) \quad (2)$$

U_m is the mean velocity and H is the channel's height.

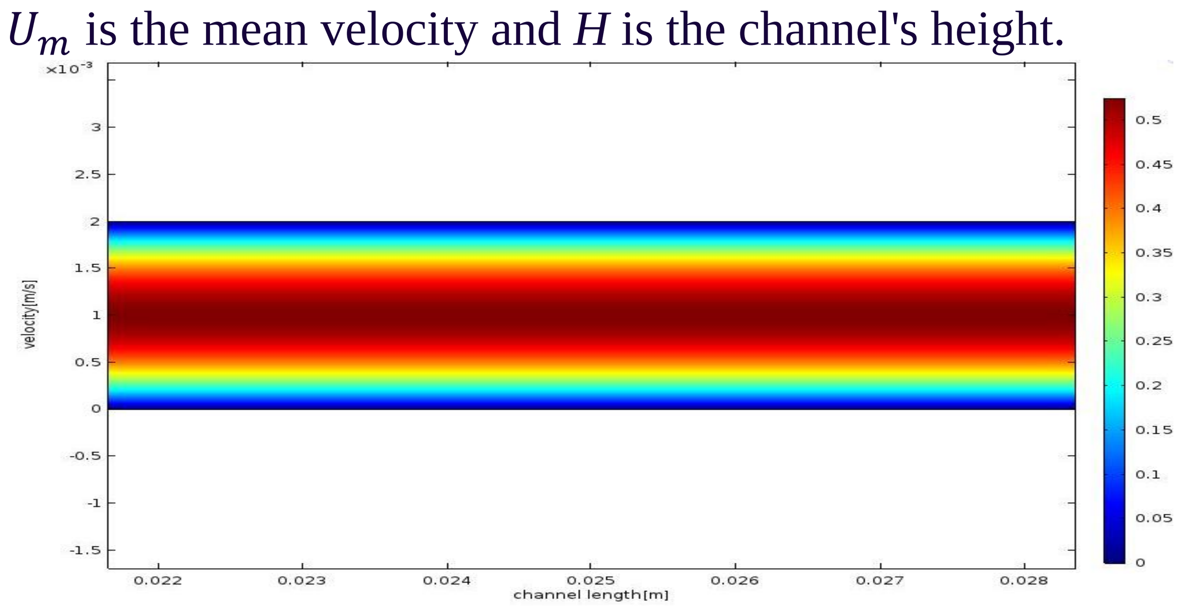
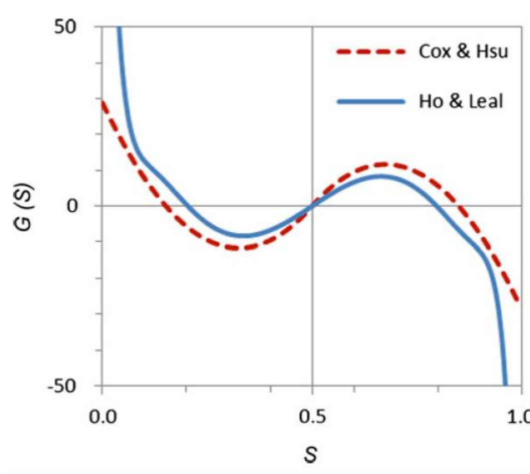


Fig. 3 - Velocity field simulation as a function of channel's height .

The migration force is a superposition of gravity force F_g and lift force F_l :



$$F_g=\frac{\pi}{6}ga^3(\rho-\rho_0) \quad (3)$$

$$F_l=\frac{\pi}{36}\rho\sigma^2a^4G(S) \quad (4)$$

Fig. 4 - Variation in lift force as a function of normalized channel's height ($S=\frac{y}{H}$) .

g is the gravitational acceleration, ρ is the particle density, ρ_0 is the medium density, σ is the medium shear rate, a is the particle's radius and *G(S)* is a dimensionless fitting function (see Fig.4).

A ***novel*** boundary condition which includes also adhesion can be written as:

$$\left[-D\vec{\nabla}C+\frac{DC}{K_BT}\left(\vec{F_g}+\vec{F_l}\right)+\vec{U}C\right]_{y=0,H}=\pm K_{dep}\frac{D}{a}C_{(y=0,H)} \quad (5)$$

The constant K_{dep} is a mass transfer coefficient that describes particle-surface interactions as well.

Analytical Model

Another goal is to have an analytical solution for particle flux. This solution is derived from boundary layer analysis which leads to the following mass conservation conjugated ordinary differential equations:

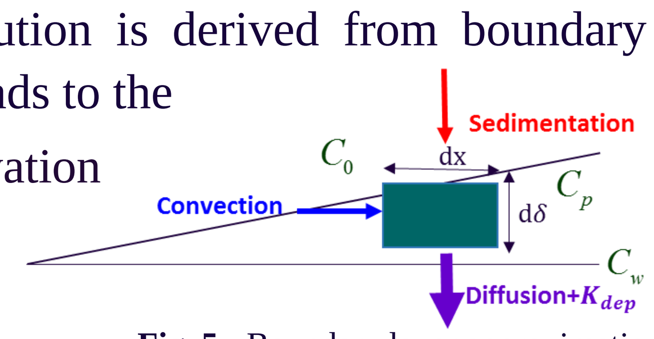


Fig. 5 - Boundary layer approximation.

$$Cv_s-D\frac{dC}{dy}=C_pv_s=J=-kC_w \quad (6)$$

$$\sigma\delta d\delta-v_sdx=-\frac{J}{C_0}dx \quad (7)$$

v_s is the sedimentation velocity, C_0 is the bulk concentration, C_w is the wall concentration, C_p is the effective concentration inside the boundary layer and $k=K_{dep}\frac{D}{a}$.

The following implicit solution is achieved:

$$x(\delta)=\frac{\sigma}{v_s}\left(\frac{1}{2}\delta(x)^2+\frac{\alpha k}{AB}\delta(x)e^{-A\delta(x)}+\frac{\alpha k}{A_2B}e^{-A\delta(x)}-\frac{\alpha k}{A^2B}\right) \quad (8)$$

Results

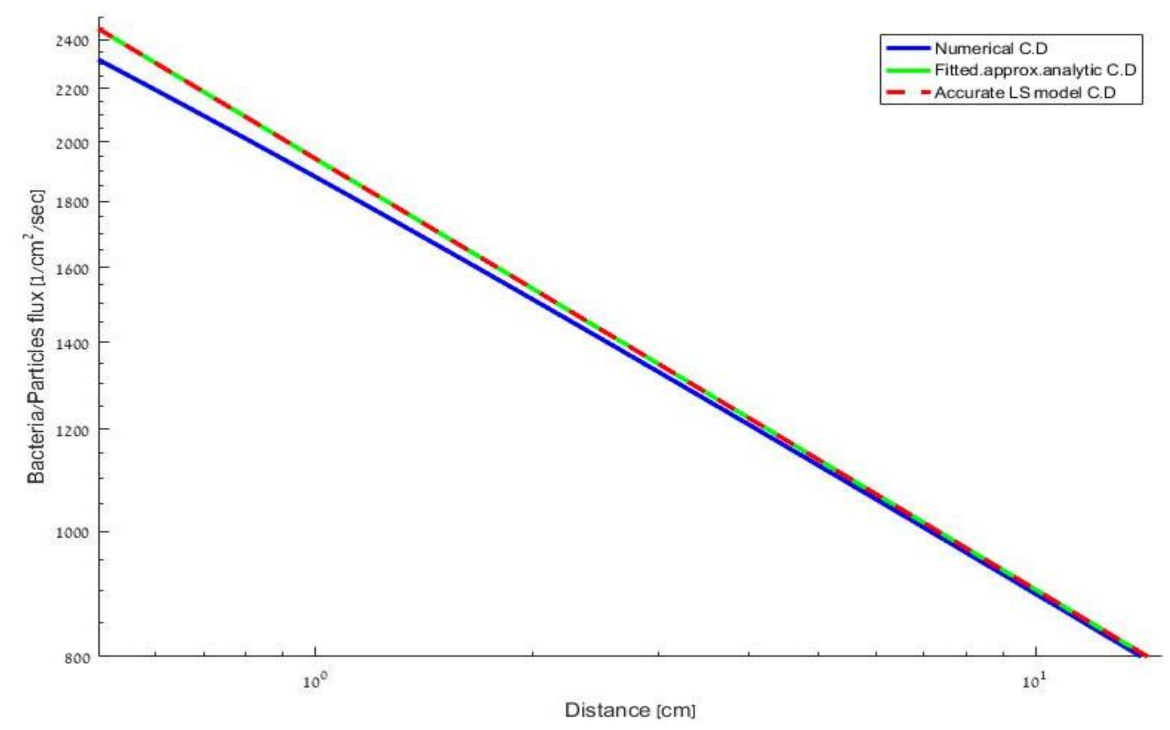


Fig. 6 - Particle flux as a function of channel distance for different models. The red dashed curve represents the SL model while the green curve is the flux obtained from equations (6-7) for the simplest case in which only diffusion and convection occur (such as in SL model). The blue curve represents the numerical solution for particle flux by COMSOL MULTIPHYSICS numerical software.

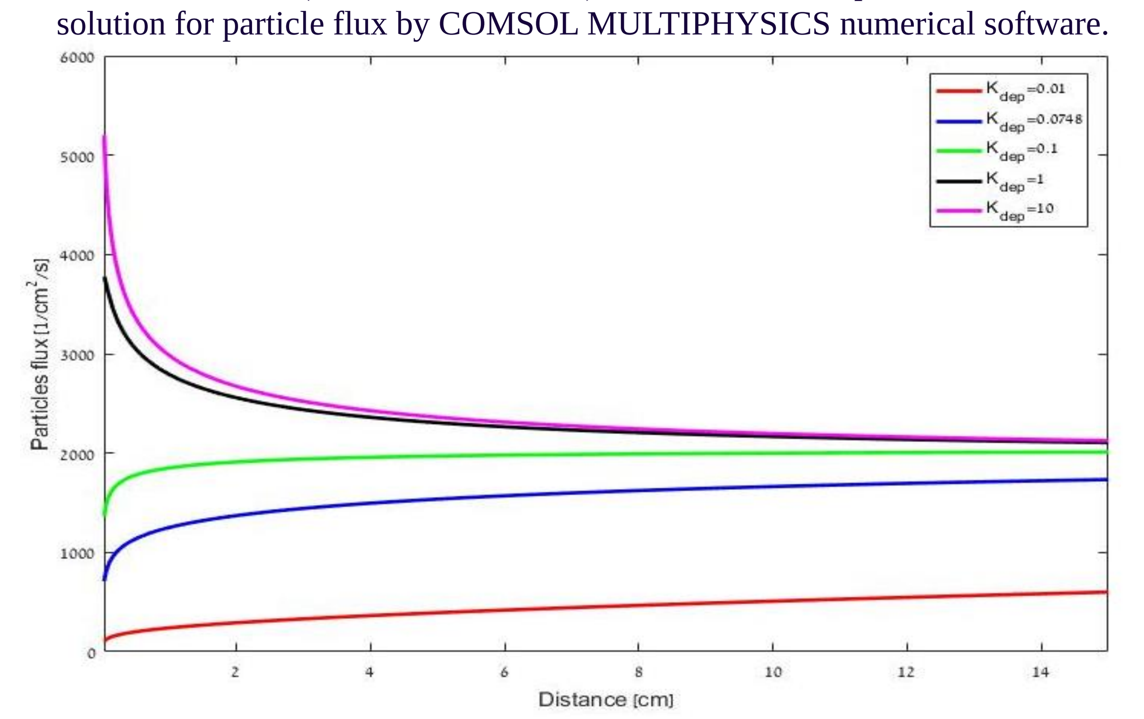


Fig. 7 - Numerical solution for Particle flux as a function of channel distance for different K_{dep} values.

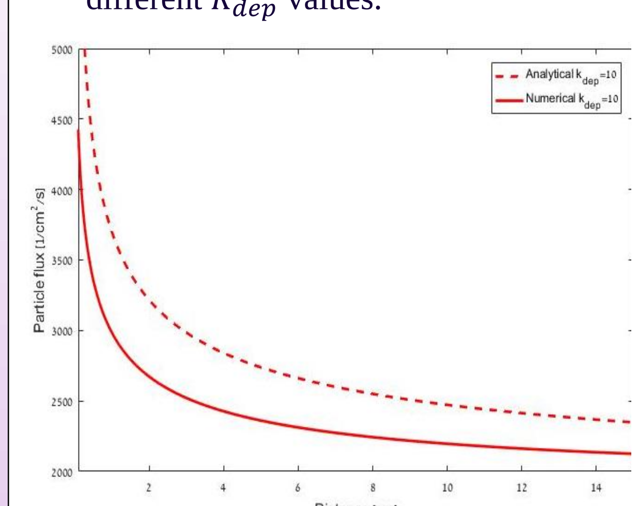


Fig. 8 - Particle flux for K_{dep}=10 in both numerical and analytical models.

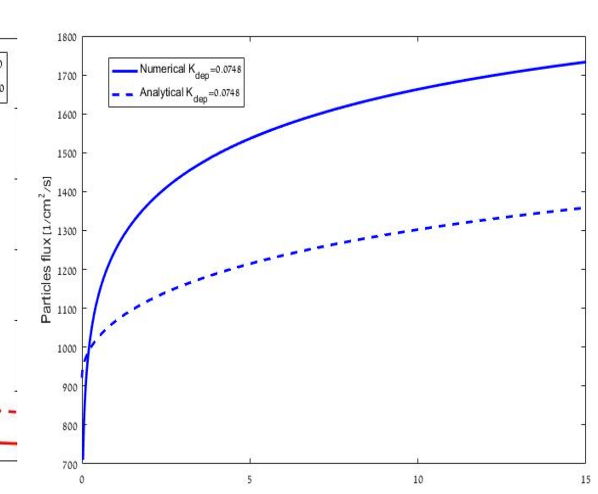


Fig. 9 - Particle flux for K_{dep}=0.0748 (Li's fitting parameter) in both numerical and analytical models.

Conclusions

- High values of the K_{dep} coefficient (of about 10 and higher) converge to the perfect sink condition.
- K_{dep} tailors the surface physics to the full mathematical model that can explain Li's results, in contrast to the SL model where the flux is always decaying with distance.
- K_{dep} includes the effects of the adhesion phenomenon within it– the missing part in the puzzle in most deposition models.
- The analytical model gives the same trends as the numerical model for both low and high values of K_{dep} with about a 20% error.

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