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APPLICATIONS OF THE FCMOM TO IN-HOMOGENEOUS SYSTEMS (PBE) AND TO KINETIC THEORY

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Outline

1. A parallel between Population Balance Equations (PBE) and Kinetic Theory (KT)
2. FCMOM governing equations
3. Application of the FCMOM to the PBE/In-Homogeneous Systems
4. Application of the FCMOM to the 2-D Boltzmann Equation (BE)

A Parallel between PBE and Kinetic Theory

How to predict the change of particle size, shape, porosity, composition?

How to describe the fluid dynamics of inelastic particles (in not too dense flows)?

particle size distribution function

$$f(\bar{\boldsymbol{\xi}}, \bar{\mathbf{x}}, t)$$

particle velocity distribution function

Internal Variables

(Size, Shape, Age, etc.)

Components of Particle Velocities

Two Fundamental Equations

Population Balance Equation:

$$\frac{\partial f_r}{\partial t} + \frac{\partial \mathbf{v} \cdot f_r}{\partial \mathbf{x}} + \frac{\partial G \cdot f_r}{\partial r} = (B - D)$$

V is particle velocity

G is the growth rate

Aggregation, breakage

Enskog-Boltzmann Equation:

$$\frac{\partial f_c}{\partial t} + \frac{\partial \mathbf{c} \cdot f_c}{\partial \mathbf{x}} + \frac{\partial \mathbf{F}_{\mathbf{tot}} \cdot f_c}{\partial \mathbf{c}} = (B - D)_{coll}$$

Particle velocity

F_{tot} external forces

Collisions

Finite domain Complete set of trial functions MOM (FCMOM)

1. PBE or BE (Boltzmann equation) in a finite domain (moving boundary problem)
2. Evolution equations of the dimensionless moments defined in the finite domain
3. Efficient reconstruction of the distribution function through orthogonal functions (closure)

FCMOM for mono-variate homogeneous processes

$f(\xi,t) =$ distribution function

$\xi = c \ (BE)$

$\xi = r \ (PBE)$

$\xi = [-\infty,\infty](BE)$
$= [0,\infty](PBE)$

$$\frac{\partial f}{\partial t} + \frac{\partial \overline{G} \cdot f}{\partial \xi} = B - D$$

$\xi = [\xi_{\min}(t), \xi_{\max}(t)]$

External forces; growth rate

Integral Terms (Collisions; aggregation, breakage)

Moving boundaries

$\overline{\xi} = [-1,1]$

$$\frac{\partial f}{\partial t} - \frac{\partial f}{\partial \overline{\xi}} \cdot \frac{1}{(\xi_{\max} - \xi_{\min})} \cdot \left[\left(\frac{d\xi_{\min}}{dt} + \frac{d\xi_{\max}}{dt} \right) + \overline{\xi} \cdot \left(-\frac{d\xi_{\min}}{dt} + \frac{d\xi_{\max}}{dt} \right) \right] + \frac{2}{(\xi_{\max} - \xi_{\min})} \cdot \left(\frac{\partial \overline{G} \cdot f}{\partial \overline{\xi}} \right) = B - D$$

Correction term for change of reference frame

Dimensionless Moments Equations

Dimensionless moments $\mu_i = \int_{-1}^{1} \overline{f} \cdot \left(\overline{\xi}\right)^i \cdot d\overline{\xi}$

Term due to the change of reference frame

$$\frac{\partial \mu_i}{\partial \overline{t}} + i \cdot \mu_{i-1} \cdot \frac{1}{\left(\xi_{max} - \xi_{min}\right)} \cdot \left(\frac{d\xi_{min}}{d\overline{t}} + \frac{d\xi_{max}}{d\overline{t}}\right) + (i+1) \cdot \mu_i \cdot \frac{1}{\left(\xi_{max} - \xi_{min}\right)} \cdot \left(-\frac{d\xi_{min}}{d\overline{t}} + \frac{d\xi_{max}}{d\overline{t}}\right) -$$

$$-\left[\overline{f_1} - (-1)^i \cdot \overline{f_{-1}}\right] \cdot \frac{1}{\left(\xi_{max} - \xi_{min}\right)} \cdot \left(\frac{d\xi_{min}}{d\overline{t}} + \frac{d\xi_{max}}{d\overline{t}}\right) - \left[\overline{f_1} - (-1)^{i+1} \cdot \overline{f_{-1}}\right] \cdot \frac{1}{\left(\xi_{max} - \xi_{min}\right)} \cdot \left(-\frac{d\xi_{min}}{d\overline{t}} + \frac{d\xi_{max}}{d\overline{t}}\right)$$

$$+ \frac{2 \cdot t_{sc}}{\left(\xi_{max} - \xi_{min}\right)} \cdot \left[\overline{G_1} \cdot \overline{f_1} - (-1)^i \cdot \overline{G_{-1}} \cdot \overline{f_{-1}}\right] -$$

$$- \frac{2 \cdot t_{sc}}{\left(\xi_{max} - \xi_{min}\right)} \cdot i \cdot \int_{-1}^{1} \overline{G} \cdot \overline{f} \cdot \left(\overline{\xi}\right)^{i-1} \cdot d\overline{\xi} = \frac{t_{sc}}{f_{sc}} \cdot \int_{-1}^{1} (B - D) \cdot \left(\overline{\xi}\right)^i \cdot d\overline{\xi}$$

Boundary Conditions

Ext. forces/growth   *Multidimensional Integrals*

$\overline{t}, \overline{f}$ = dimensionless values t_{sc}, f_{sc} = scale factors

$\overline{G_1}, \overline{f_1}, \overline{G_{-1}}, \overline{f_{-1}}$ = boundary values

Distribution function reconstruction/Closure

Truncated series expansion of orthonormal functions (complete set):

$$\overline{f}\left(\overline{\xi},\overline{t}\right) \approx \sum_{n=0}^{M-1} c_n\left(\overline{t}\right)\cdot\phi_n\left(\overline{\xi}\right)$$

M = number of moments

Dependency on external variables → μ_i

Dependency on internal variables (velocity, size)

1) Good properties of convergence: the distribution function is well represented with few moments

2) The truncated series expansion provides the closure in the FCMOM

PBE in Homogeneous Conditions

$$\frac{\partial f(\xi,t,\mathbf{x})}{\partial t}+\underbrace{\frac{\partial v_{p,j}(t,\mathbf{x})\cdot f(\xi,t,\mathbf{x})}{\partial x_j}}_{0}-\underbrace{\frac{\partial}{\partial x_j}\left[D_{pt}(\xi,t,\mathbf{x})\cdot\frac{\partial f(\xi,t,\mathbf{x})}{\partial x_j}\right]}_{0}=-\frac{\partial G(\xi,t,\mathbf{x})\cdot f(\xi,t,\mathbf{x})}{\partial \xi}+B(\xi,t,\mathbf{x})-D(\xi,t,\mathbf{x})$$

Convection — Diffusion — Growth — Aggregation, Breakage

$$\frac{\partial f(\xi,t,\mathbf{x})}{\partial t}=-\frac{\partial G(\xi,t,\mathbf{x})\cdot f(\xi,t,\mathbf{x})}{\partial \xi}+B(\xi,t,\mathbf{x})-D(\xi,t,\mathbf{x})$$

Growth — Aggregation, Breakage

- Mono-variate homogeneous systems: Chem Eng Sci, Solution of PBE by MOM in finite size domains, 63, 2624-2640, 2008
- Bi-variate homogeneous systems: Ind Eng Chem Res, Solution of bivariate PBE using the FCMOM, 48(1), 262-273, 2009

Validation Cases (Monovariate Distributions)

- Growth (linear, constant, diffusion-controlled): analytical solutions
- Growth (constant, diffusion-controlled) +Primary Nucleation: analytical solutions
- Growth (diffusion-controlled) +Nucleation (primary and secondary) +Solute mass balance: experimental data
- Dissolution: analytical solution
- Aggregation (constant, linear, product, Smoluchowski continuum kernels): analytical solutions and self-preserving solution for the Smoluchowski continuum kernel
- Aggregation and Growth (constant, linear kernels and constant and linear growth): analytical solutions
- Breakage (symmetric breakage, power-law breakage function, homogeneous type breakage kernels): analytical solutions

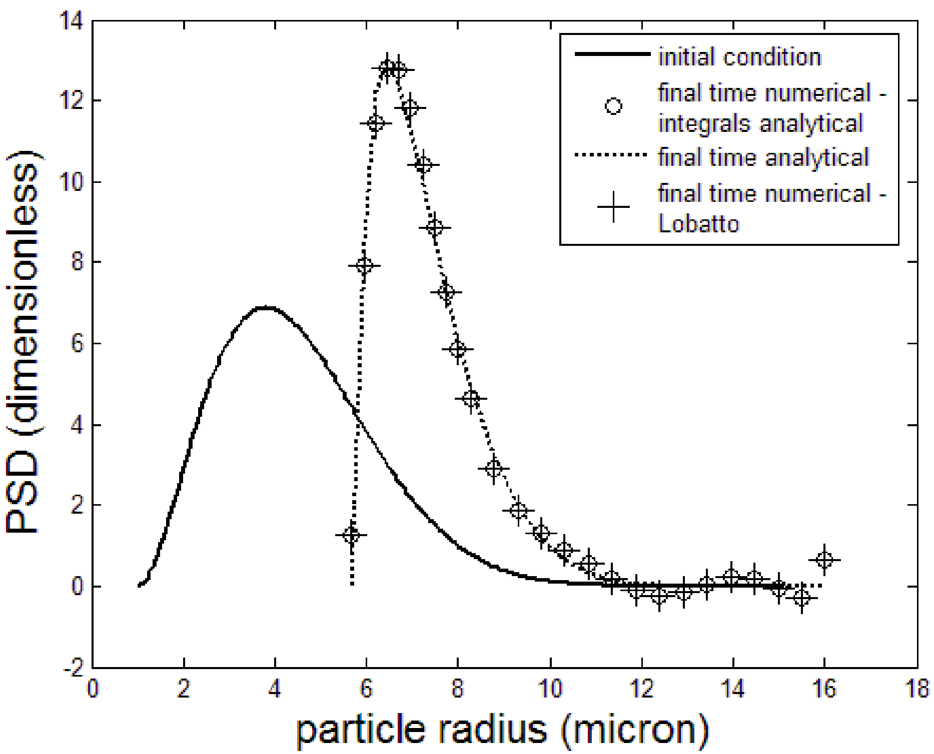
Diffusion Controlled Growth

$$G = \frac{dr}{dt} = \frac{K}{r}$$

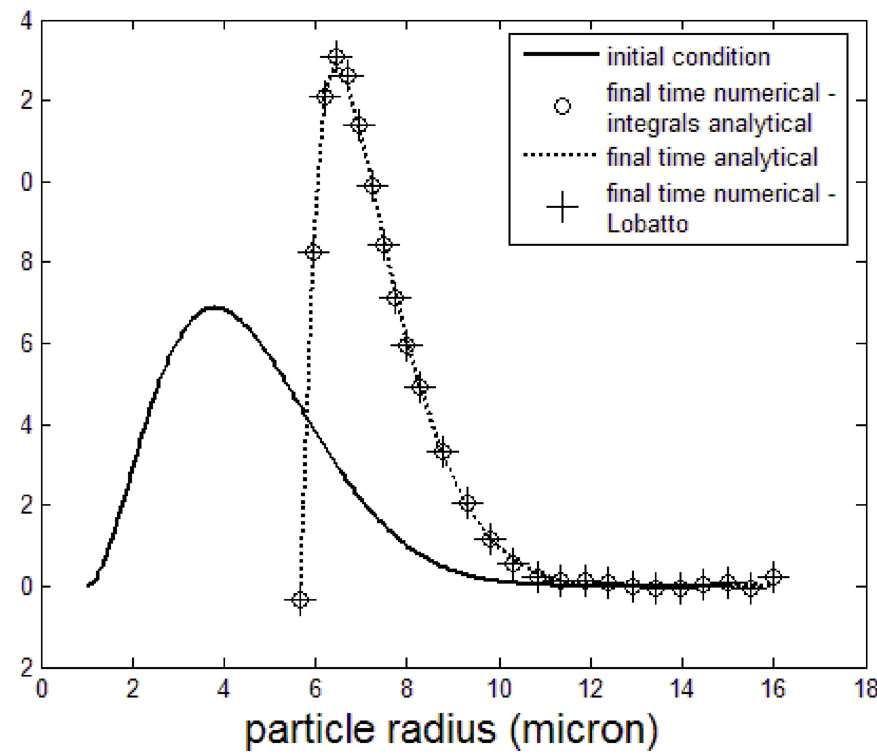
$$K = 0.78 \text{ micron}^2/\text{sec}$$

$$t_{fin} = 20 \text{ sec}$$

Clouds: particle radius > 1 micron (McGraw)



8 moments



10 moments

Aggregation models

1. **Smoluchowski equation:** particles of any size are produced and aggregate.

2. **Finite Smoluchowski equation:** a finite domain is defined. Particles of any size can be produced but not all the aggregations are possible: aggregations creating particles larger than the maximum size are neglected (similar to method of classes).

3. **Oort-Hulst equation:** v' particles and v particles aggregate (v'< v); v' particles break in monomers and aggregate to v particles

$$\frac{\partial f(v,t)}{\partial t} = -\frac{\partial f(v,t)\cdot \int_0^v v' \cdot K(v,v')\cdot f(v',t)\cdot dv'}{\partial v} - \int_v^\infty K(v,v')\cdot f(v,t)\cdot f(v',t)\cdot dv'$$

Net gain of particles aggregating

Loss of particles breaking in monomers

Dubovski (J. Phys. A, 32, 781-793, 1999) compared 1) vs. 3):

in 1), aggregation front propagates at infinite rate;

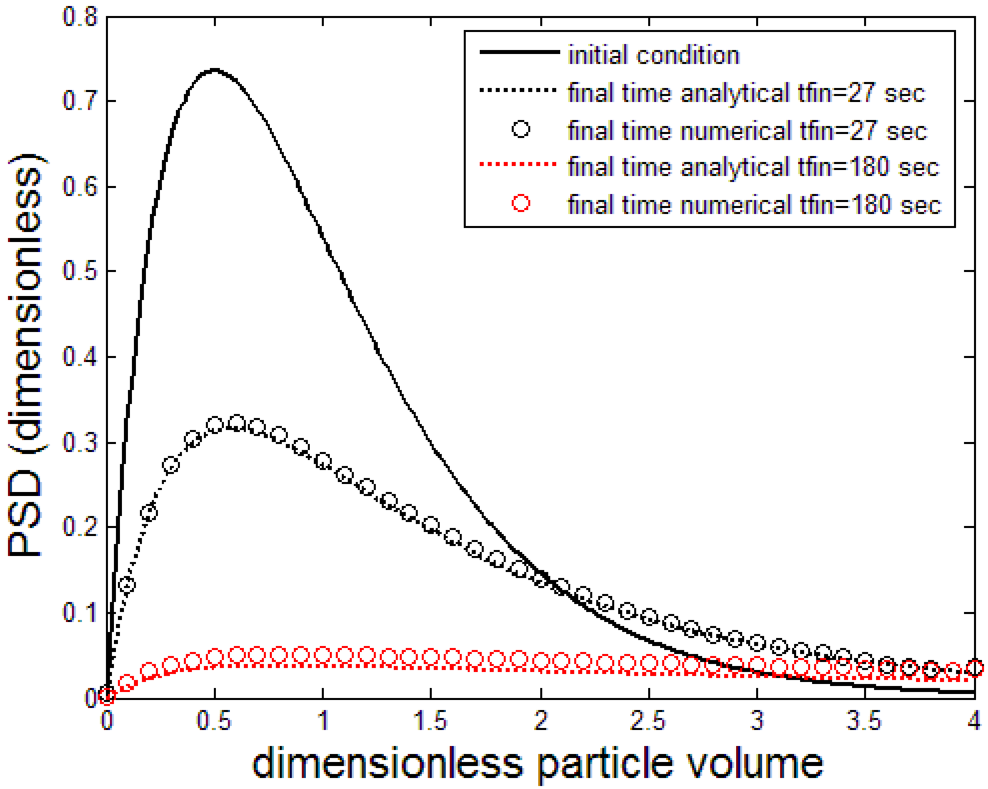
in 3), aggregation front moves at finite rate, unless mass conservation law breaks down

Aggregation: constant kernel $K=K_0$

Initial condition for PSD: Gaussian-like distribution

$$\overline{f} = \left(\frac{v_{\max}}{v_{av}}\right) \cdot \frac{(\upsilon+1)^{(\upsilon+1)}}{\Gamma(\upsilon+1)} \cdot \left(\frac{v}{v_{av}}\right)^{\upsilon} \cdot \exp\left[-\frac{v}{v_{av}} \cdot (\upsilon+1)\right]$$

$$\upsilon = 1, v_{av} = 4.189 \cdot (10)^{-15}\ \mathrm{m}^3, K_0 = 1.8 \cdot (10)^{-10}\ \frac{\mathrm{m}^3}{\mathrm{s}}, \left(\frac{v_{\max}}{v_{av}}\right) = 4, N_{in} = \frac{(10)^9}{4.189}\ \frac{\text{particles}}{\mathrm{m}^3}$$



For finite Smoluchowski equation:

- *Number of moments = 8*
- *Increasing the ratio* $\left(\frac{v_{\max}}{v_{av}}\right)$ *it converges to the solution of the Smoluchowski equation*

For Oort-Hulst equation:

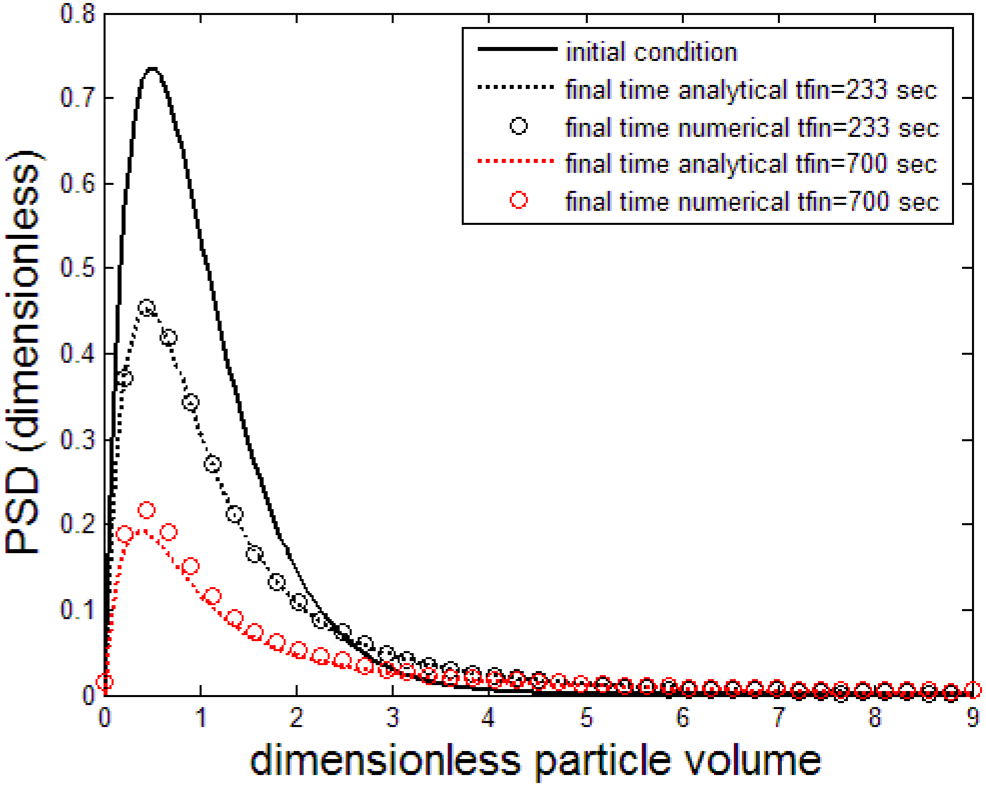
- *Number of moments = 10*
- *Aggregation front can be tracked*

Aggregation: sum kernel $K=K_0*(v+v')$

Initial condition for PSD: Gaussian-like distribution

$$\overline{f}=\left(\frac{v_{\max}}{v_{av}}\right)\cdot\frac{(\upsilon+1)^{(\upsilon+1)}}{\Gamma(\upsilon+1)}\cdot\left(\frac{v}{v_{av}}\right)^{\upsilon}\cdot\exp\left[-\frac{v}{v_{av}}\cdot(\upsilon+1)\right]$$

$$\upsilon=1, v_{av}=4.189\cdot(10)^{-15}\,\mathrm{m}^3, K_0=1.53\cdot(10)^3\,\frac{1}{\mathrm{s}}, \left(\frac{v_{\max}}{v_{av}}\right)=9, N_{in}=\frac{(10)^9}{4.189}\frac{\text{particles}}{\mathrm{m}^3}$$



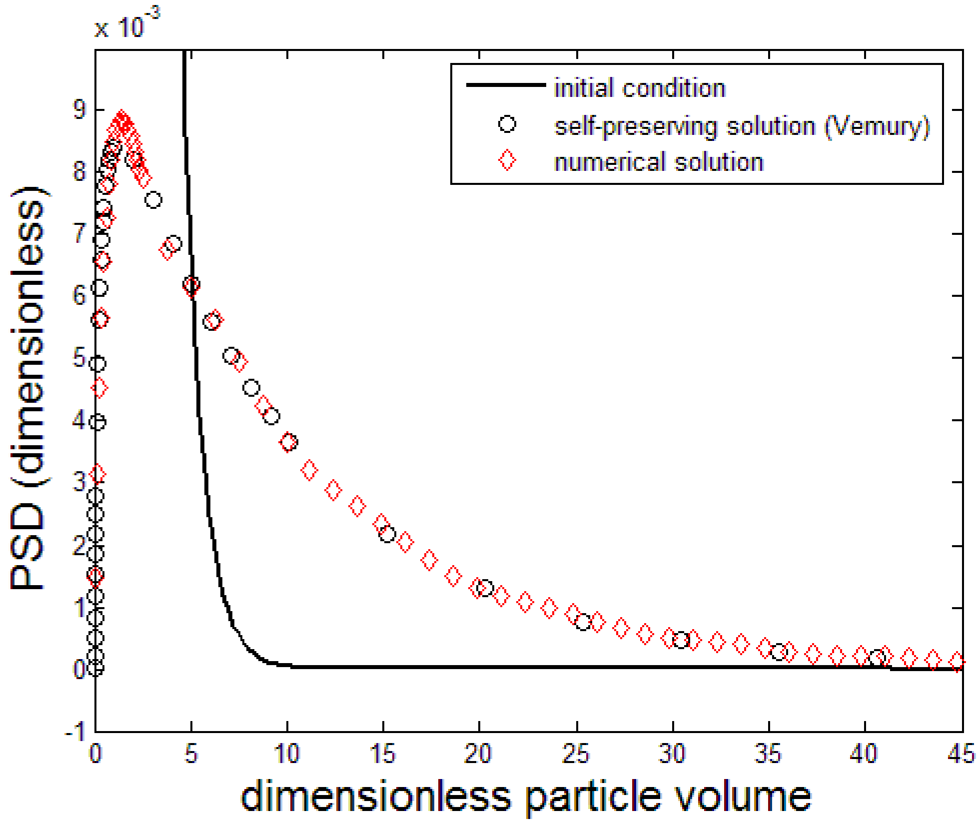
For finite Smoluchowski equation:

- *Number of moments = 12*
- *Increasing the ratio $\left(\frac{v_{\max}}{v_{av}}\right)$ it converges to the solution of the Smoluchowski equation*

Aggregation: Smoluchowski Kernel - Continuum Regime

$$K = \frac{2 \cdot T \cdot K_{BOLTZ}}{3 \cdot \mu} \cdot \left[2 + \left(\frac{v_i}{v_j} \right)^{\frac{1}{3}} + \left(\frac{v_j}{v_i} \right)^{\frac{1}{3}} \right]$$

Initial condition for PSD: Exponential distribution

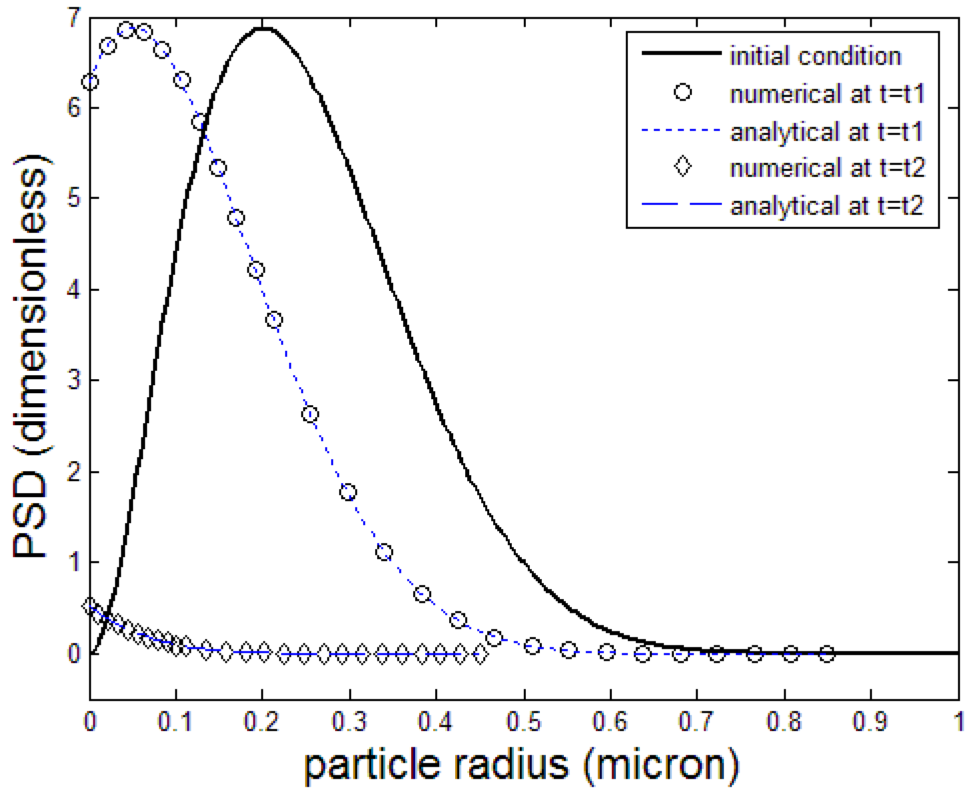


For finite Smoluchowski equation:

- *Increasing the ratio $\left(\frac{v_{\max}}{v_{av}}\right)$ it converges to the solution of the Smoluchowski equation*
- *With Smoluchowski kernel, $\left(\frac{v_{\max}}{v_{av}}\right)$ must be high (50)*

Particle Dissolution

Constant dissolution rate, 10 moments



1) *Solution with other MOM is problematic for particle dissolution*

2) *Even in this case, results are excellent with FCMOM*

PBE in In-homogeneous Conditions

Assumption: convective velocity not dependent on particle size (internal variable)

0 0

$$\frac{\partial f(\xi,t,\mathbf{x})}{\partial t}+\frac{\partial v_{p,j}(t,\mathbf{x})\cdot f(\xi,t,\mathbf{x})}{\partial x_j}-\frac{\partial}{\partial x_j}\left[D_{pt}(\xi,t,\mathbf{x})\cdot\frac{\partial f(\xi,t,\mathbf{x})}{\partial x_j}\right]=-\frac{\partial G(\xi,t,\mathbf{x})\cdot f(\xi,t,\mathbf{x})}{\partial \xi}+B(\xi,t,\mathbf{x})-D(\xi,t,\mathbf{x})$$

Convection *Diffusion* *Growth* *Aggregation, Breakage*

$$\frac{\partial f(\xi,t,\mathbf{x})}{\partial t}+\frac{\partial v_{p,j}(t,\mathbf{x})\cdot f(\xi,t,\mathbf{x})}{\partial x_j}-\frac{\partial}{\partial x_j}\left[D_{pt}(\xi,t,\mathbf{x})\cdot\frac{\partial f(\xi,t,\mathbf{x})}{\partial x_j}\right]=0$$

Convection *Diffusion*

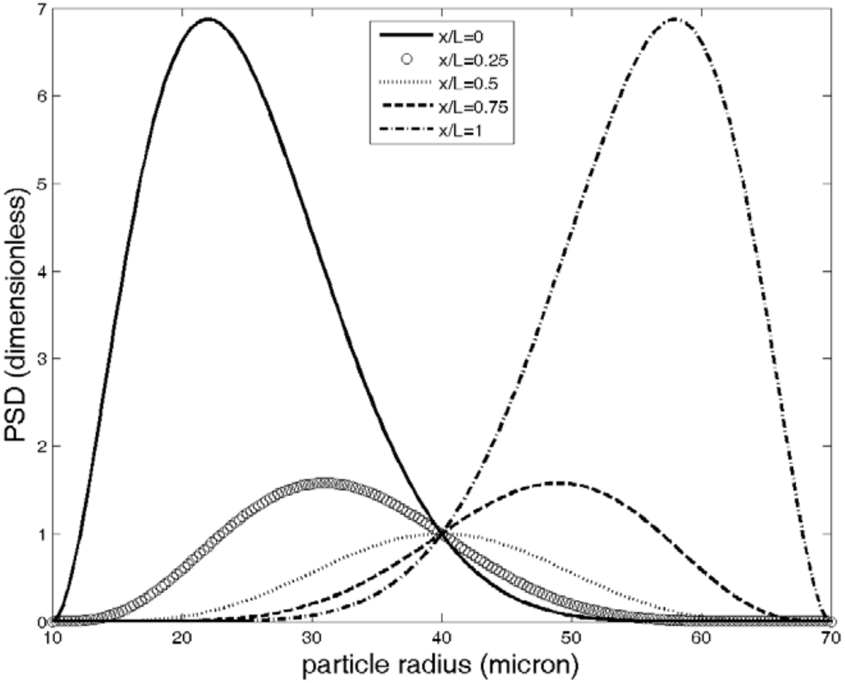
$$\frac{\partial \mu_i}{\partial t}+\frac{\partial v_{p,j}\cdot\mu_i}{\partial x_j}-\frac{\partial}{\partial x_j}\left[\int_{-1}^{1} D'_{pt}\cdot\frac{\partial \overline{f}'}{\partial x_j}\cdot\left(\overline{\xi}\right)^i\cdot d\overline{\xi}\right]=-\left(MB+MB_{conv}+MB_{diff1}+MB_{diff2}+MB_{diff3}\right)$$

Convection *Diffusion* *Moving Boundaries*

Ind Eng Chem Res, Solution of PBE by the FCMOM for In-homogeneous systems, DOI: 10.1021/ie901407x.

Size-Independent Diffusivity

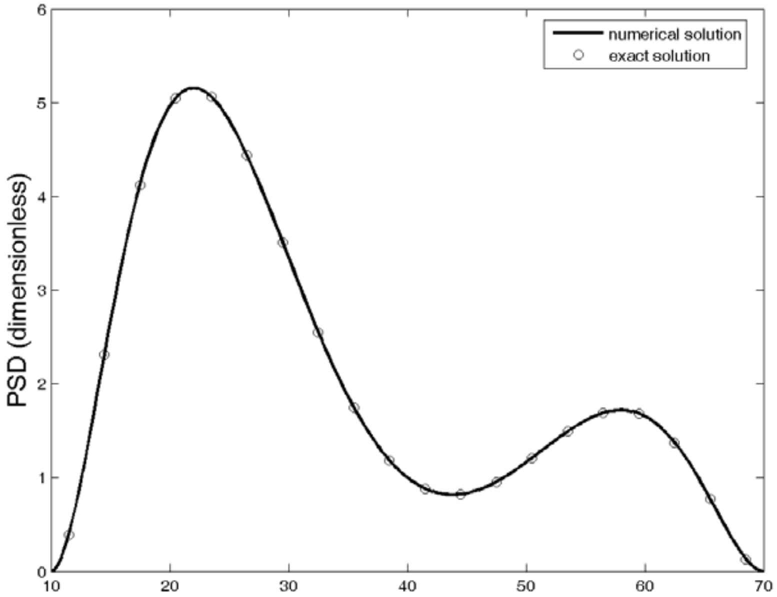
$$D_{pt} = D_{ft} \approx 10^{-3}\,\frac{\mathrm{m}^2}{\mathrm{s}}$$



No need of closure

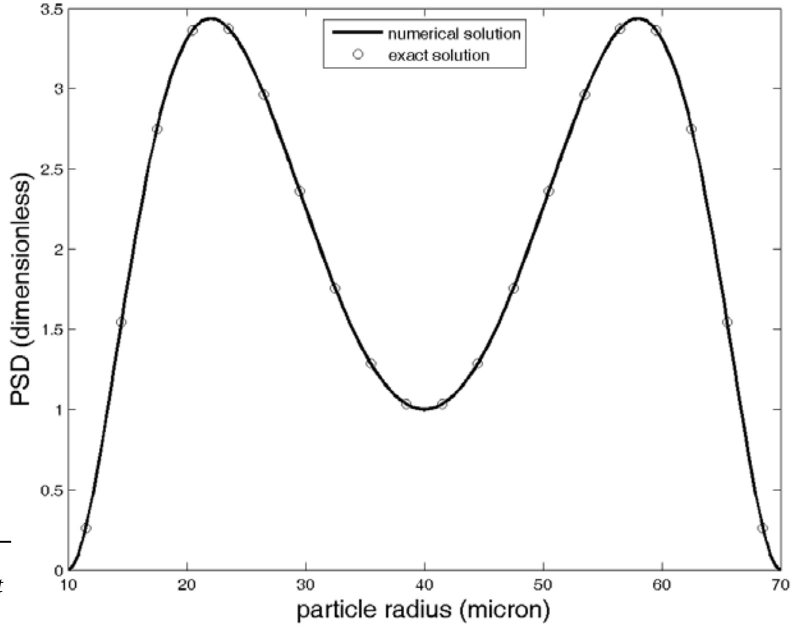
$$\frac{x}{L} = 0.25$$

$$t_{final} = \frac{L^2}{D_{ft}}$$



$$\frac{x}{L} = 0.5$$

$$t_{final} = \frac{L^2}{D_{ft}}$$



Size-Dependent Diffusivity: Closure Problem

Tchen's theory

$$D_{pt}(\xi) = D_{ft} \cdot \frac{1 + b^2 \cdot \frac{\tau_p}{T_L}}{1 + \frac{\tau_p}{T_L}}$$

$$\tau_p = \frac{\left(2 \cdot \frac{\rho_p}{\rho_f} + 1\right) \cdot (2 \cdot \xi)^2}{36 \cdot \nu_t}$$

$$T_L \cong 0.8 \cdot \frac{k_t}{3 \cdot \varepsilon_t}$$

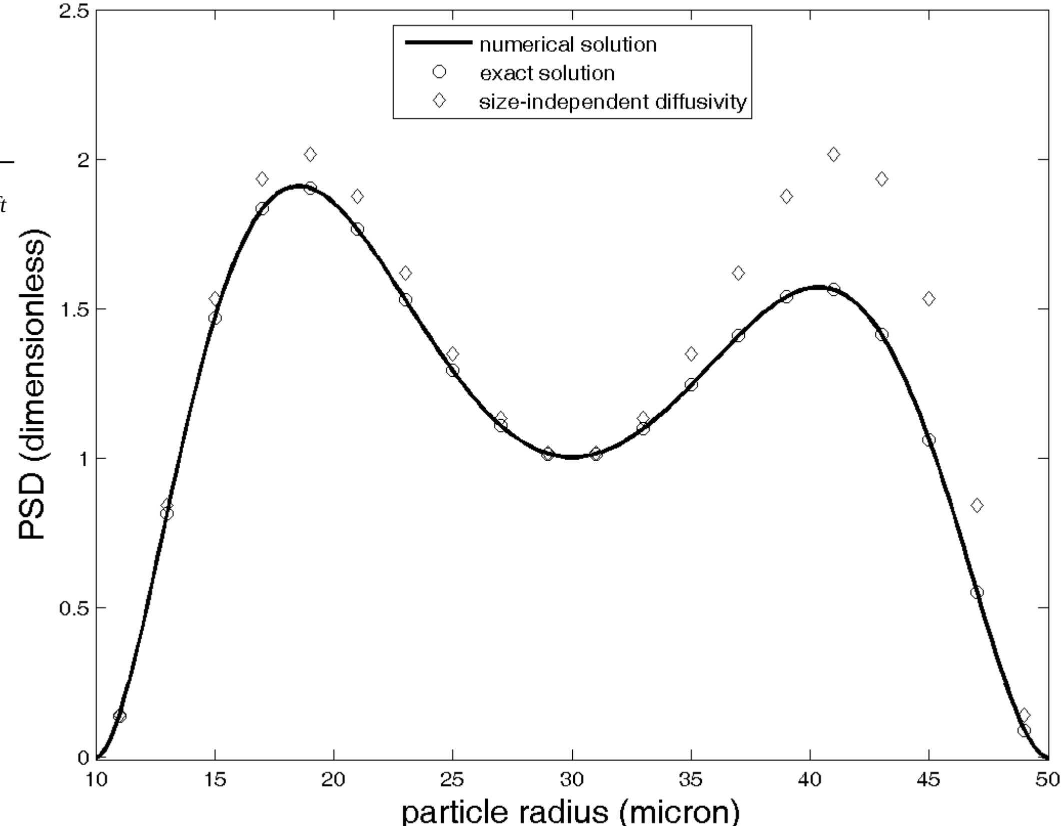
$$b = \frac{3}{2 \cdot \frac{\rho_p}{\rho_f} + 1}$$

$$D_{ft} \approx 10^{-3} \frac{\text{m}^2}{\text{s}}$$

$$\frac{x}{L} = 0.5$$

$$t = \frac{1}{10} \cdot \frac{L^2}{D_{ft}}$$

Closure problem solved correctly



Convection:Axial Effects vs PSD at Inlet

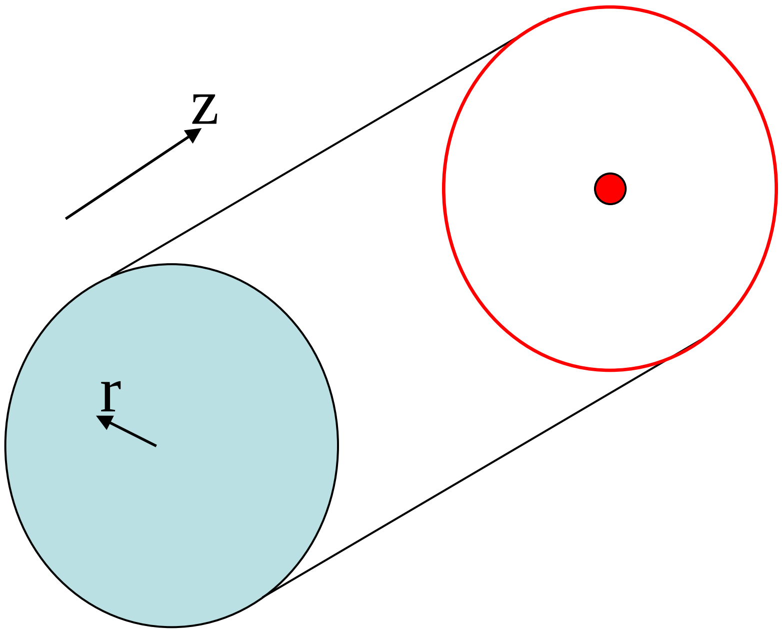
Dilute Gas Solid Pipe Flow (Laminar Flow); r-z coordinates.

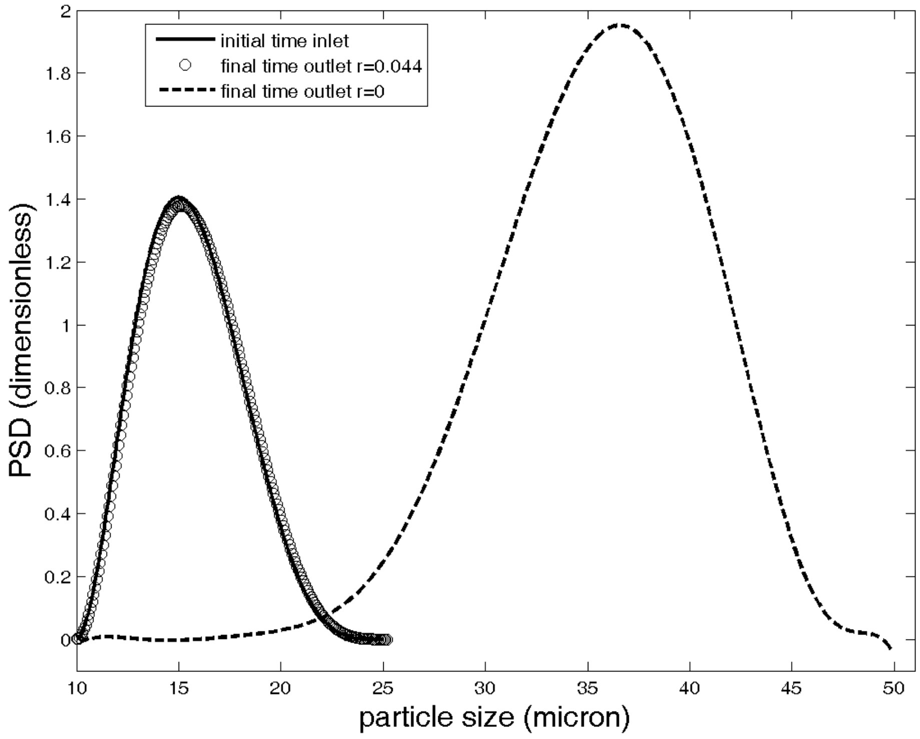
Light particles follow the gas flow.

The PSD at the inlet is switched after that the gas-phase reaches steady-state.

Initial and inlet PSD are radially uniform.

$$t_{final} = \frac{L}{v_{g,\max}}$$



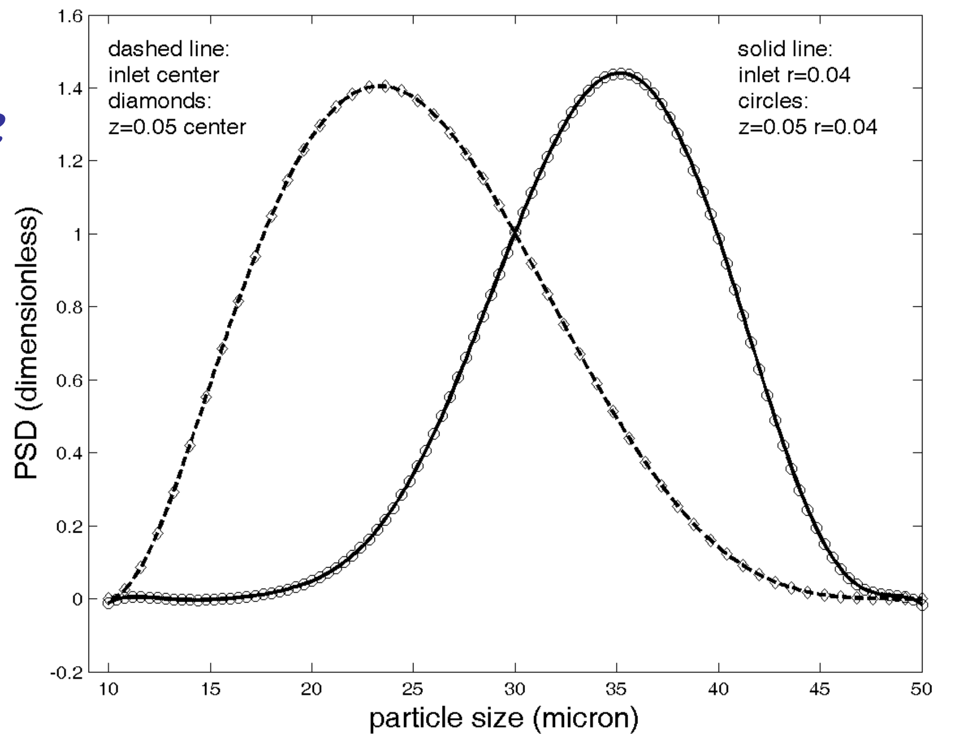


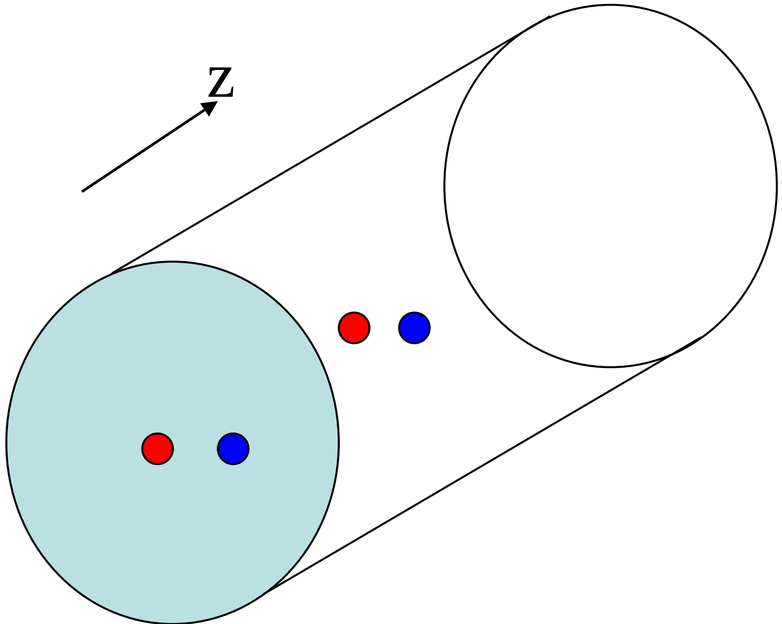
Convection-Radial Effects

Initial = inlet PSD: both are the same and not uniform radially

Gas in Steady State Conditions.

Radial components of the velocity are zero.

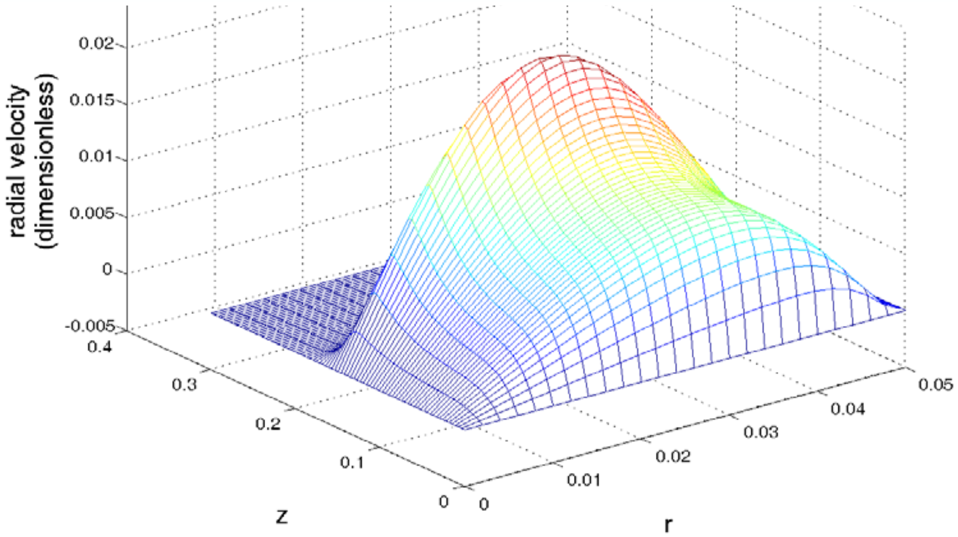




$$\frac{\partial \xi_{\max}}{\partial t} = \underset{i=x,y,z}{\mathrm{Sum}}\left(-\frac{\partial \xi_{\max}}{\partial x_i} \cdot u_{p,i,\max} \right)$$

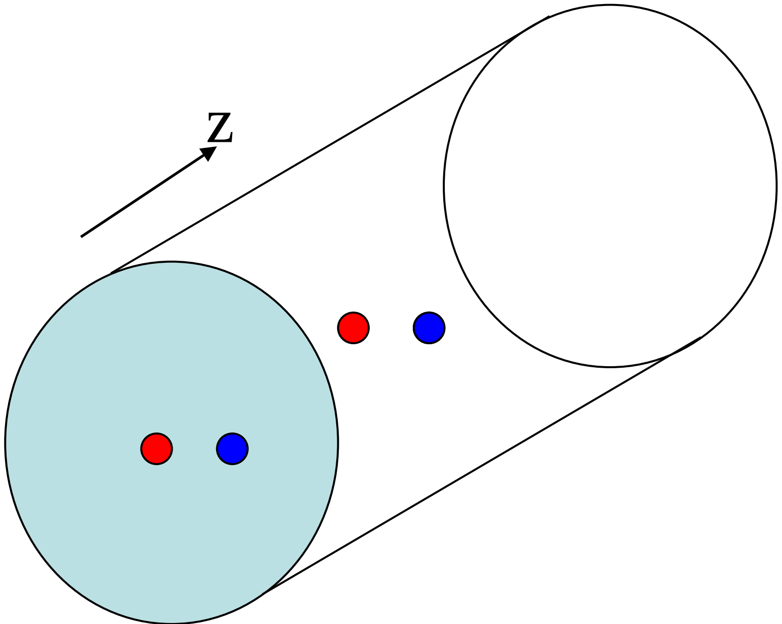
$$\frac{\partial \xi_{\min}}{\partial t} = \underset{i=x,y,z}{\mathrm{Sum}}\left(-\frac{\partial \xi_{\min}}{\partial x_i} \cdot u_{p,i,\min} \right)$$

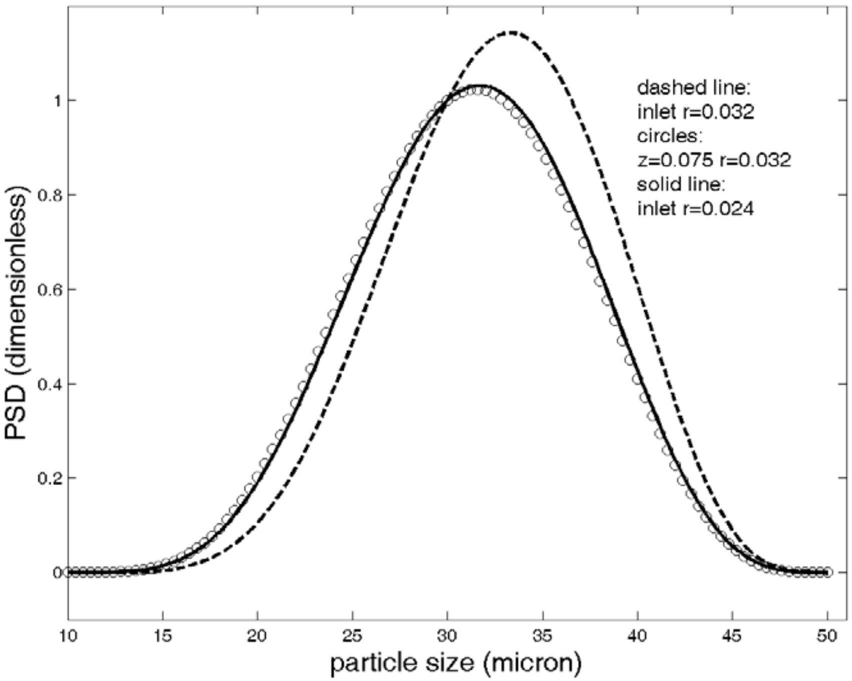
Convection- Radial Effects in Unsteady Conditions



Un-Steady State Conditions.

Radial components of the velocity are not-zero.





Conclusions (PBE)

1. *FCMOM for PBE: efficient algorithm (low computational effort); provides accurate PSD reconstructions.*
2. *Ready for CFD applications (high temperature CO_2 capture processes using magnesium oxide sorbents; particle porosity is the internal variable)*
3. *In multivariate applications: the domains are always well defined.*
4. *Finishing touches: a) size-dependent convective velocity; b) PSD first derivative convergence*

2-D Boltzmann Equation

$$\frac{\partial f_c}{\partial t} + \frac{\partial \mathbf{c} \cdot f_c}{\partial \mathbf{x}} + \frac{\partial \mathbf{F_{tot}} \cdot f_c}{\partial \mathbf{c}} = \left(B - D\right)_{coll}$$

Particle velocity   *F_{tot} external forces*   *Collisions*

Terms of B-D (due to collisions) are:

$$B = \int\limits_{\mathbf{g}\bullet\mathbf{k}>0} \int \left[\frac{1}{e^2} \cdot f_c\left(\mathbf{c}', \mathbf{x}, t\right) \cdot f_c\left(\mathbf{c}_1', \mathbf{x}, t\right)\right] \cdot D_P \cdot \left(\mathbf{g} \cdot \mathbf{k}\right) \cdot d\mathbf{k} \cdot d\mathbf{c_1}$$

$$D = \int\limits_{\mathbf{g}\bullet\mathbf{k}>0} \int \left[f_c\left(\mathbf{c}, \mathbf{x}, t\right) \cdot f_c\left(\mathbf{c_1}, \mathbf{x}, t\right)\right] \cdot D_P \cdot \left(\mathbf{g} \cdot \mathbf{k}\right) \cdot d\mathbf{k} \cdot d\mathbf{c_1}$$

D_P = particle diameter; $\mathbf{g}$ = relative velocity; $\mathbf{k}$ = unit vector

e = restitution coefficient; $\mathbf{c_1}$ = second particle velocity;

$\mathbf{c}', \mathbf{c}_1'$ = post collision velocities

2-D Boltzmann equation is a bi-variate PBE, in which:

- *Internal variables are particle velocities and, therefore, the "growth rates" are the external forces F_{tot}*

Limits and dimensionless numbers

Kn (Knudsen):

- *High Kn – dilute conditions: Closure, Convection*
- *Low Kn – collision dominated: Normal Solutions, Collision integrals.*

M (Mach number):

- *Subsonic/supersonic*
- *Discontinuities*

Other "layers":

- *Boundary Layer (Bimodal distributions)*
- *Initial layer*

High Knudsen – Closure Problem

$$\frac{\partial f_c}{\partial t} + \frac{\partial \mathbf{c} \cdot f_c}{\partial \mathbf{x}} = 0 \quad \Rightarrow \quad \frac{\partial \mu_i}{\partial t} + \frac{c_{1,h} - c_{1,l}}{2} \cdot \frac{\partial \mu_{i+1}}{\partial \mathbf{x}} = 0$$

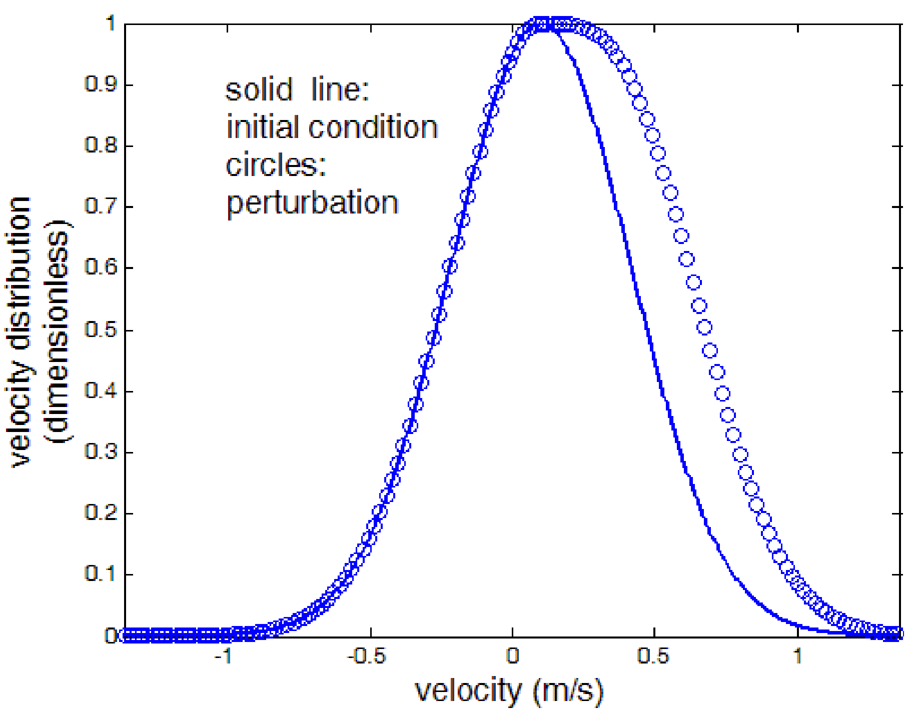
Not moving boundaries

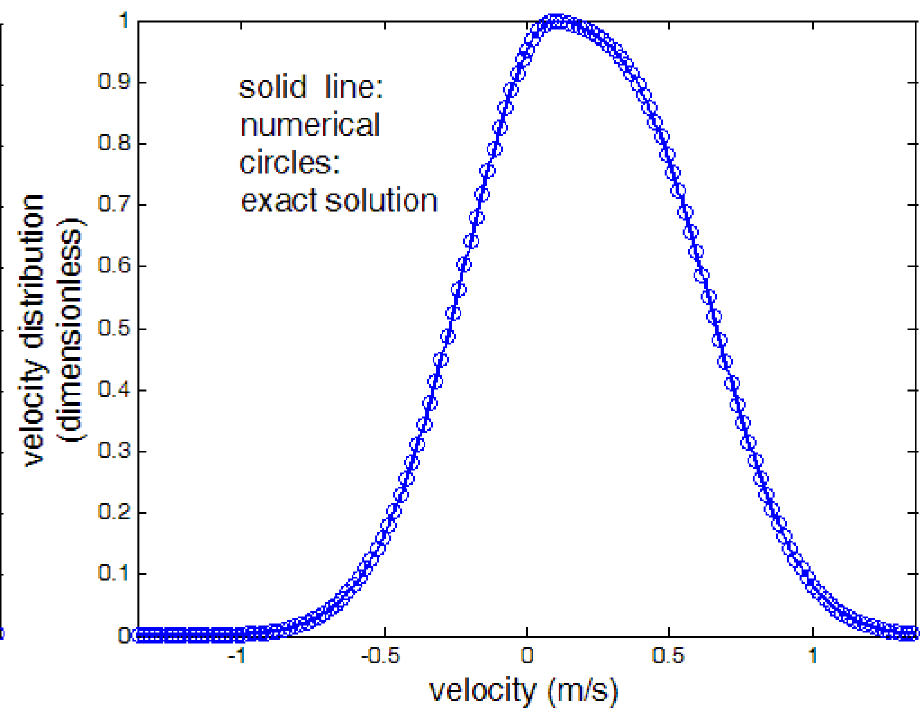
A ———— B

(perturbation)

1-D

Granular system (low Mach)





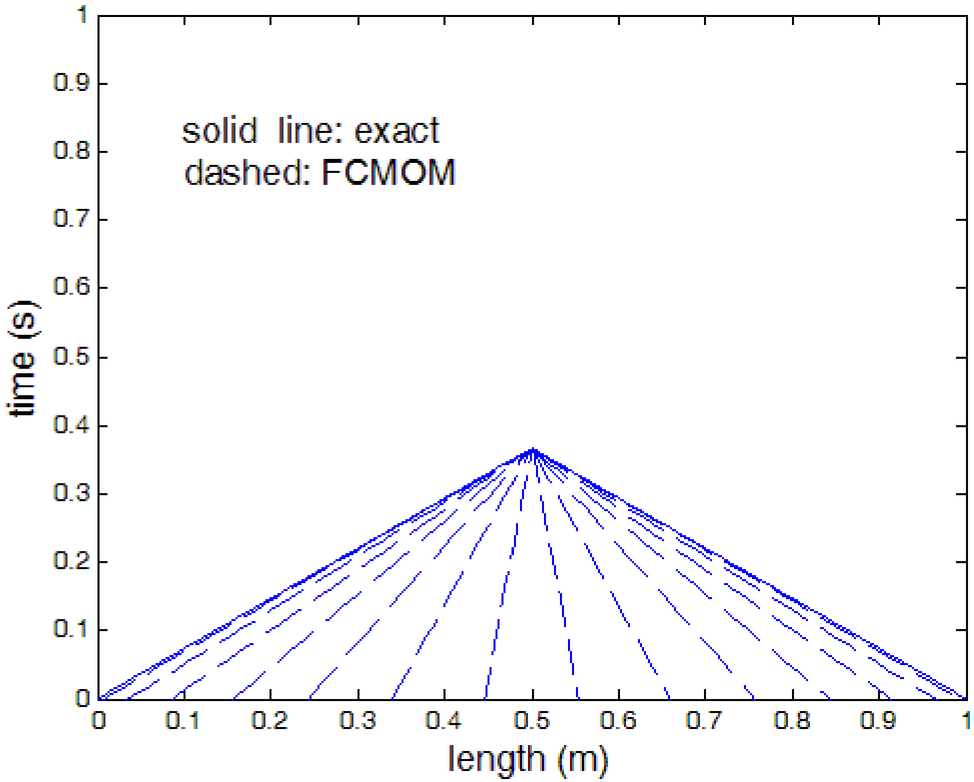
Hyperbolic Structure

$$\frac{\partial \mu_i}{\partial t} + \frac{c_{1,h} - c_{1,l}}{2} \cdot \frac{\partial \mu_{i+1}}{\partial x} = 0 \ + \ \text{FCMOM Closure}$$ ⇒ *Boundaries not moving: linear hyperbolic system*

- *In general, non-linear hyperbolic system with sources (collision integrals and external forces)*
- *Finite Signals-Finite Velocities*
- *Well-posed problem*
- *Hyperbolic systems numerics (based on characteristics): Godunov method, Riemann problem*
- *Spatial discontinuities*

Domain of Dependence

Granular system (low Mach)

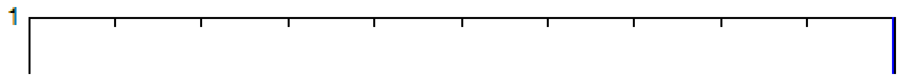


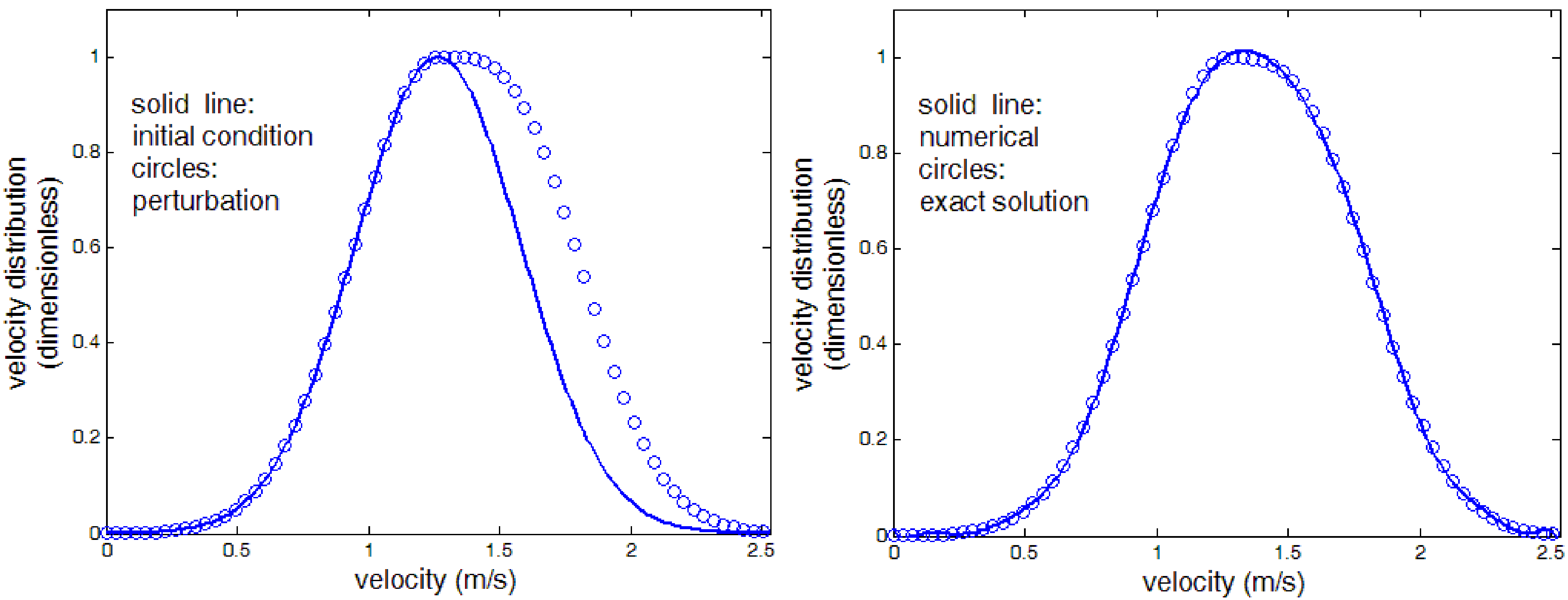
CFL condition

Closure correct if the domain of dependence is correct

High Mach numbers

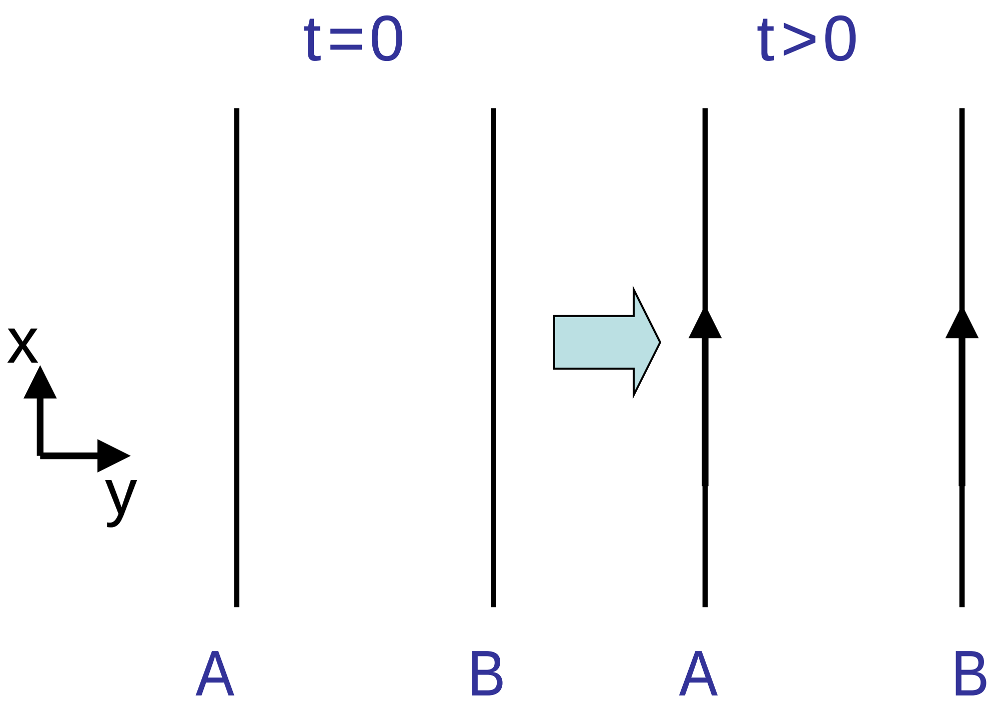
Granular system (high Mach)





Boundary conditions can be correctly set

Bivariate case: Start-up problem



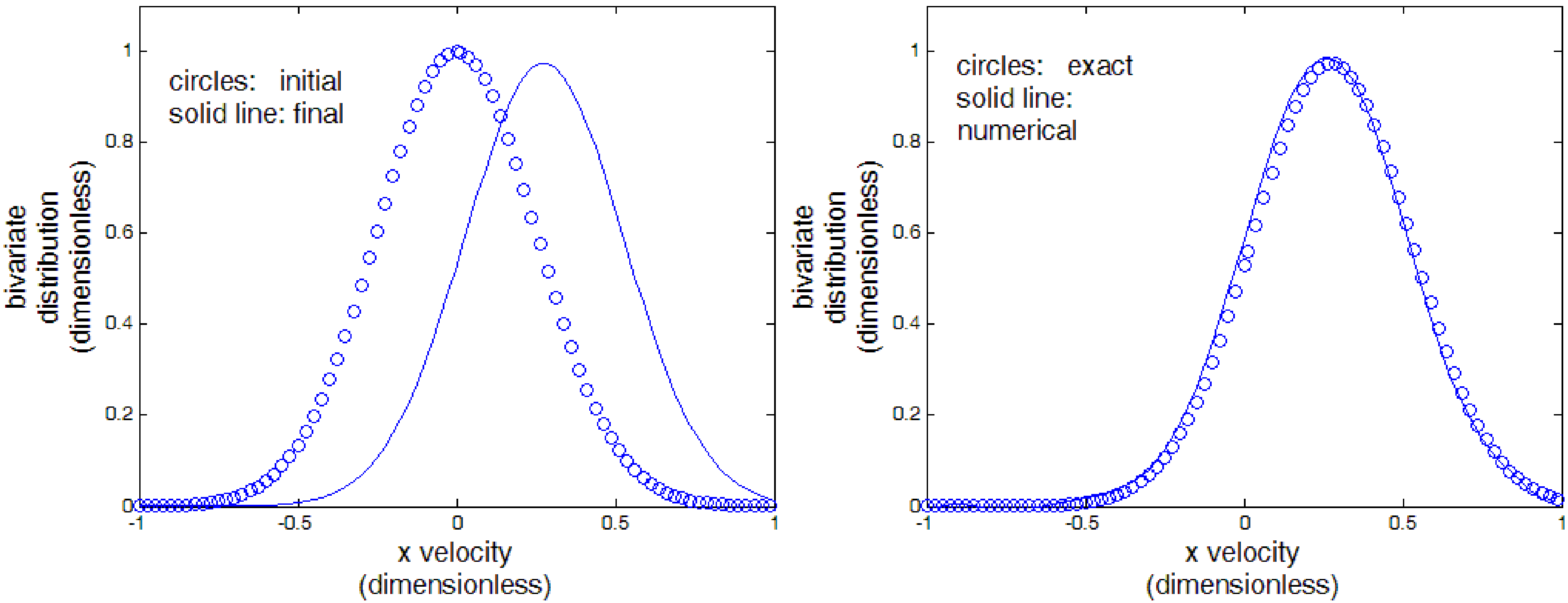
Infinite walls A and B move with velocity U_x

High Knudsen number (collisionless)

Diffuse reflection boundary conditions: the velocities reflected by the wall follow a Maxwellian distribution around U_x

Start-up problem: results

$$D_P = 100\mu,\ \text{Granular Temperature} \square\ 0.1\frac{m^2}{s^2}$$



Slice for c_y (velocity perpendicular to the walls)=0

A Finite Boltzmann Model

Homogeneous conditions

$$B = \int_{\mathbf{g}\bullet\mathbf{k}>0} \int \left[\frac{1}{e^2} \cdot f_c\left(\mathbf{c}', \mathbf{x}, t\right) \cdot f_c\left(\mathbf{c}_1', \mathbf{x}, t\right) \right] \cdot D_P \cdot \left(\mathbf{g}\square\mathbf{k}\right) \cdot d\mathbf{k} \cdot d\mathbf{c}_1$$

$$\frac{\partial f_c}{\partial t} = \left(B - D\right)_{coll}$$

$$D = \int_{\mathbf{g}\bullet\mathbf{k}>0} \int \left[f_c\left(\mathbf{c}, \mathbf{x}, t\right) \cdot f_c\left(\mathbf{c}_1, \mathbf{x}, t\right) \right] \cdot D_P \cdot \left(\mathbf{g}\square\mathbf{k}\right) \cdot d\mathbf{k} \cdot d\mathbf{c}_1$$

1. Classical Boltzmann Model (CBM): particles of any velocity range can collide and are obtained by collisions.
2. Finite Boltzmann Model (FBM): a finite domain is defined. Particles of any velocity range can be produced but not all the collisions are possible: collisions creating particle velocities larger than the maximum velocity are neglected.

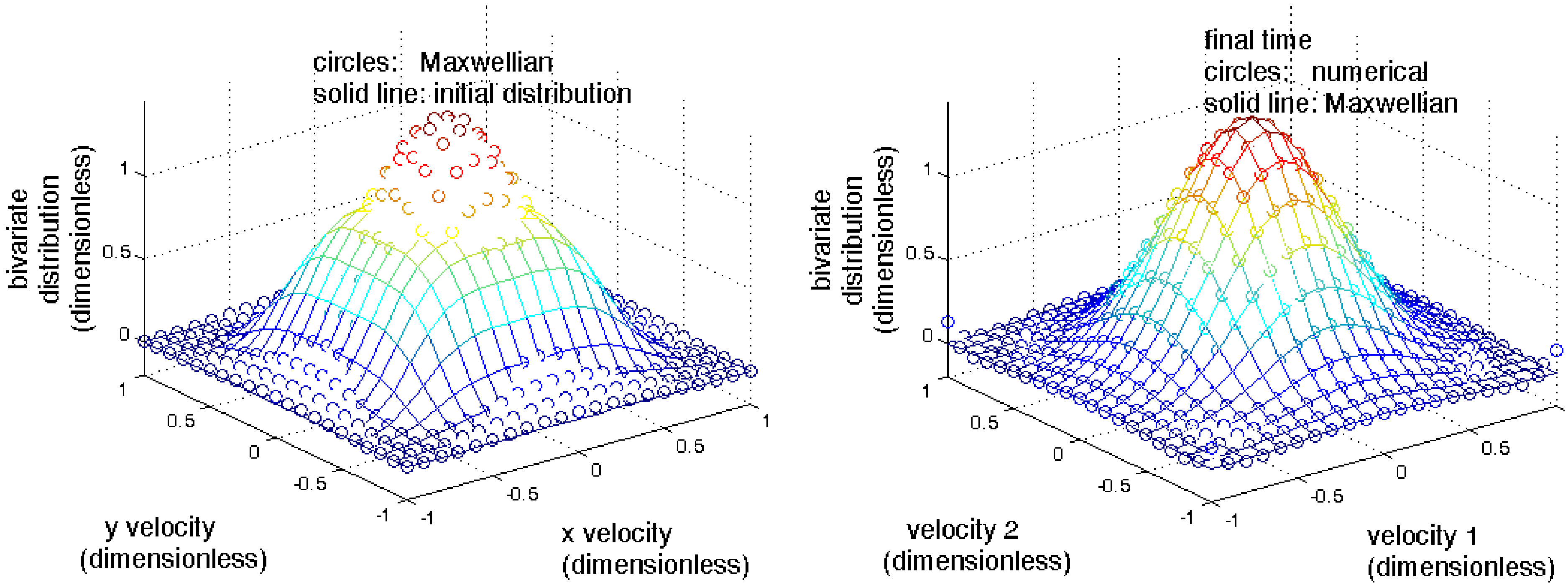
Increasing the finite domain, the solution of the FBM converges to the solution of the CBM

Solutions in Homogeneous Conditions

1. Elastic Particles: the system relaxes to the Maxwellian state (from an initial condition which can be not-Maxwellian).
2. Inelastic Particles: after sufficiently long times, the system approaches the Homogeneous Cooling State solution (for 2-D systems: Brey, Cubero, Ruiz-Montero, Physical Review E, 59 (1), 1256-1258, 1999).

Relaxation to the Equilibrium State (Elastic Particles)

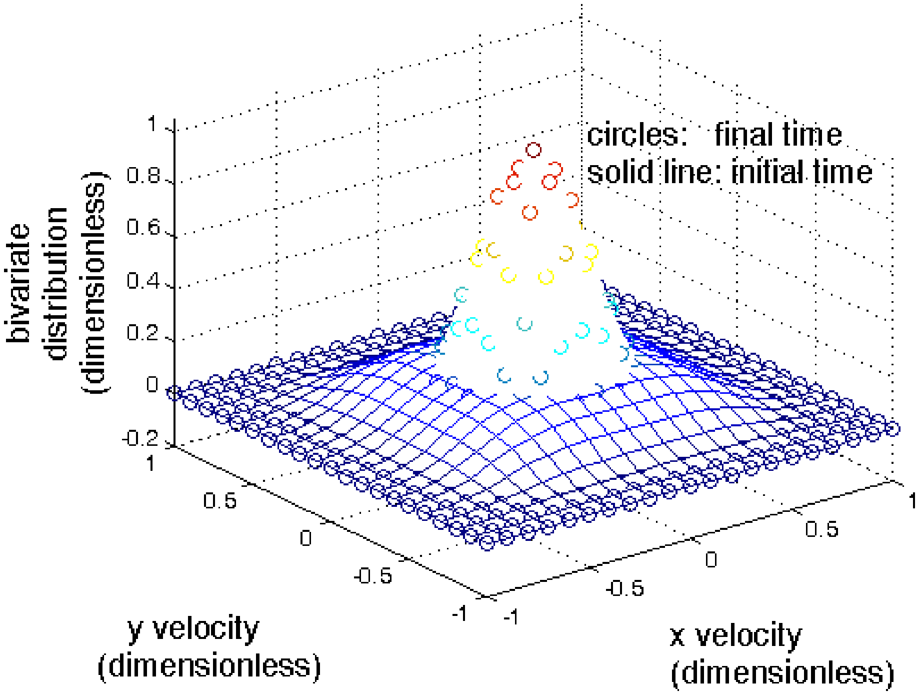
$D_P = 100\mu$, Granular Temperature $\approx 0.2\frac{m^2}{s^2}$

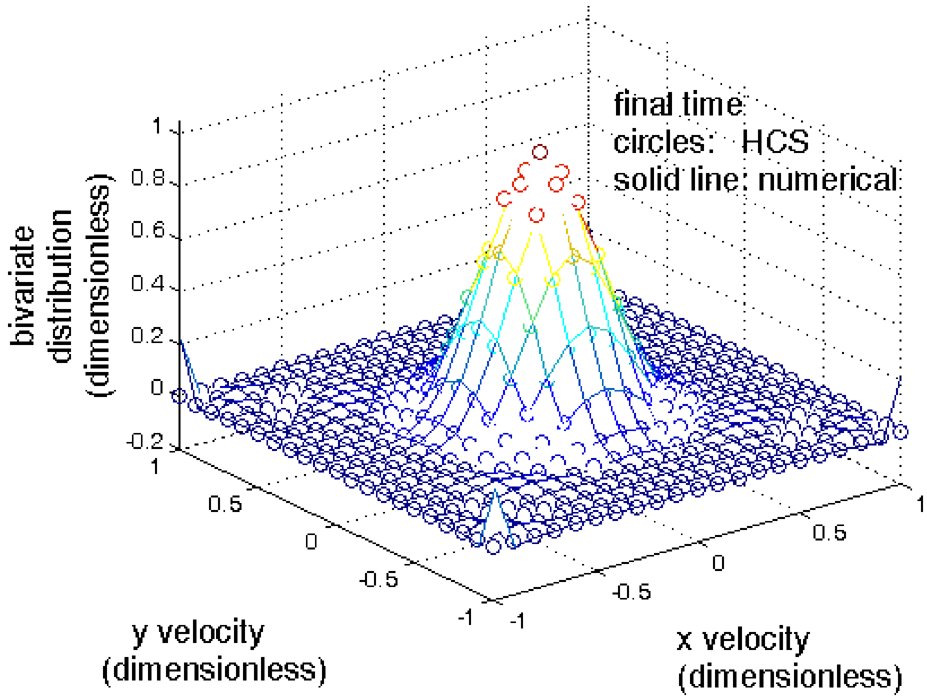


Good agreement with the exact solution with moments up to 10th order (high energy tails to be improved increasing the number of moments and/or with different trial functions)

HCS Solution (Inelastic Particles)

$D_P = 100\mu$, Initial Granular Temperature □ $0.2\frac{m^2}{s^2}$, Restitution coefficient □ 0.95





Solution approaches the exact solution, but there are oscillations in the reconstruction.

BE needs to be rescaled -sqrt(T)- before applying the FCMOM

Conclusions (KE) and Acknowledgements

1. FCMOM for kinetic theory: still efficient, accurate reconstructions and well defined domains.
2. In kinetic theory: particle velocity distribution convergence, hyperbolic structure, well posed problem, closure.
3. Different regimes: high/low Knudsen numbers, subsonic/supersonic, boundary layers, discontinuities.
4. Future plan: high energy tails reconstruction must be improved (especially in HCS solution); investigation of moving boundaries/non-linearities; 3-D BE.

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