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QUASI-SMOLUCHOWSKI EQUATION AND DEPOSITION OF MACRO-NANO PARTICLES ONTO A SURFACE

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INTRODUCTION

Smoluchowski Equation (S.E.)

The Smoluchowski equation is a population balance equation, describing temporal evolution of particulates' concentrations, applicable to the study of particulate dynamics and morphology such as formation of particles, bubbles, sprays, clouds and galaxies, processes of polymerization, flocculation, fragmentation, charge transfer and evolution of microbial population.

The S.E. is a set of non-linear coupled partial differential equations, by which microscopic description of particulate interactions explains how macroscopic parameters evolve in space and time. The microscopic interactions are subsumed into the agglomeration rate kernel b. In this study the macroscopic parameter is $N(x)$, the number concentration of clusters of size x at time t. Discrete and continuous forms of the S.E. are:

$$\mathrm{SE_{Discrete}}: \quad \frac{\partial N_k}{\partial t} = +\frac{1}{2}\sum_{i=1}^{k-1} N_{k-i} b^{i\to k-i} N_i - N_k \sum_{i=1}^{\infty} b^{i\to k} N_i$$

$$\mathrm{SE_{Continuous}}: \quad \frac{\partial N(x)}{\partial t} = +\frac{1}{2}\int_0^x N(x-y).b(x-y,y).N(y)\,dy - N(x)\int_0^\infty b(x,y).N(y)\,dy$$

Eq. 1. Smoluchowski Equation (S.E.)

The microscopic description of particulate interactions from which kernel b is derived, can be governed on the basis of the following microscopic phenomena:

Brownian diffusion, Gravitational collection Van der Waals forces, Viscous forces, Fractal geometry, Thermophoresis, Electric charge, etc.

Quasi-Smoluchowski Equation (Q.S.E.)

A set of extra equations to the conventional S.E. accounts for poly-disperse particles entering to the physical system of particle-surface. These particles enter to the system to either deposit on to a free surface or form aggregates to the existing clusters deposited before.

In the S.E., collision kernels are derived based on theories describing the microscopic phenomena such as Brownian diffusion and then the macroscopic parameters are obtained by the solution to the S.E. system.

As opposed to what is conventional in the S.E., here we observe the macroscopic parameters to obtain the kernels. Discrete and continuous forms of the S.E. are shown in Eq. 2 where the macroscopic parameters (number concentrations N_k, $N(x)$ and N_p) can be functions of space and time (s,t).
Theoretical comparisons and classifications of different flows are possible by solving the QSE describing macroscopic transport phenomena to a surface under flow, such as:

- Formation/adhesion of biofilms, organisms or bacteria on different materials and surfaces
- Volcanic ash deposited on the ground
- Particle impaction process in particle impactors
- Mass and charge transfers
- Surface characterization

$$\mathrm{QSE_{Discrete}}: \begin{cases} \dfrac{dP_i}{dt} = N_{p_i}(s,t) \\ \dfrac{\partial N_k}{\partial t} = \displaystyle\sum_{i=1}^{k-1}\left(+a^{i\to k-i}N_{p_i} - a^{i\to k-i+1}N_{p_i}\right) + \frac{1}{2}\sum_{i=1}^{k-1} N_{k-i} b^{i\to k-i} N_i - N_k \sum_{i=1}^{\infty} b^{i\to k} N_i \end{cases}$$

$$\mathrm{QSE_{Continuous}}: \begin{cases} \dfrac{dP(y)}{dt} = N_p(y,s,t) \\ \dfrac{\partial N(x)}{\partial t} = \displaystyle\int_0^x \left(a(x-y,y).N_p(y) - a(x-y,y).N_p(y)\right) dy + \frac{1}{2}\int_0^x N(x-y).b(x-y,y).N(y)\,dy - N(x)\int_0^\infty b(x,y).N(y)\,dy \end{cases}$$

Eq. 2. Quasi Smoluchowski Equation (Q.S.E.)

Illustration of Terms

$(i=1,k=1) \;\Rightarrow\; a^{i\to k-i} = a^{1\to 0}$

$(i=1,k=2) \;\Rightarrow\; a^{i\to k-i} = a^{1\to 1}$

$(i=1,k=3) \;\Rightarrow\; a^{i\to k-i} = a^{1\to 2}$
$(i=2,k=3) \;\Rightarrow\; a^{i\to k-i} = a^{2\to 1}$

$(i=1,k=4) \;\Rightarrow\; a^{i\to k-i} = a^{1\to 3}$
$(i=2,k=4) \;\Rightarrow\; a^{i\to k-i} = a^{2\to 2}$
$(i=3,k=4) \;\Rightarrow\; a^{i\to k-i} = a^{3\to 1}$

$(i=1,k=n) \;\Rightarrow\; a^{i\to k-i} = b^{1\to n-1}$
$(i=2,k=n) \;\Rightarrow\; a^{i\to k-i} = a^{2\to n-2}$
$\left(i=\frac{n}{2},k=n\right) \;\Rightarrow\; a^{i\to k-i} = a^{\frac{n}{2}\to\frac{n}{2}}$

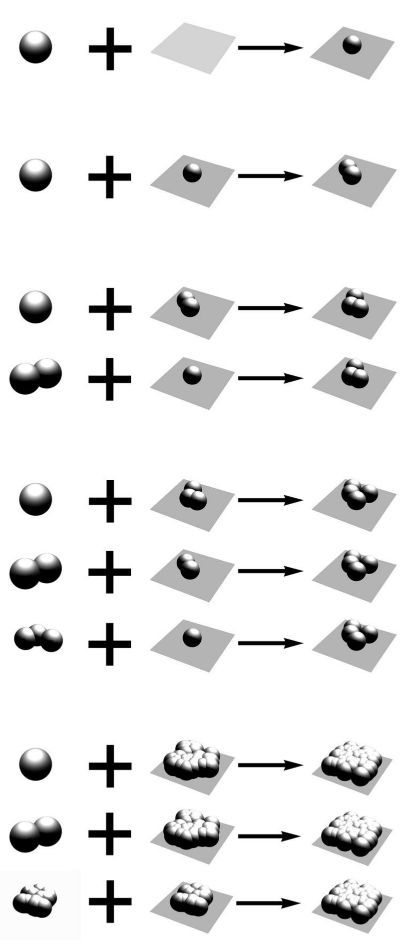

FIGURE 1. Binary collisions from space to surface

N_{p_i}: Rate of particles added from space to the surface

$b^{i\to k-i}$: Probability of i-particle clusters forming agglomerates to $(k-i)$-particle clusters, (On the surface).

$a^{i\to k-i}$: Probability of i-particle clusters forming agglomerates to $(k-i)$-particle clusters, (From space to the surface).

$$\underbrace{\sum_{i=1}^{k-1}\left(+a^{i\to k-i}N_{p_i}\right)}_{\text{Formation of k-particle clusters}} \qquad \underbrace{\frac{1}{2}\sum_{i=1}^{k-1} N_{k-i} b^{i\to k-i} N_i}_{\text{Birth of k-particle clusters}}$$

$$\underbrace{\sum_{i=1}^{k-1}\left(a^{i\to k-i+1}N_{p_i}\right)}_{\text{Loss of k-particle clusters}} \qquad \underbrace{N_k \sum_{i=1}^{\infty} b^{i\to k} N_i}_{\text{Death of k-particle clusters}}$$

$(i=1,k=2) \;\Rightarrow\; b^{i\to k-i} = b^{1\to 1}$

$(i=1,k=3) \;\Rightarrow\; b^{i\to k-i} = b^{1\to 2}$
$(i=2,k=3) \;\Rightarrow\; b^{i\to k-i} = b^{2\to 1}$

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$\left(i=\frac{n}{2},k=n\right) \;\Rightarrow\; b^{i\to k-i} = b^{\frac{n}{2}\to\frac{n}{2}}$

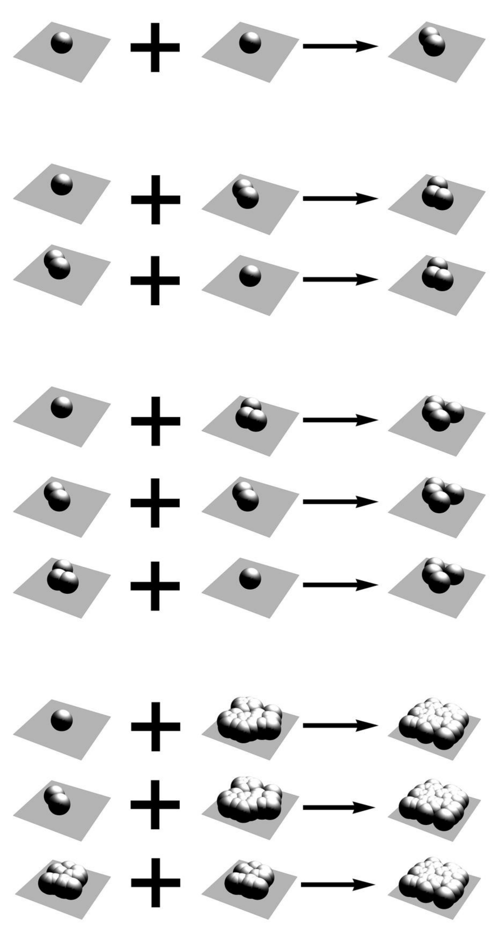

FIGURE 2. Binary collisions on the surface

Statement of a Simple Problem as an application

Synthetic mono-disperse spherical particles were released with zero initial velocity at the upper wall in a cubic domain. The rate of deposition onto the lower wall due to Brownian motion and an imaginary force was known. It was assumed that the imaginary force propels particles toward the larger clusters (an attractive force proportional to the size of the clusters). We see the output of the simulation or the deposited particles through time. We are interested in probability kernels. Fig. 3 shows deposited clusters in an instance.

Solution Procedure

Using clustering methods in each time step, size and number of clusters deposited on the surface (circles in Fig.3) were estimated. This also gives an estimation of rate of change in clusters' size. Assuming time invariant kernels, discrete form of Eq. 2 was used to form an over-determined system of linear equations with respect to the kernels a. Solving the system, an estimation of probability kernels were obtained and compared to the their actual values. This method can be applied in classifications according to different kernel functions at hand.

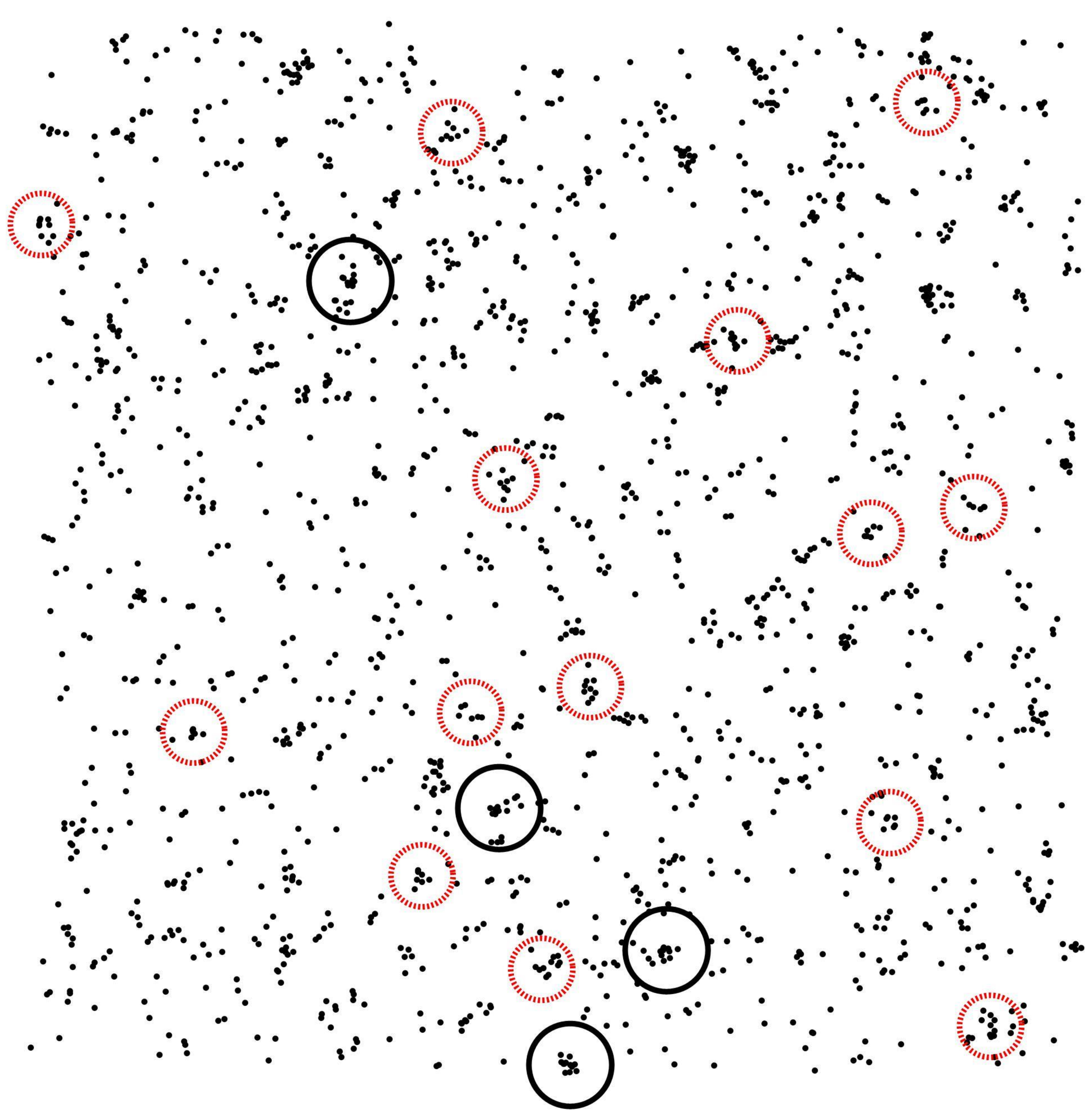

FIGURE 3. Clusters deposited on the surface. 10-p clusters circled black and 6-p clusters circled dashed red.

Results

Probability kernels calculated and governing equations derived are given in Fig. 4 and Eq. 3 respectively.

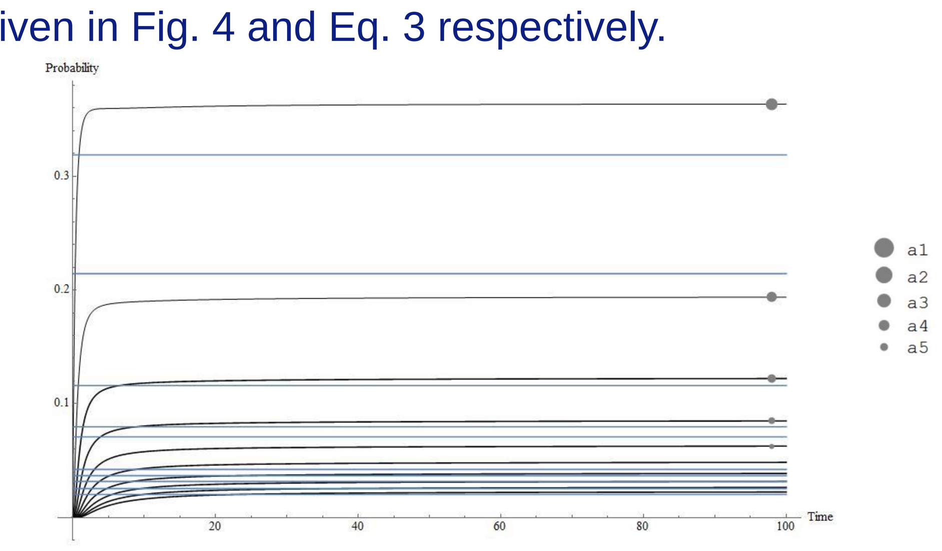

FIGURE 4. Probability kernels, given and approximated

$$\frac{d}{dt}N_1(t) = 0.999 \quad N_{p,1}(t) - 0.31356 \quad N_{p,1}(t), \qquad \frac{d}{dt}N_6(t) = 0.05269\,N_{p,1}(t) - 0.048416 \quad N_{p,1}(t),$$
$$\frac{d}{dt}N_2(t) = 0.31356\,N_{p,1}(t) - 0.205375\;N_{p,1}(t), \qquad \frac{d}{dt}N_7(t) = 0.04841\,N_{p,1}(t) - 0.038624\;N_{p,1}(t),$$
$$\frac{d}{dt}N_3(t) = 0.20537\,N_{p,1}(t) - 0.112166\;N_{p,1}(t), \qquad \frac{d}{dt}N_8(t) = 0.03862\,N_{p,1}(t) - 0.031594\;N_{p,1}(t),$$
$$\frac{d}{dt}N_4(t) = 0.11216\,N_{p,1}(t) - 0.074825\,N_{p,1}(t), \qquad \frac{d}{dt}N_9(t) = 0.03159\,N_{p,1}(t) - 0.026361\,N_{p,1}(t),$$
$$\frac{d}{dt}N_5(t) = 0.07482\,N_{p,1}(t) - 0.052695\,N_{p,1}(t), \qquad \frac{d}{dt}N_{10}(t) = 0.026361\,N_{p,1}(t) - 0.02235\,N_{p,1}(t),$$

Eq. 3. Governed equations based on the calculated kernels

CONCLUSIONS

We theorized and derived governing equations (QSE) of cluster growth and deposition on a surface versus time. One application of the governing equations could be in classification of different physical phenomena according to the probability kernels by which the observed data will be best described. For a synthetic deposition as a test example, we extracted the probability kernels which were in agreement with the given probabilities by which the data were produced.