The friction coefficient of fractal aggregates in the continuum and transition regimes

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Objectives

- To introduce a methodology for the calculation of the friction coefficient of fractal aggregates by solving a diffusion equation.

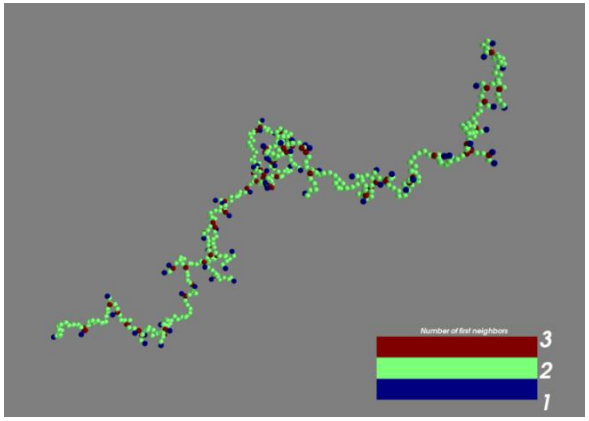
- Advantages:
  i. Numerical solution of a simpler equation (Laplace vs Stokes)
  ii. Easy to implement computationally

- Relate geometric and dynamic properties of fractal aggregates

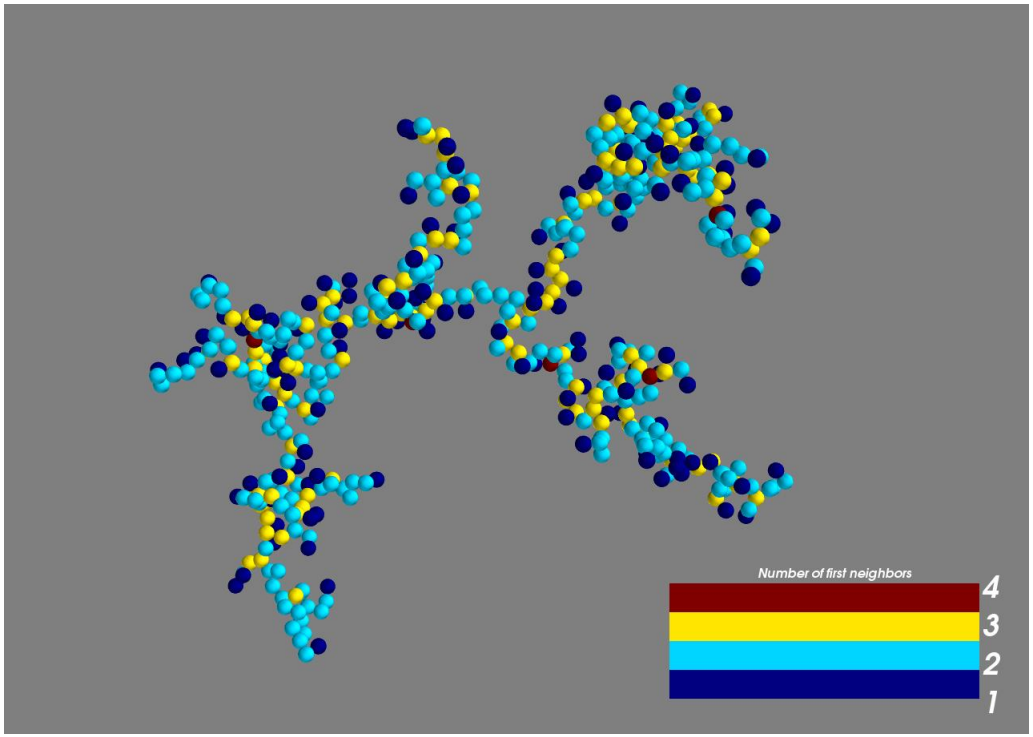
Fractal aggregates (I)

- Aerosols and colloids form fractal-like structures

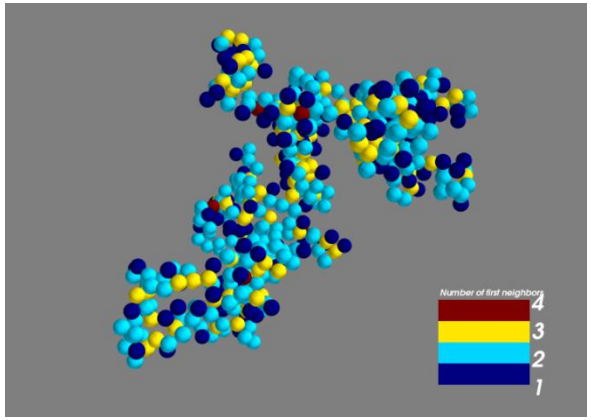
512 monomers, D_f=1.5 and k_f=1.3, R_g=53.7



512 monomers, D_f=1.8 and k_f=1.3, R_g=27.6



512 monomers, D_f=2.1 and k_f=1.3, R_g=17.2



Fractal aggregates (II)

- **Scaling law**

$$N = k_f \left(\frac{R_g}{R_1}\right)^{d_f}$$

N: number of monomers
k_f: fractal prefactor
R_g: radius of gyration
R_1: monomer radius
d_f: fractal dimension

- **Cluster-cluster aggregation algorithm**

  i. Satisfy exactly the scaling law
  ii. Prescribed fractal dimension (d_f) and fractal prefactor (k_f)
  iii. No monomer overlapping

- **Insert the structures from Matlab in Comsol Multiphysics with the tool Livelink**

Friction coefficient of fractal aggregates in the continuum regime (I)

- **Knudsen number is 0 ($Kn=\lambda/R_1$)**
- **Stokes friction coefficient (continuum regime):**

$$f_N = \frac{1}{B_N} = 6\pi\mu R_h$$

B_N: Mechanical mobility
R_h: Hydrodynamic radius

- **Experimentally observed (*Keller et al., 2000*):**

$K_N \cdot B_N$=constant Independent of particle material, shape and size

K_N: Collision rate between gas molecules and an aggregate. We assume that sticking coefficient is 1

- **From Stokes friction coefficient (*Isella and Drossinos, 2011*):**

$$\frac{K_N}{K_1} = \frac{f_N}{f_1} = \frac{R_h}{R_1}$$

(R_m=R_h in the continuum regime)

Friction coefficient of fractal aggregates in the continuum regime (II)

- **Collision rate between gas molecules and an aggregate:**

$$K_N = \int_s J \cdot \hat{s}\, dS$$

J: Diffusive flux of the gas towards the aggregate
s: unit vector perpendicular to S
dS: surface element

- **Diffusive flux:**

$$J = -D_g \nabla \rho$$

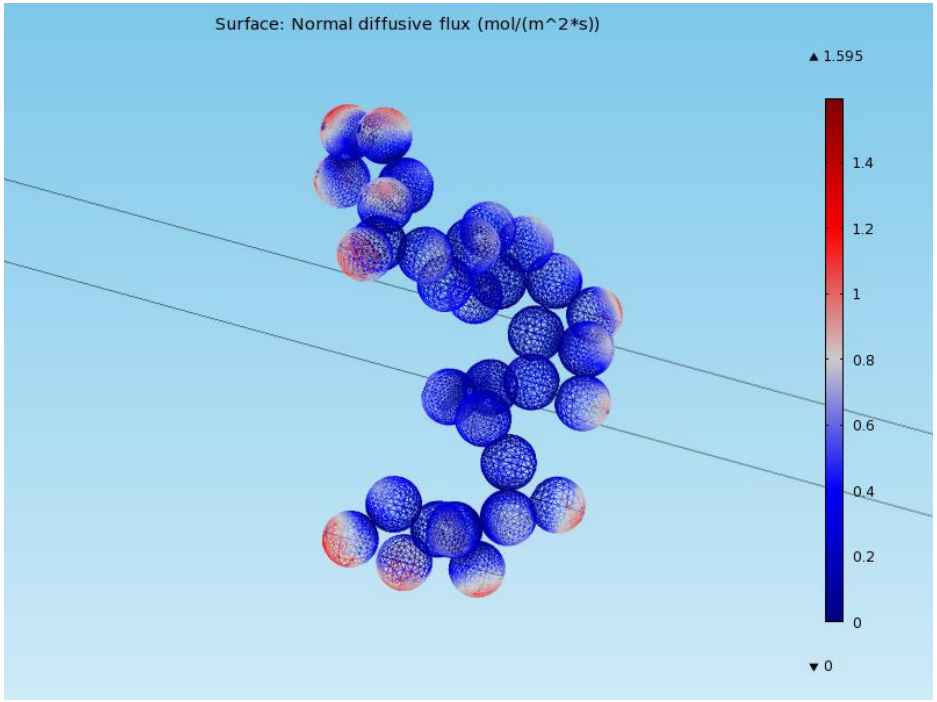
D_g: gas self-diffusion coefficient
ρ: gas density

- **Dirichlet boundary conditions:**

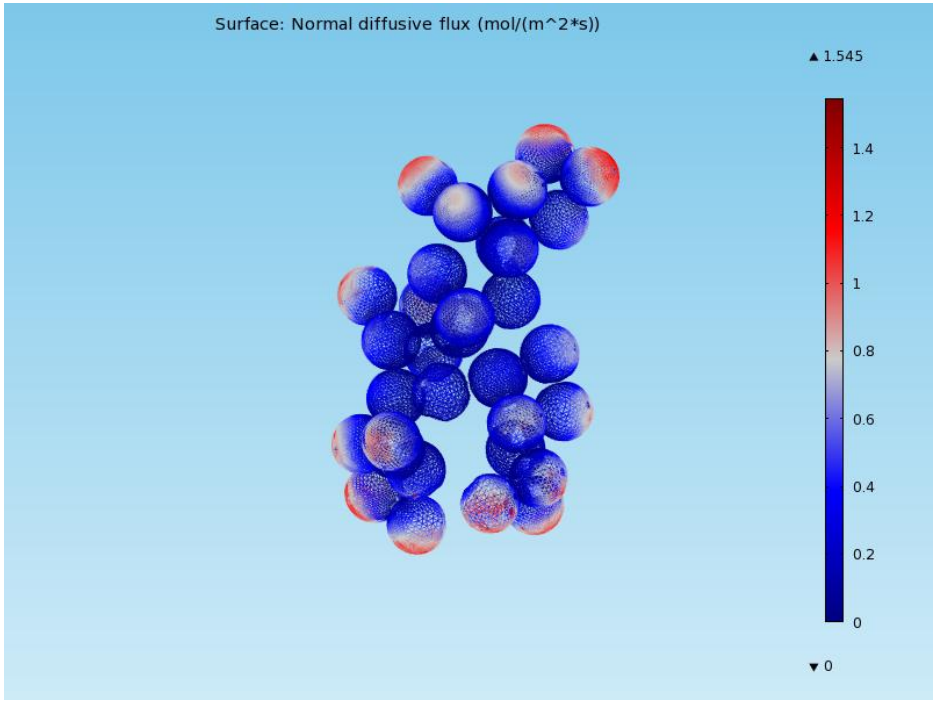
i. On the aggregate surface: $\varrho = 0$
ii. Far away from the aggregate (on an outer sphere): $\varrho = 1$

Use of Comsol Multiphysics

$N = 32 - d_f = 1.8 - k_f = 1.3$

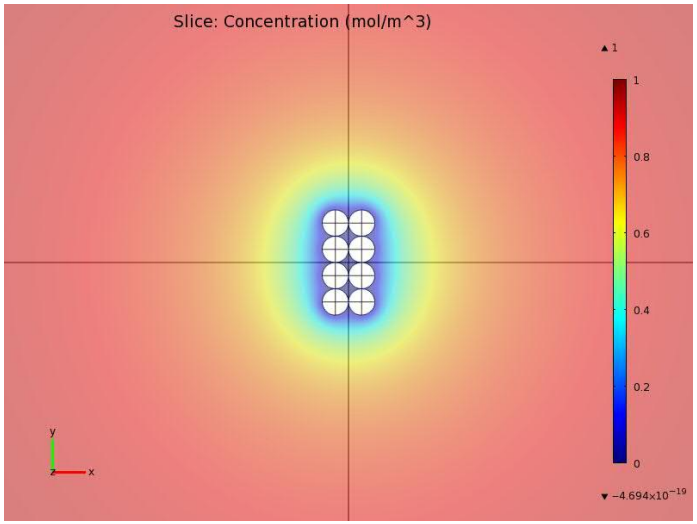


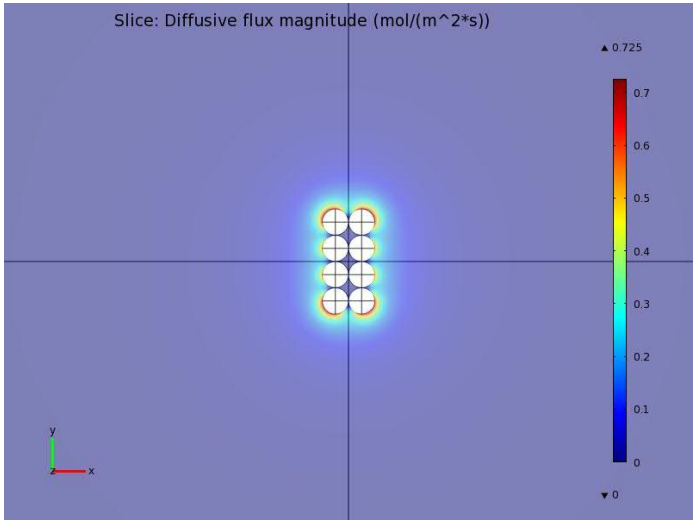
$N = 32 - d_f = 2.1 - k_f = 1.3$



- Transport of diluted species or PDE with 2 Dirichlet boundary conditions.
- Free tetrahedral mesh: Extra fine
- Surface integration: Diffusive flux
- Surface integration either on the whole fractal or on each monomer

Simulations and results for simpler structures





Straight chains

Straight chains	Dahneke (1982), experimental fit	Collision rate
4-monomers	0.507	0.507
8-monomers	0.390	0.389

More complex structures: cube and rectangle solved analytically by Filippov (2000)

Structures (8-monomers)	Filippov(2000), analytical calculation	Collision rate
Cube (2*2*2)	0.293	0.290
Rectangle (2*4*1)	0.361	0.366

Slip flow regime

- **Small Knudsen numbers ($0 < Kn \leq 0.2$)**
- **In the transition regime** $$f_N(Kn) = \frac{f_N(0)}{C(N, Kn)}$$

  where C(N, Kn) is the Cunningham correction factor

$$C(1, Kn) = 1 + AKn \text{ and } A = 1.234 + 0.414 \exp\left(-\frac{0.876}{Kn}\right) \text{ (Millikan, 1923)}$$

- **We relate the collision rate to the friction coefficient**

$$C(N, Kn) = \frac{f_N(0)}{f_N(Kn)} = \frac{K_N(0)}{K_N(Kn)}$$

Boundary conditions and the Comsol Multiphysics use

- **Robin boundary condition (Radiation boundary condition)**

$$\rho(R_1) = \alpha(Kn) \left.\frac{d\rho}{dr}\right| R_1$$ On the aggregate surface

$$\rho = 1$$ Far away from the aggregate surface

We solve a PDE with flux/source and dirichlet boundary conditions.

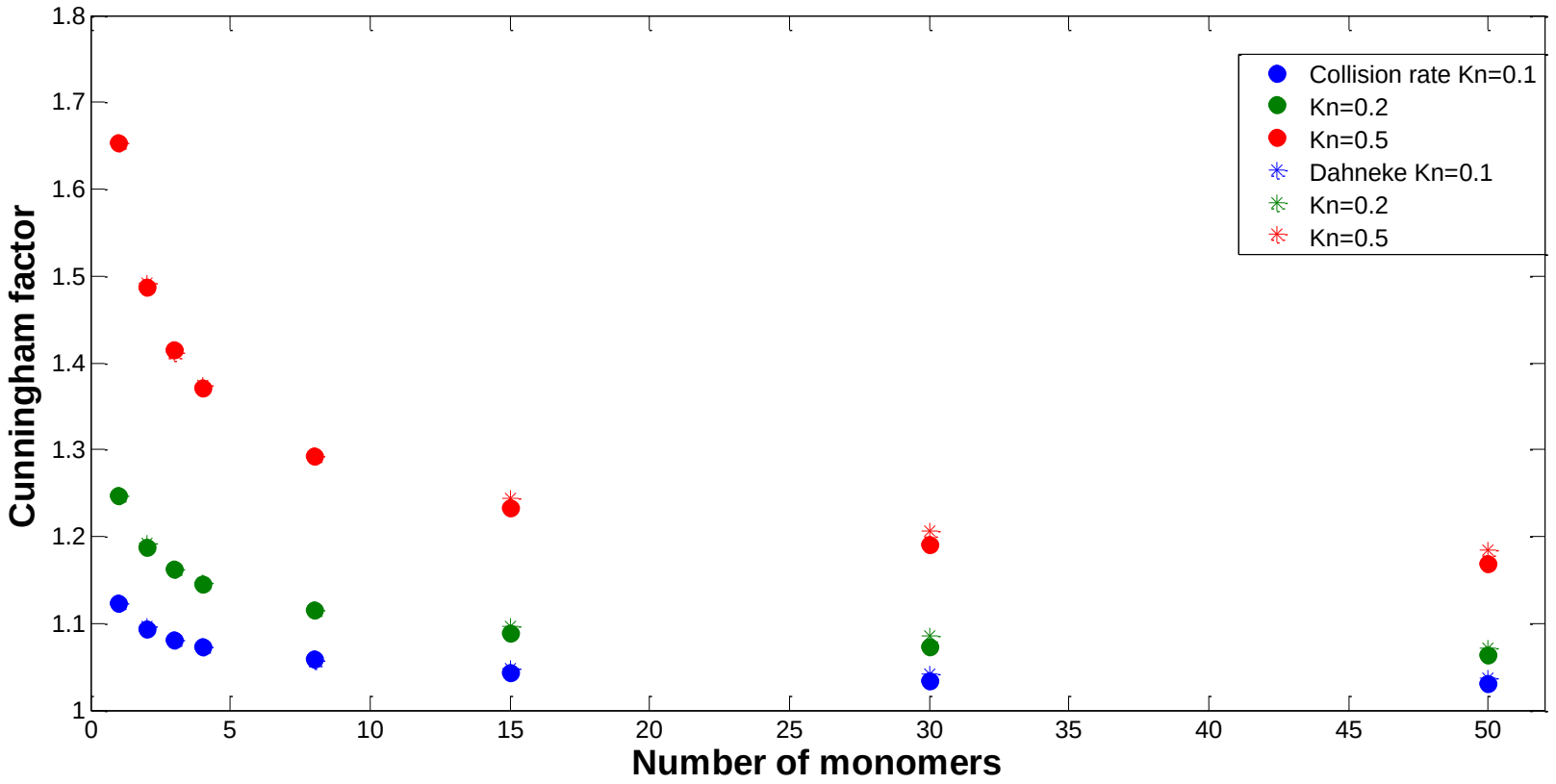
- **The $\alpha(Kn)$ is calculated for a monomer**

$$\rho(r) = \rho_\infty \left[1 - \frac{1}{1+\frac{\alpha}{R_1}} \frac{R_1}{r}\right] \qquad \Rightarrow K_1(Kn) = \frac{K_1(0)}{1+\frac{\alpha}{R_1}}$$

$$\Rightarrow \frac{\boldsymbol{\alpha}}{\boldsymbol{R_1}} = \frac{\boldsymbol{K_1(0)}}{\boldsymbol{K_1(Kn)}} - \mathbf{1} = \frac{\boldsymbol{f_1(0)}}{\boldsymbol{f_1(Kn)}} - \mathbf{1} = \boldsymbol{C(1, Kn)} - \mathbf{1}$$

- **Boundary absorption/impedance term: $q = 1/\alpha$**

Straight chains



- Comparison with Dahneke's (1982) results for the Cunningham factor of straight chains in different Knudsen numbers
- Maximum deviation 1.3%

Conclusions

- A methodology was introduced and validated for the calculation of the friction coefficient of fractal aggregates in the continuum and the slip flow regimes by solving a diffusion equation.
- There is a very good agreement with literature values for straight chains and more complex structures with maximum Kn=0.5.
- Comsol Multiphysics was used to solve the diffusion equation with complex boundary conditions on fractal-like surfaces.
- Comsol Multiphysics can be used for the integrations either on the whole surface of fractal aggregates or for individual monomers of a fractal.