Computational Aerosol Transport

Aerosol Phase Space Tracking to Predict Size-Specific Concentration Distribution and Deposition in Space and Time

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Overview

- Aerosol characterization
- The transport equation
- Simulation of coagulation and deposition
- Simulation of dynamic aerosol transport in confined space + validation of code
- Applications
  - Design of portable wireless aerosol detector
  - Transport in the lung

Introduction

Definition and Characterization of Aerosols

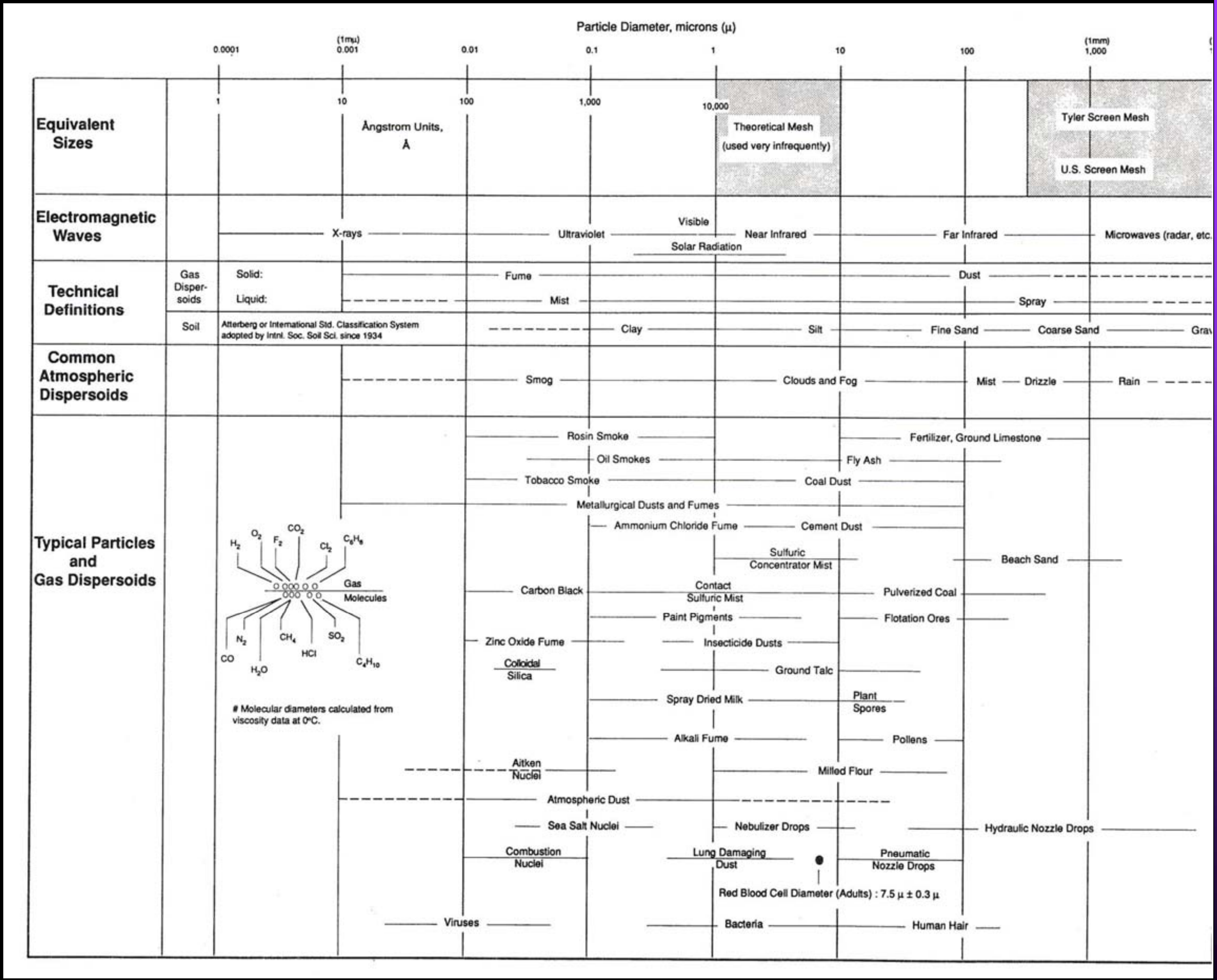
- Definition of Aerosol
  - A colloidal system of fine solid or liquid particles suspended in gas
- Size, Concentration
  - Diameter of particles ranges from 10^{-9} to 10^{-3} m
  - Typical concentration in air is 10^{3} (clean air) to 10^{5} (polluted air) [particle/cc]

- Characterization
  - Volume concentration [μm^3/cc]
  - Mass concentration [μg/cc]
  - Number concentration [particles/cc]
  - Surface concentration [μm^2/cc]
- Volume distribution as property of interest
  - Conserved quantities are easier to treat when solving the transport equation
  - But, large variation in magnitude (~20 orders)

Applications

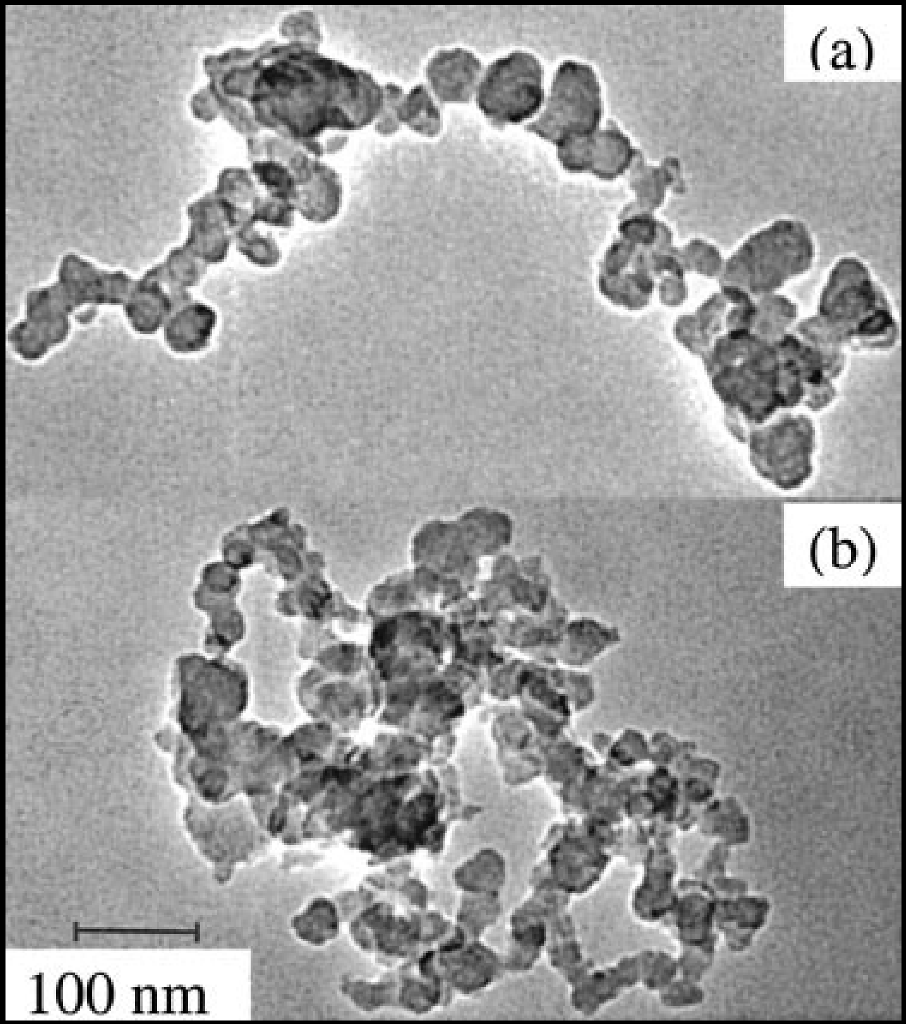
- Homeland Security
  - NBC aerosol dispersion in confined and open spaces
- Nuclear Safety
  - Understanding aerosol evolution and transport is critical importance in estimating and controlling nuclear accidents.
- Indoor Air Quality
  - Air pollutants such as radon, radon daughter product, volatile organic compounds can easily attach to aerosol particles and inhalation of those may cause significant health hazard.
- Atmospheric Science
  - The formation of fog and cloud, ozone depletion and solar-radiative interactions depend strongly on particulate generation and transport process
- Aerosol Medicine and Toxicology
  - Systemic and local delivery of therapeutic and imaging agents

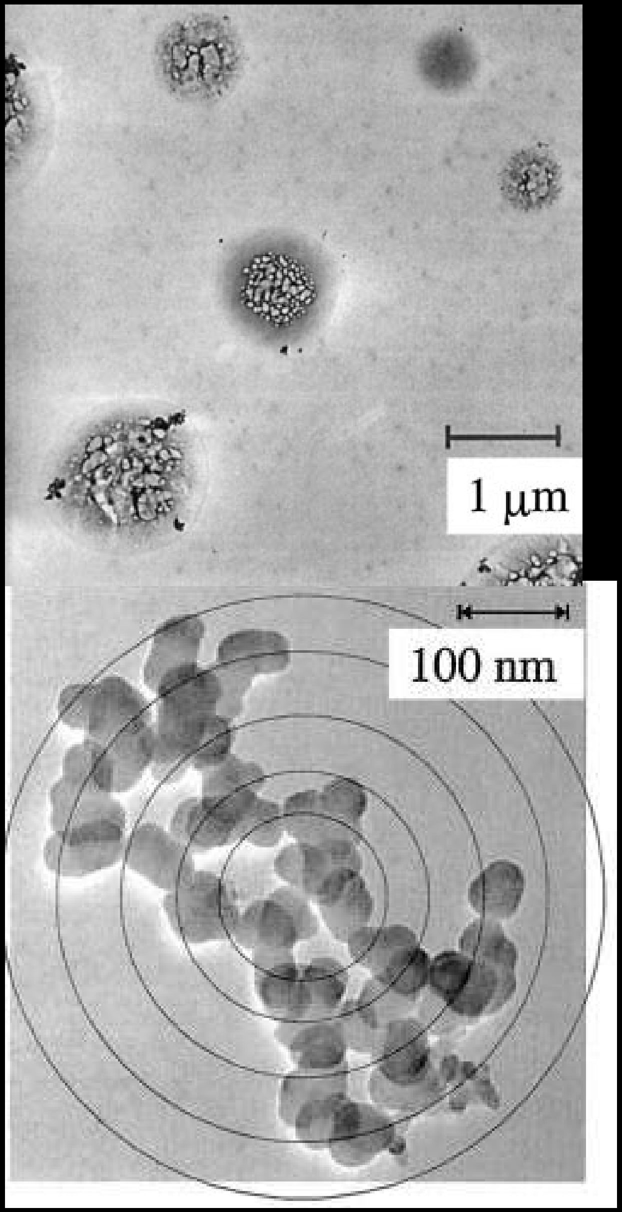
The Aerosol Size Spectrum



Particle Morphology

coagulation





Courtesy of C Xiong and SK Friedlander, UCLA

Transport Phenomena

- Convective transfer
- Diffusion
- Deposition, resuspension
- Thermophoresis
- Electrophoresis
- Sedimentation (gravitational settling)
- Coagulation
- Condensation, evaporation

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Problem Statement for Aerosol Transport

- Aerosol spectrum changes *en route*
  - Especially near-field
- Significant aerosol physics far field
  - Phoretic effects, condensation, evaporation, gravitational settling, deposition, etc.
- Intricate thermal-hydraulics
- Low air velocities but high gradients
- No current comp. model considers all

Current Aerosol Models

- Confined spaces
  - CONTAM / COMIS: simple mass balance with well-mixed hypothesis, no aerosol dynamics.
  - MAEROS: coagulation with geometric constraint, homogeneous turbulence, no transport.
- Outdoors
  - HPAC: size specific deposition and removal but no dynamics. Deposition via dep. velocities.
- Dummy particles in all computational models except for MAEROS

Objective

- Develop a comprehensive computational tool to predict the aerosol phase space n(v,**r**,t) using full physics
  - Based on first principles – Boltzmann Eq.
  - Coagulation treatment using sectional approach
  - Deposition handled via boundary layer theory
  - Convective and diffusive transport
  - Thermophoresis, electrophoresis
  - Condensation and evaporation
  - Confined or open atmospheres w/ obstructions
  - Time dependent source term, including $\delta(t-t_o)$

Aerosol Transport Equation

Distribution Function and Method of Solving the Transport Equation

Aerosol characterization

- Differential property: $$q(v,t) = \alpha\, v^{\gamma} n(v,t)$$
  - Volume concentration [(μm)³/cc]
  - Mass concentration [μg/cc]
  - Number concentration [particles/cc]
- Integral property: $$Q(t) = \int_0^{\infty} q(v,t)\,dv$$
- Number concentration is not conserved

Aerosol Distribution Function

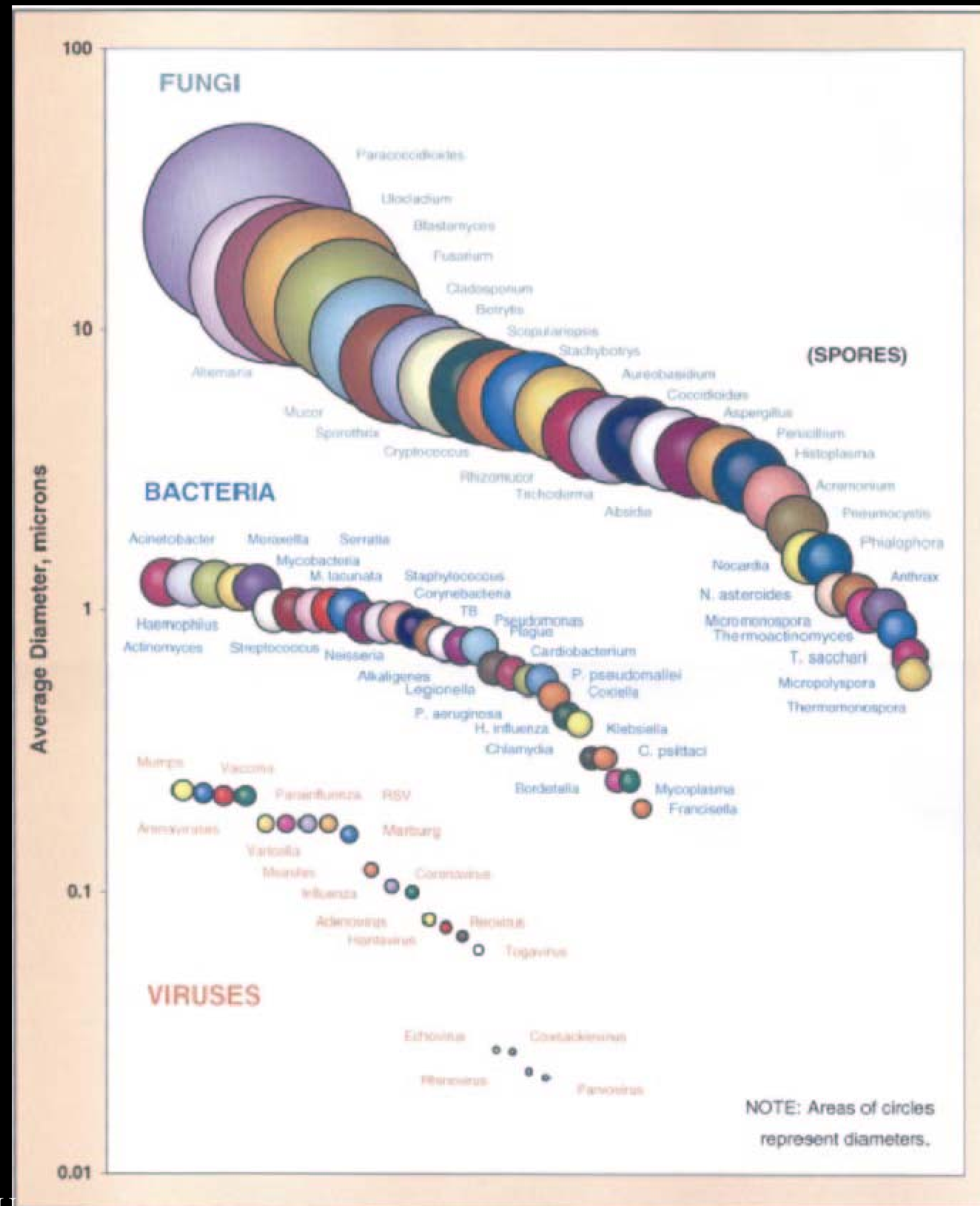
- Log-Normal Distribution Function

$$n(d) = \frac{N}{\sqrt{2\pi}\,\ln(\sigma_g)d} \exp\left[\frac{[\ln(d) - \ln(d_g)]^2}{2[\ln(\sigma_g)]^2}\right]$$

n(d)= number of particle per unit volume
at particle diameter d;
N = total number of particles;
d_g = median diameter of aerosol;
σ_g = geometric standard deviation.

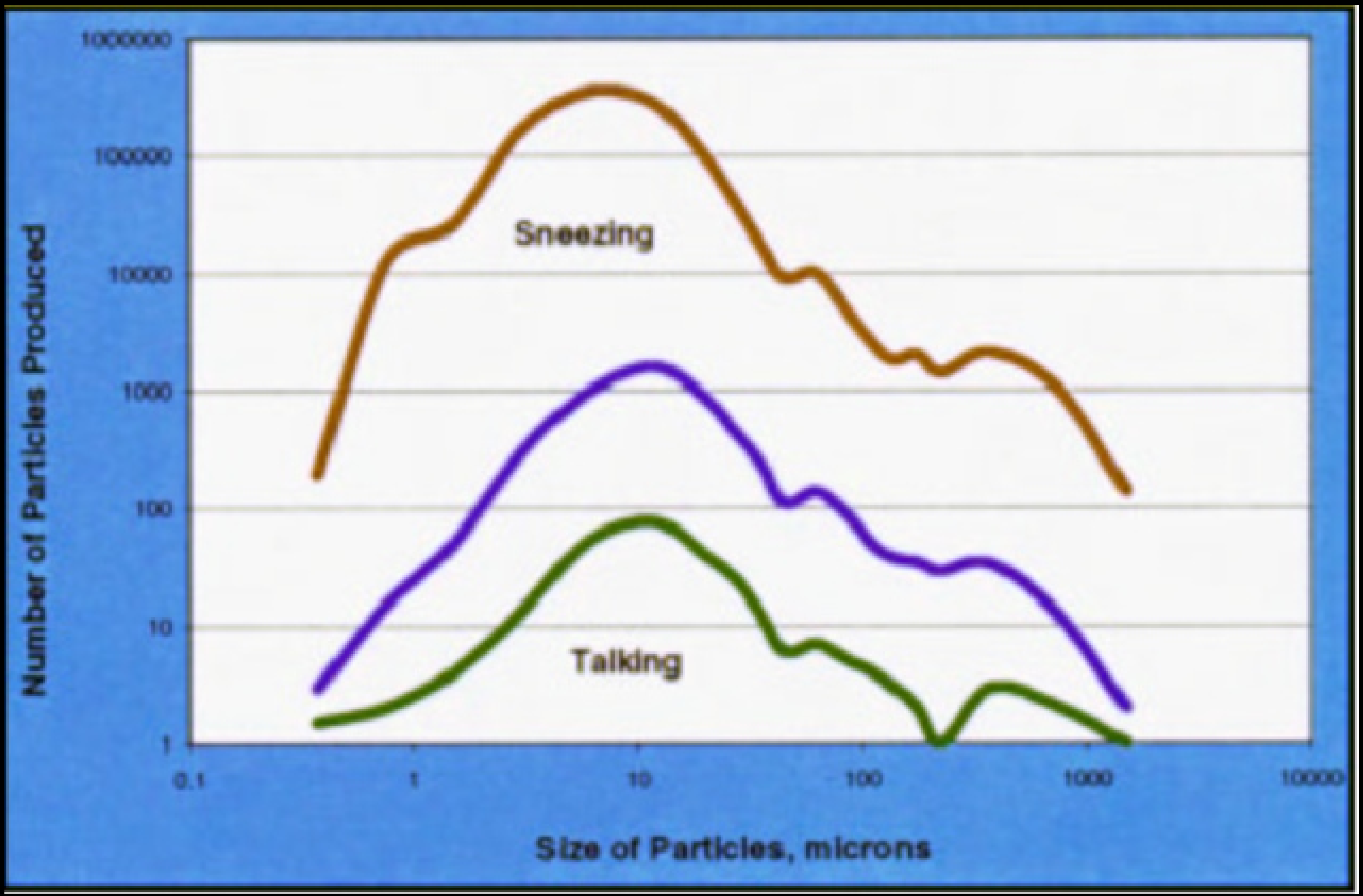
Bio-aerosols and Microbes

- Anthrax: 1.0 μ
- Corona virus: 0.1 μ
- Narrow distribution
  - σ_g = 1.02 to 1.05



Courtesy of WJ Kowalski and W Bahnfleth, Penn State U.

Respiratory Aerosol Generation



Courtesy of WJ Kowalski and W Bahnfleth, Penn State U.

Aerosol Transport Equation

$$\frac{\partial q(v,\vec{r},t)}{\partial t} + \nabla \cdot [\vec{U}(v,\vec{r},t) q(v,\vec{r},t)] - \nabla \cdot [D(v,\vec{r},t) \nabla q(v,\vec{r},t)]$$
$$+ \frac{\partial}{\partial v}[I(v,\vec{r},t) q(v,\vec{r},t)] = S(v,\vec{r},t) + \left(\frac{\partial q(v,\vec{r},t)}{\partial t} \right)_{coag}$$

U = velocity of aerosol

D = diffusion coefficient

I = rate of growth due to condensation and evaporation

S = independent source term

On to Coagulation

Method of Solution

- Treat coagulation using the sectional method; Coagulation appears as source.
- Solve coagulation under uniform mixing first.
- Reduce compartment size.
- Add convective transfer, sweep the domain
- Add phoretic effects, deposition, etc.
- Assumption: No slip in the convective term
- Neglected in this version:
  - Condensation & evaporation
  - Diffusion when convective velocity is large

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Coagulation

- Binary collision or many-body problem?
  - morphology
- Non-linear Integro-differential equation

$$\left(\frac{\partial n(v,t)}{\partial t}\right)_{coag} = \frac{1}{2}\int_0^v du K(u,v-u)n(u,t)n(v-u,t) - n(v,t)\int_0^\infty du K(u,v)n(u,t)$$

K(u,v) = coagulation kernel. Represents the physical process of collision between two particles. Typical processes leading to coagulation are e.g., Brownian motion, gravitational settling, and turbulence.

Source term in the Transport Equation

Some Coagulation Kernels:

Brownian coagulation

$$K_B(u,v) = \frac{2kT}{3\mu}\left(2 + \left(\frac{u}{v}\right)^{1/3} + \left(\frac{v}{u}\right)^{1/3}\right)$$

k = Boltzmann's constant

T = temperature of surrounding fluid

μ = fluid dynamic viscosity

u and v are volumes of particles

Gravitational coagulation

$$K_G(u, v) = \frac{\rho\, g}{6\mu}\left(\frac{3}{4\pi}\right)^{1/3}(v^{2/3} + u^{2/3})\left|v^{2/3}C_v - u^{2/3}C_u\right|$$

ρ = density of particle

g = gravitational acceleration

C_v and C_u are Cunningham coefficients for slip correction

Kernels in transition flow regimes:

- Rapidly becoming intractable
- Combined Brownian and Gravitational kernel:

$$\frac{K_{BG}(u,v)}{K_B(u,v)+K_G(u,v)} = \frac{4\pi}{\beta(\beta+4)}\sum_{n=0}^{\infty}(2n+1)\frac{I_{n+\frac{1}{2}}\left(\frac{\beta}{2}\right)}{K_{n+\frac{1}{2}}\left(\frac{\beta}{2}\right)}$$

$$\beta \propto uv\left|u^2 - v^2\right|, \quad \beta \in (0, >> 1)$$

Discrete Coagulation Equation

- Integral quantity of aerosol property in section *l*

$$Q_l = \int_{v_{l-1}}^{v_l} q(v,t)\,dv$$

- Discrete coagulation equation

$$\frac{\partial Q_l}{\partial t} = \frac{1}{2}\sum_{i=1}^{l-1}\sum_{j=1}^{l-1} {}^{1}\beta_{i,j,l} Q_i Q_j - Q_l \sum_{i=1}^{l-1} {}^{2}\beta_{i,l} Q_i - \frac{1}{2}\,{}^{3}\beta_{l,l} Q_l^2 - Q_l \sum_{i=l+1}^{m} {}^{4}\beta_{i,l} Q_i$$

Sectional coagulation coefficients

Symbol	Condition	Sectional coefficient
${}^{1}\beta_{i,j,l}$	2✁l✁m 1✁i<l 1✁j<l ${}^{1}\beta_{i,j,l}={}^{1}\beta_{j,i,l}$	$\int_{v_{i-1}}^{v_i}\int_{v_{j-1}}^{v_j}\frac{\theta(v_{l-1}<u+v<v_l)(u+v)K(u,v)}{uv(v_i-v_{i-1})(v_j-v_{j-1})}dudv$
${}^{2}\beta_{i,l}$	2✁l✁m i<l ${}^{2}\beta_{i,l}$⑤${}^{2}\beta_{l,i}$	$\int_{v_{i-1}}^{v_i}\int_{v_{l-1}}^{v_l}\frac{[\theta(u+v>v_l)u-\theta(u+v<v_l)v]K(u,v)}{uv(v_i-v_{i-1})(v_l-v_{l-1})}dudv$
${}^{3}\beta_{l,l}$	1✁l✁m	$\int_{v_{l-1}}^{v_l}\int_{v_{l-1}}^{v_l}\frac{\theta(u+v>v_l)uK(u,v)}{uv(v_l-v_{l-1})^2}dudv$
${}^{4}\beta_{i,l}$	1✁l<m i>l ${}^{4}\beta_{i,l}$⑤${}^{4}\beta_{l,i}$	$\int_{v_{i-1}}^{v_i}\int_{v_{l-1}}^{v_l}\frac{uK(u,v)}{uv(v_i-v_{i-1})(v_l-v_{l-1})}dudv$

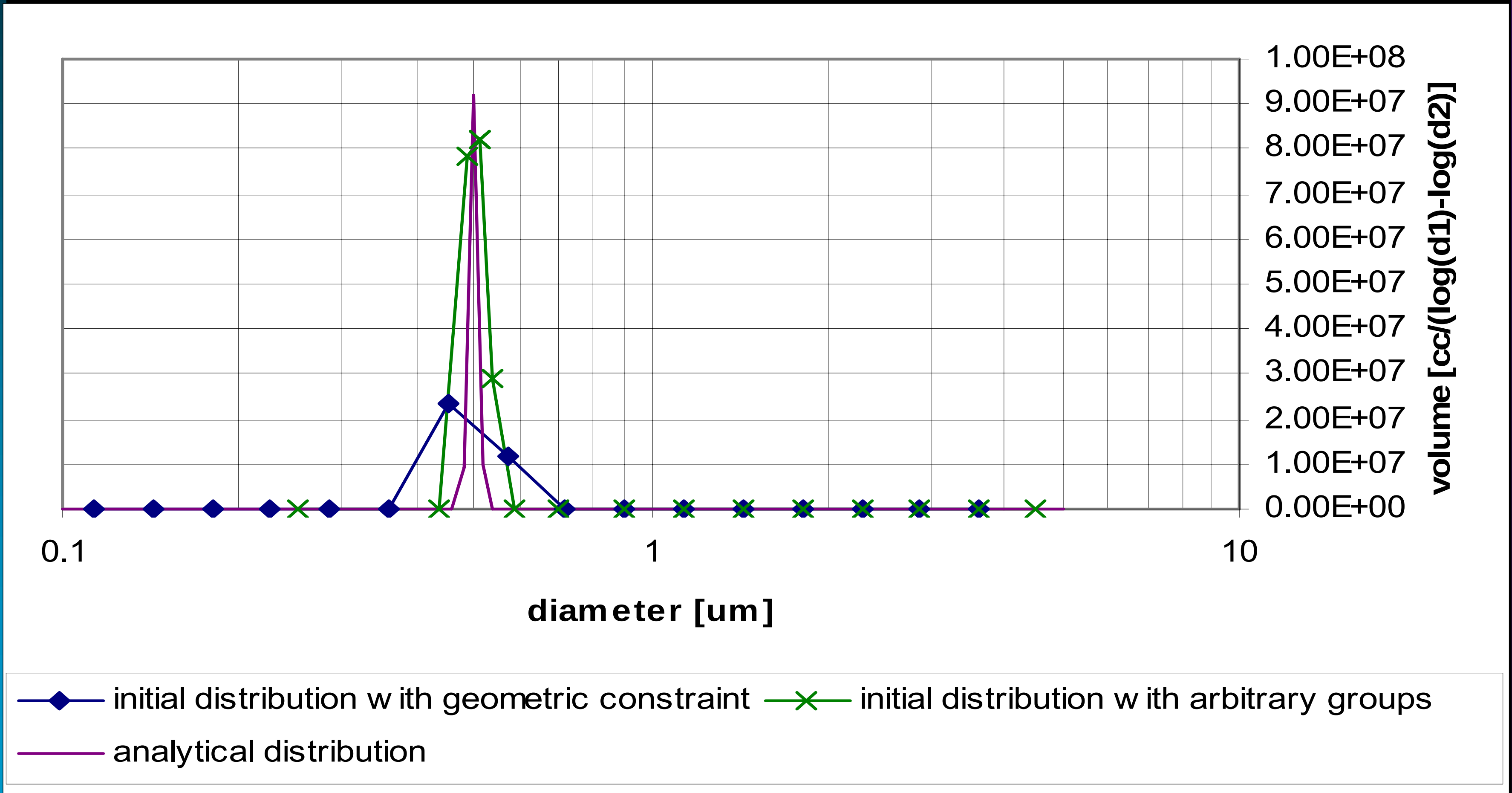
Simulation of coagulation and deposition

- Coagulation: sectional representation
  - Logarithmic groups (geometric constraint)

$$v_l \geq 2 v_{l-1}$$

  - Advantage:
    - Flux into group l is possible only from group $l-1$. This reduces the computational cost of $\beta_{i,j,l}$
  - Disadvantage:
    - It is not possible to resolve narrow distributions predominant for bio and therapeutic aerosols
  - SAEROSA: Arbitrary sectionalization

Fit of a Narrow Distribution IC

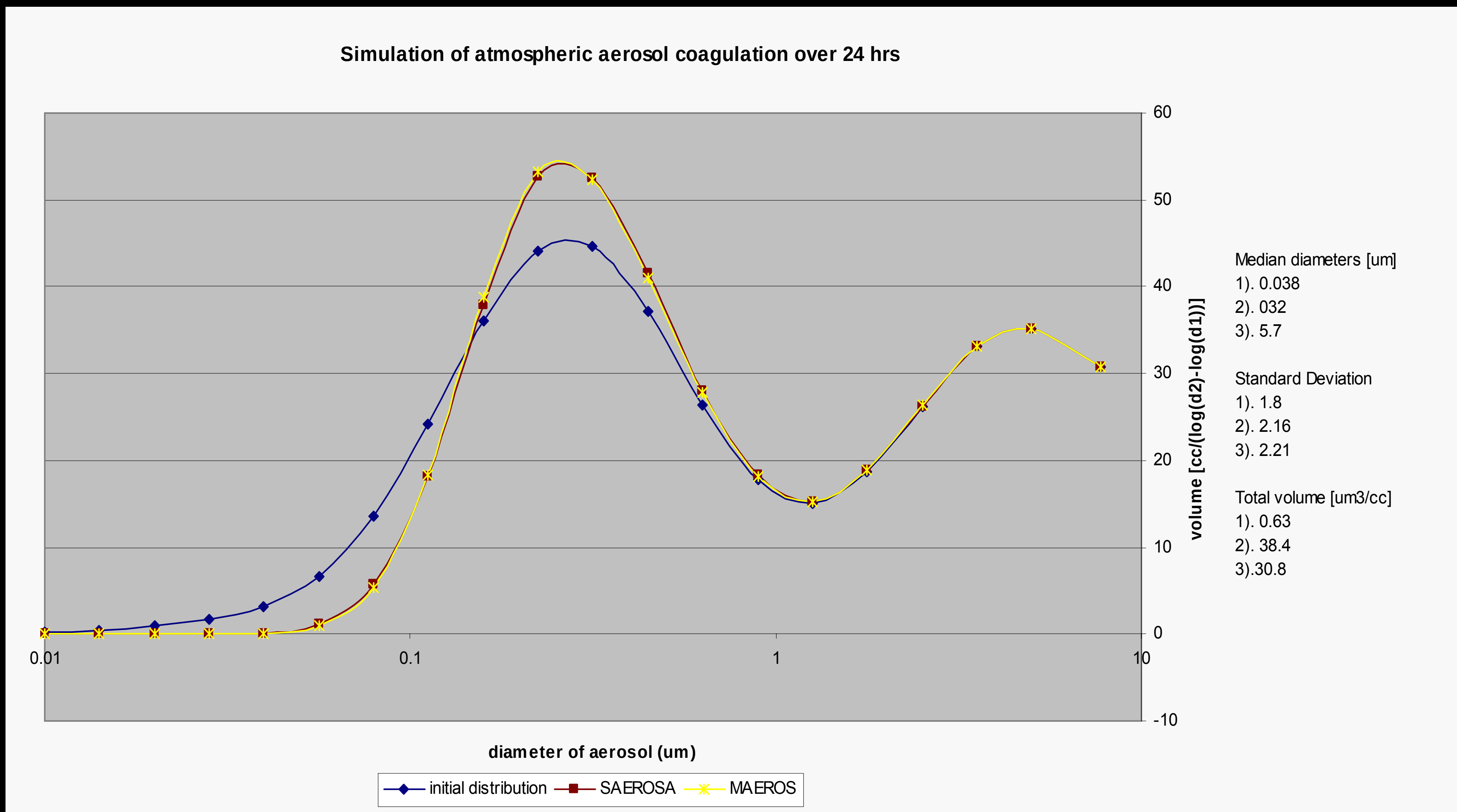


Model Comparison

Name		SAEROSA	MAEROS
Capability	Coagulation	YES	YES
	Deposition	YES	YES
	Condensation	NO	YES
	Species	Single	Multi-species
Group structure	Sectional Method	Arbitrary	Geometric Constraint
	Maximum Groups	Unlimited	20 groups
Kernel treatment		True kernels	Sum kernels
Numerical scheme		R-K, 5-6^{th} Adaptive Δt	R-K, 4-5^{th}
Computational time	(for 24hr simulation with 20 groups)	~1 min	~1 min

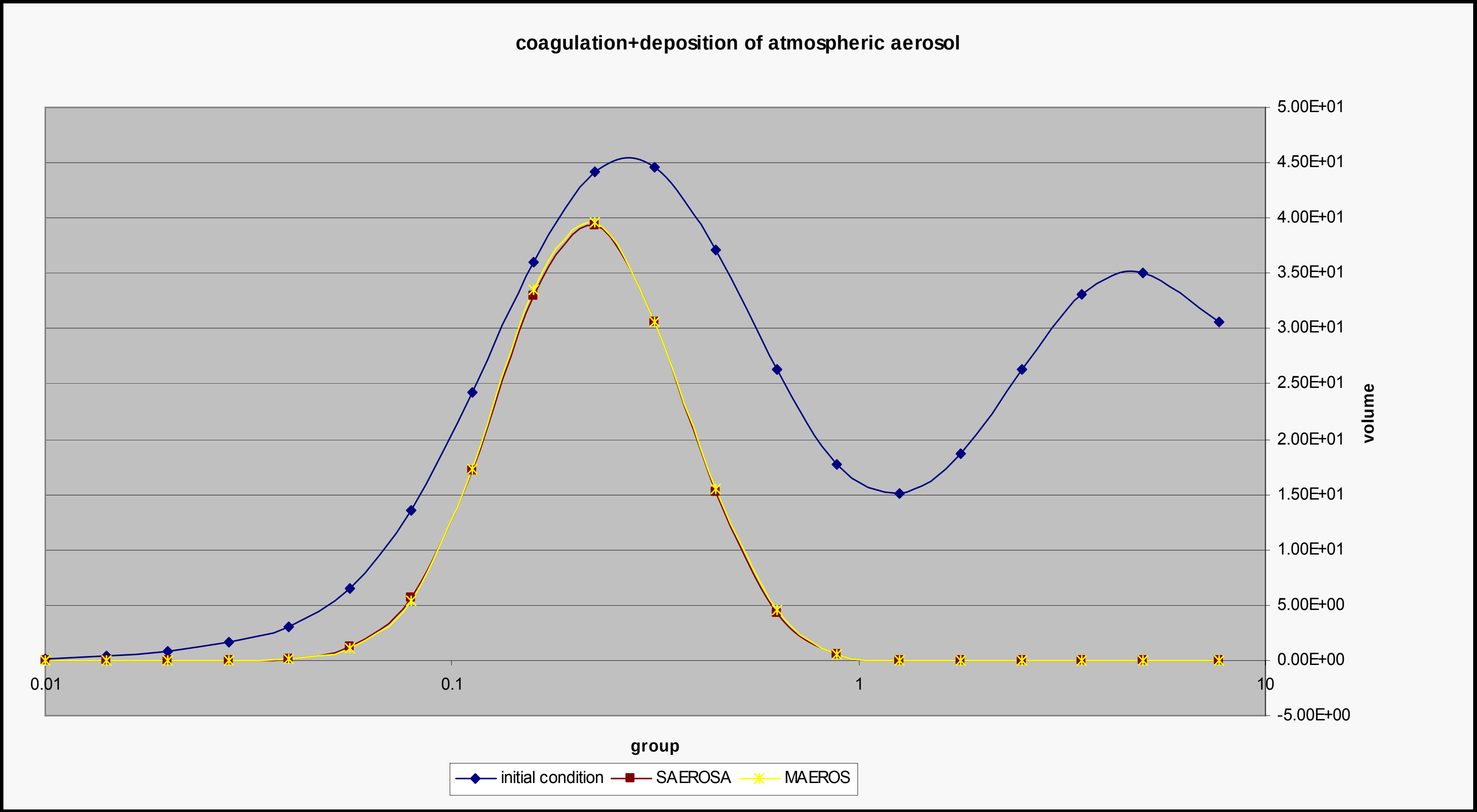
Coagulation Benchmark 1

without deposition



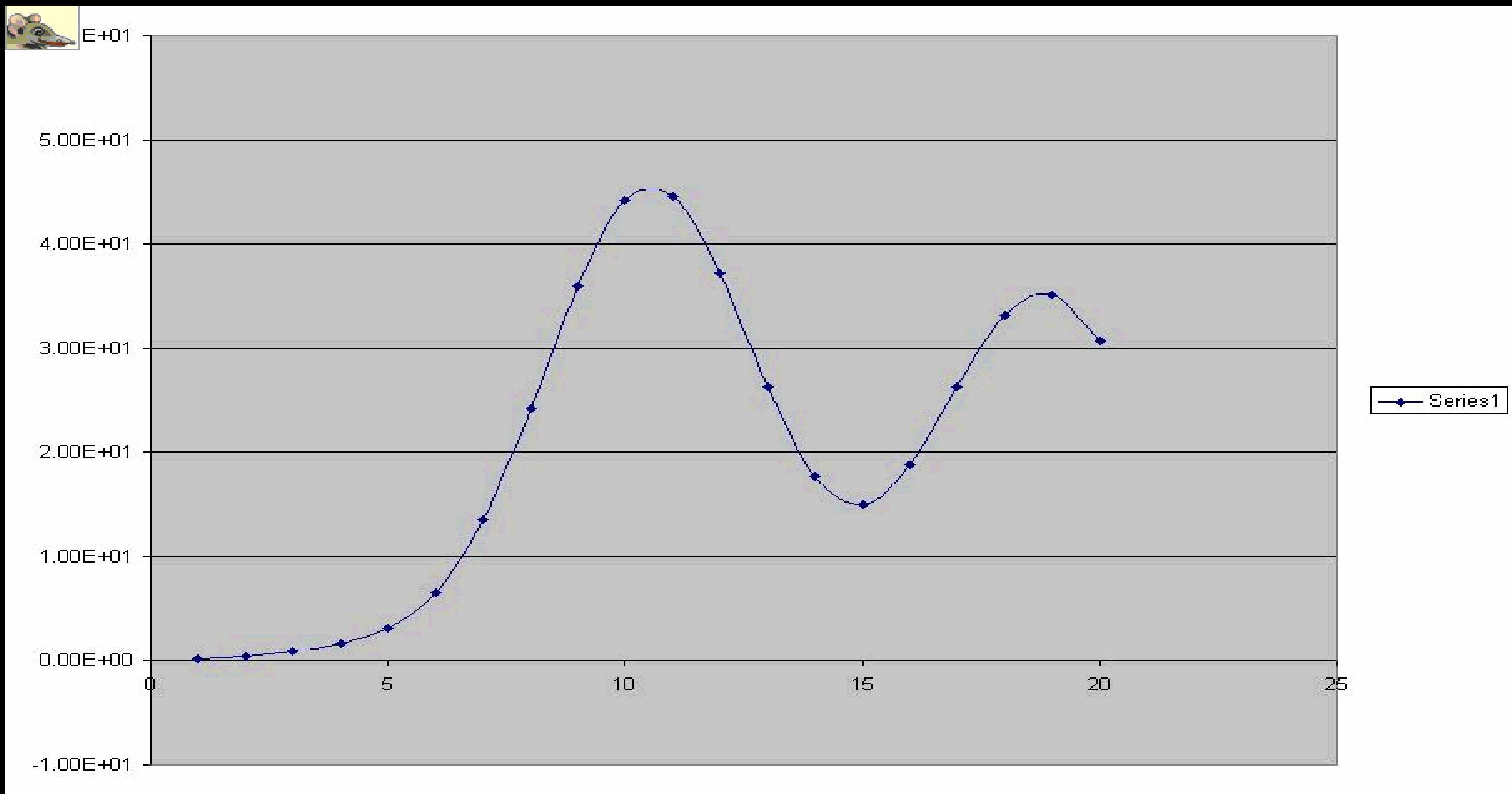
Coagulation Benchmark 2

with deposition



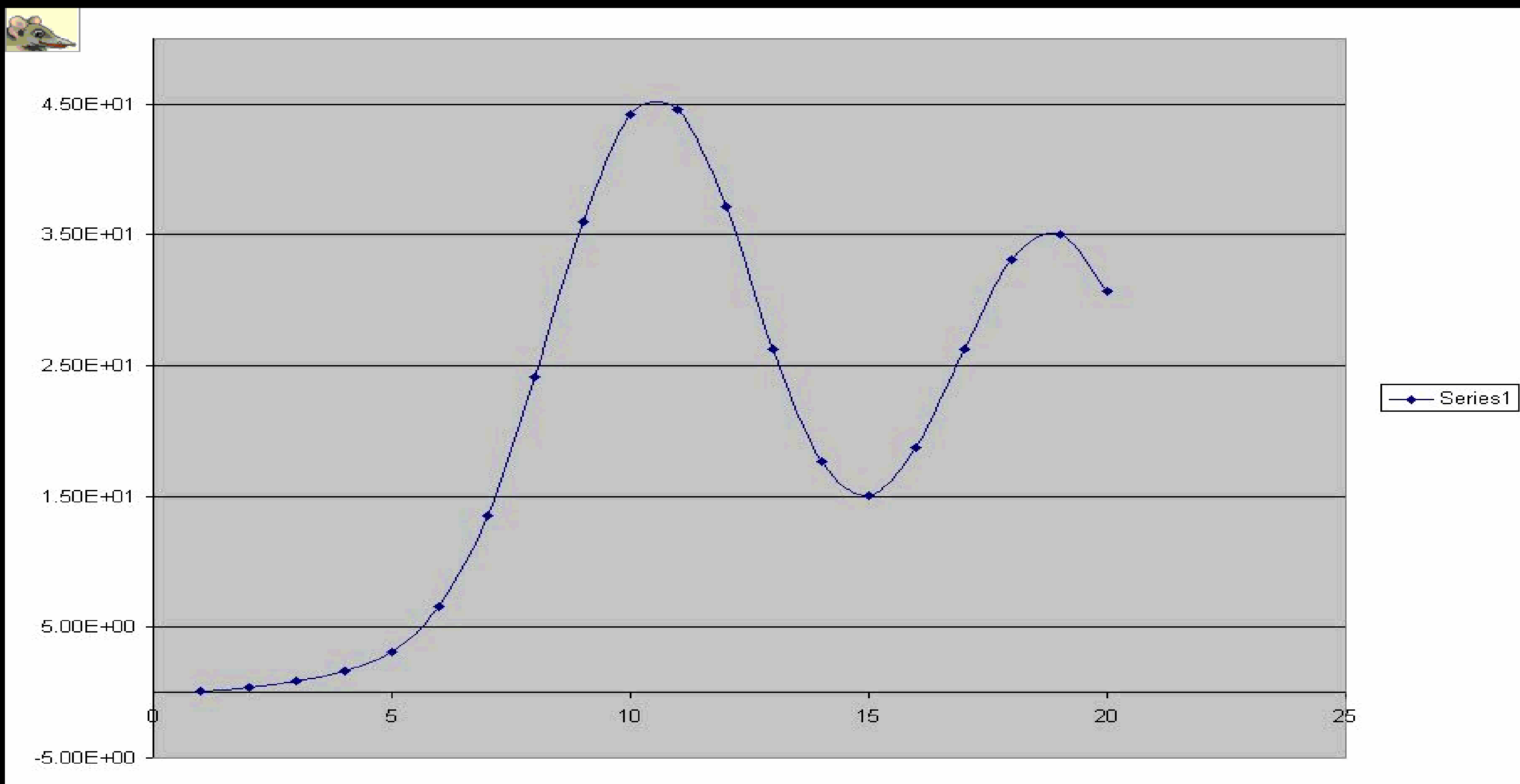
Visualizing the Time Evolution

Coagulation



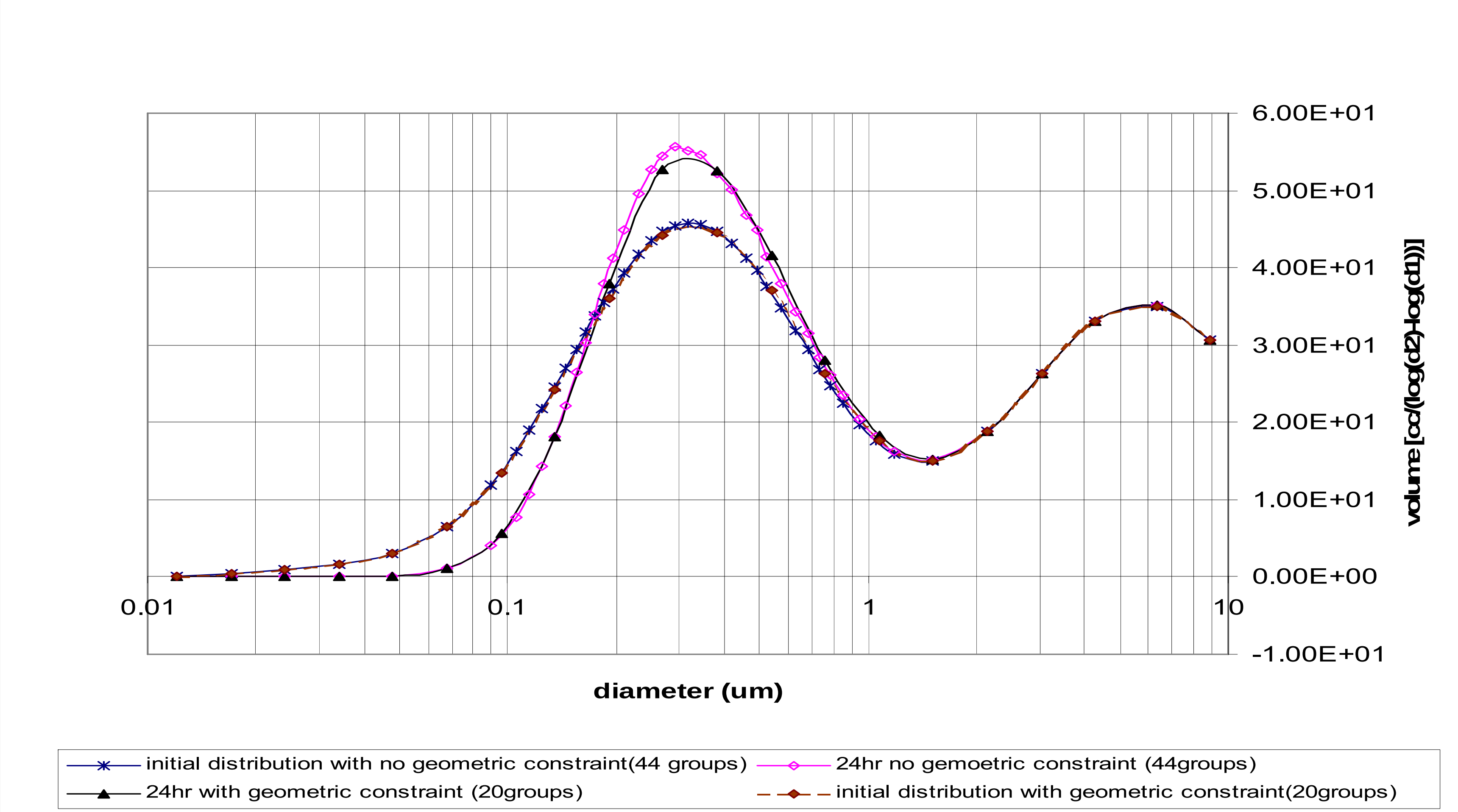
Visualizing Time Evolution (cont.)

Coagulation +Deposition



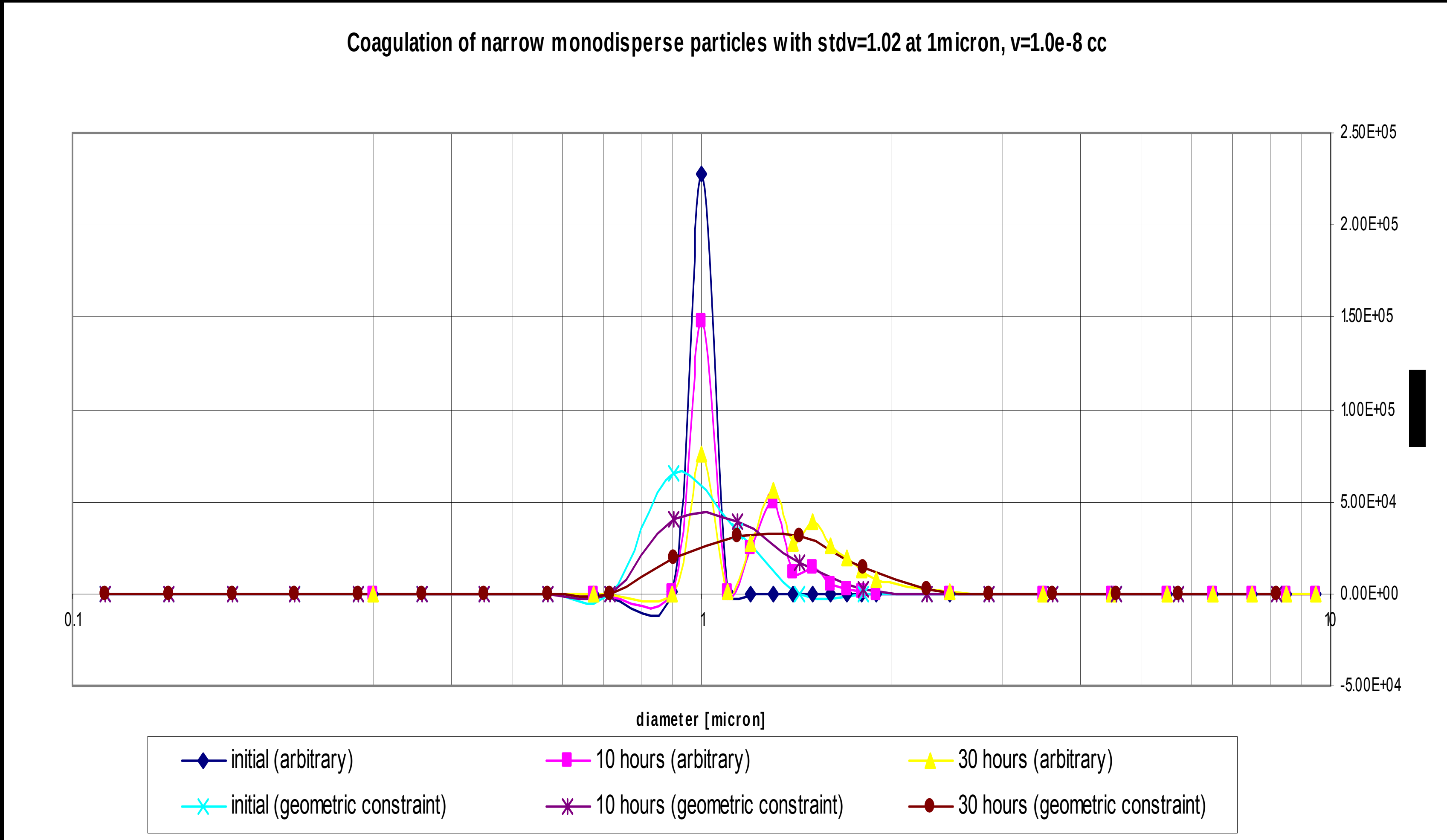
Effect of arbitrary sections

On urban aerosol, without deposition



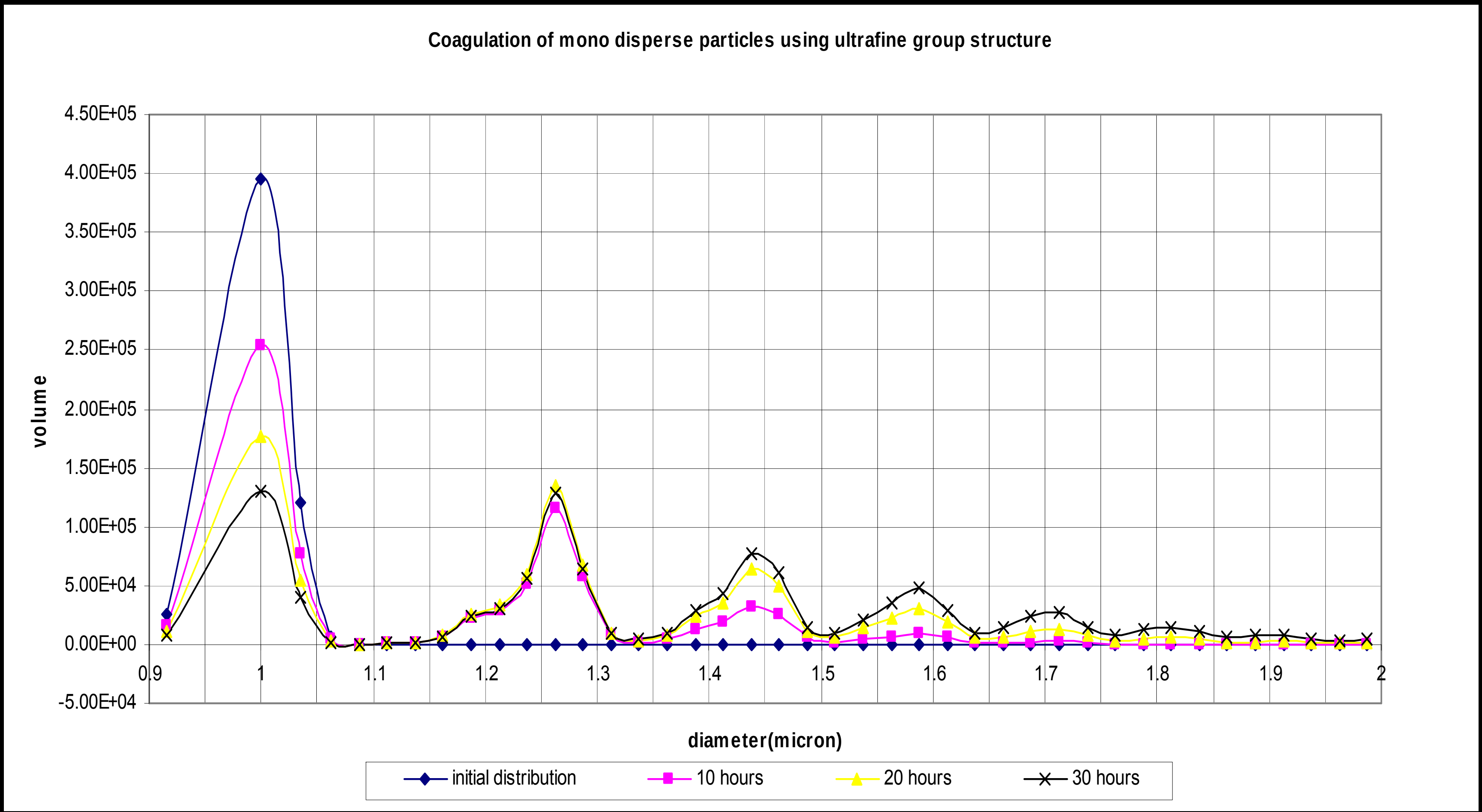
Effect of arbitrary sections

On near delta function source



Ultra-fine group structure

Near delta function source



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Aerosol transport in confined spaces
The CAEROT code

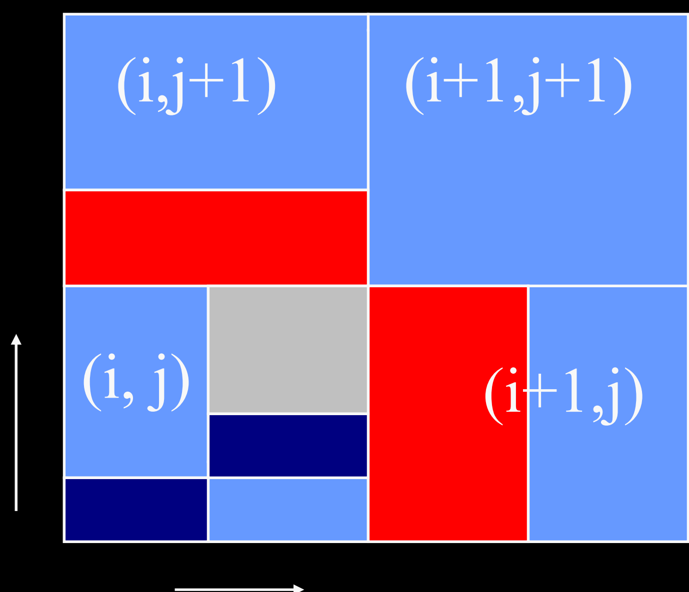
- Inclusion of convective transport and geometry into SAEROSA
  - Spatial discretization
  - Production of velocity field by using external CFD code
  - Advanced nodal method using hybrid Eulerian-Lagrangian treatment
- Time & space-dependent source and sink
- Code validation against experiments

Advanced Nodal Method

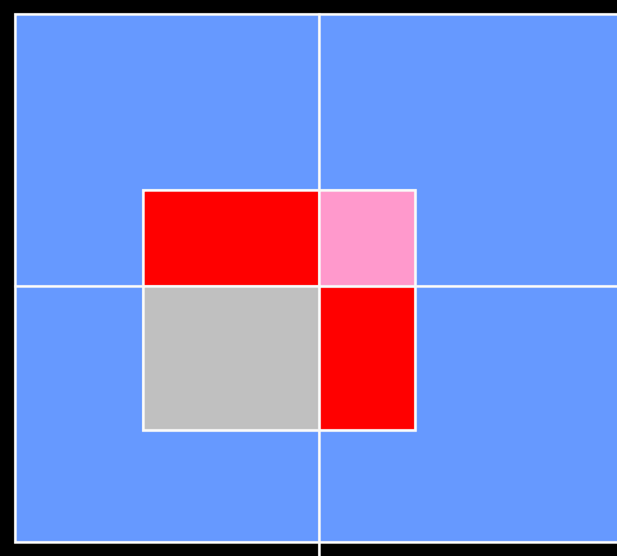
Hybrid Eulerian-Lagrangian

- In 2D case
  - Transport from (i,j) to(i+1,j+1) along stream lines
  - Less diffusive, faster convergence

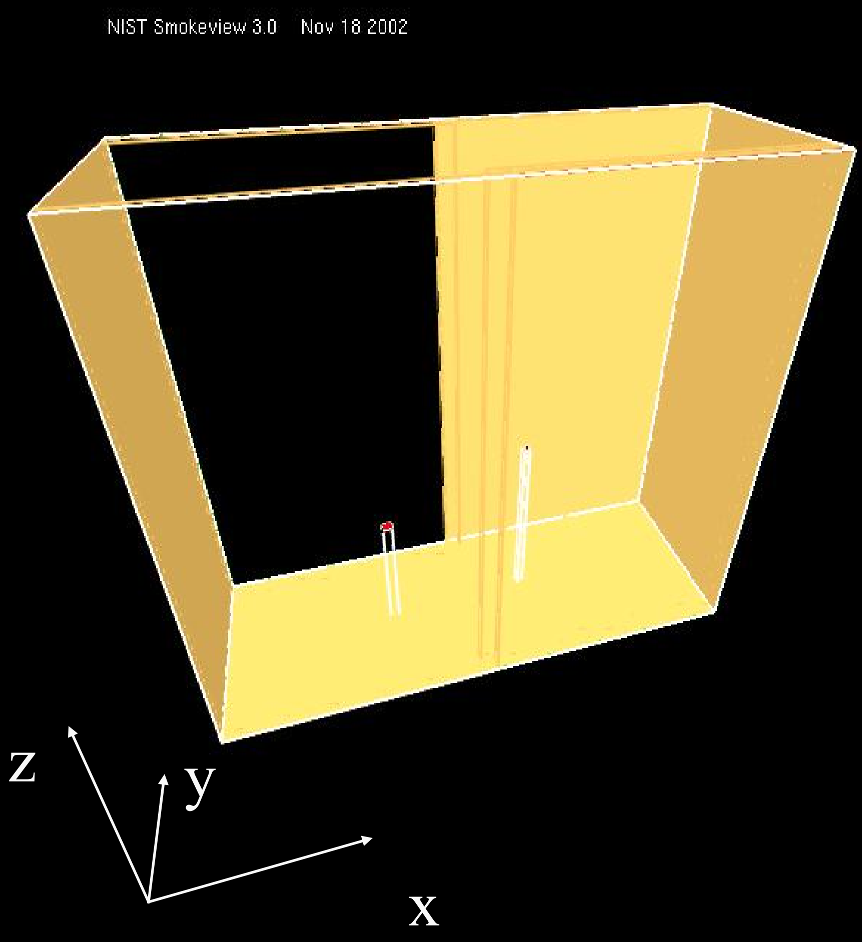
Finite difference



Stream tube model



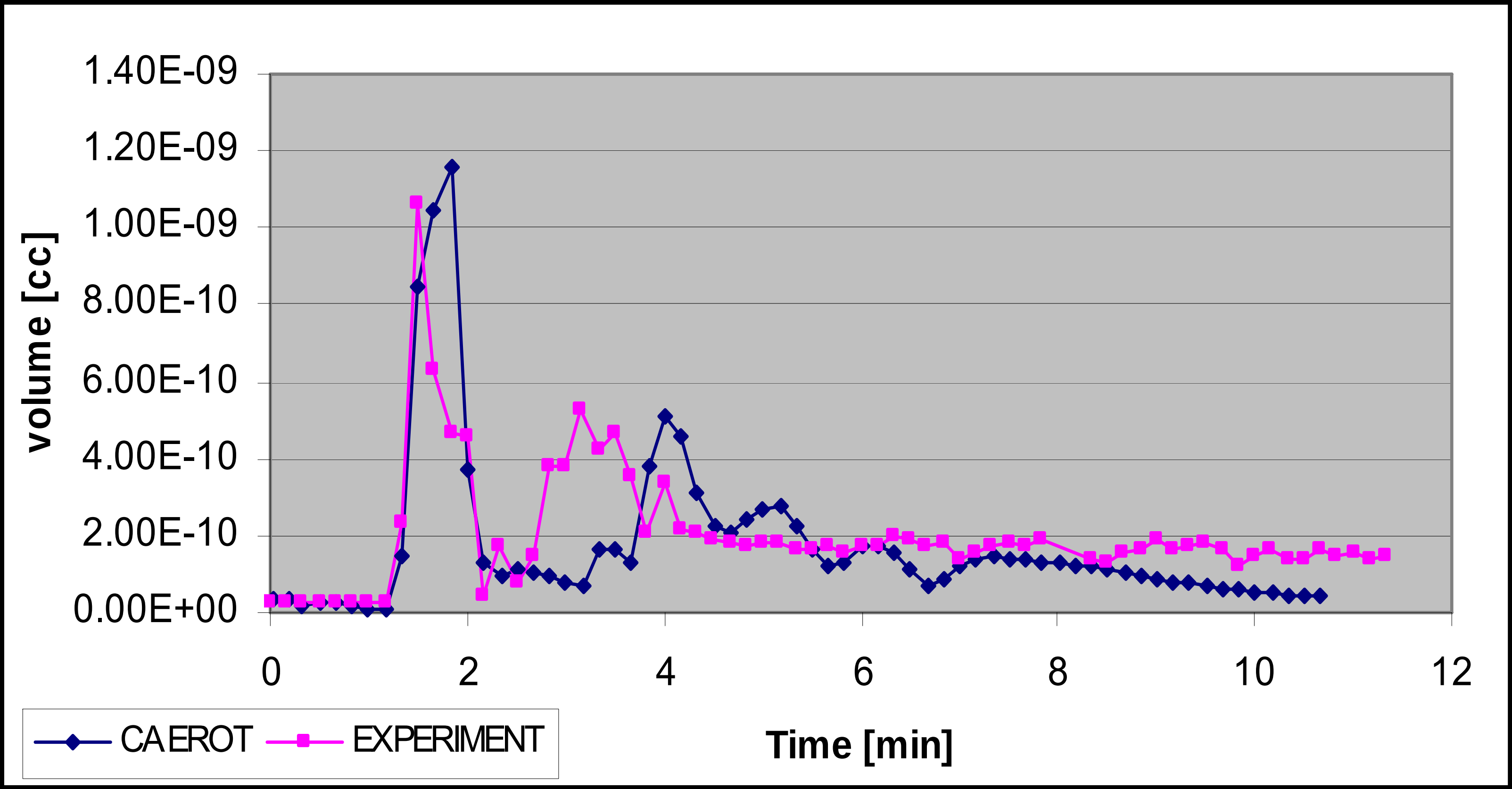
Validation Experiments in an Environment Chamber



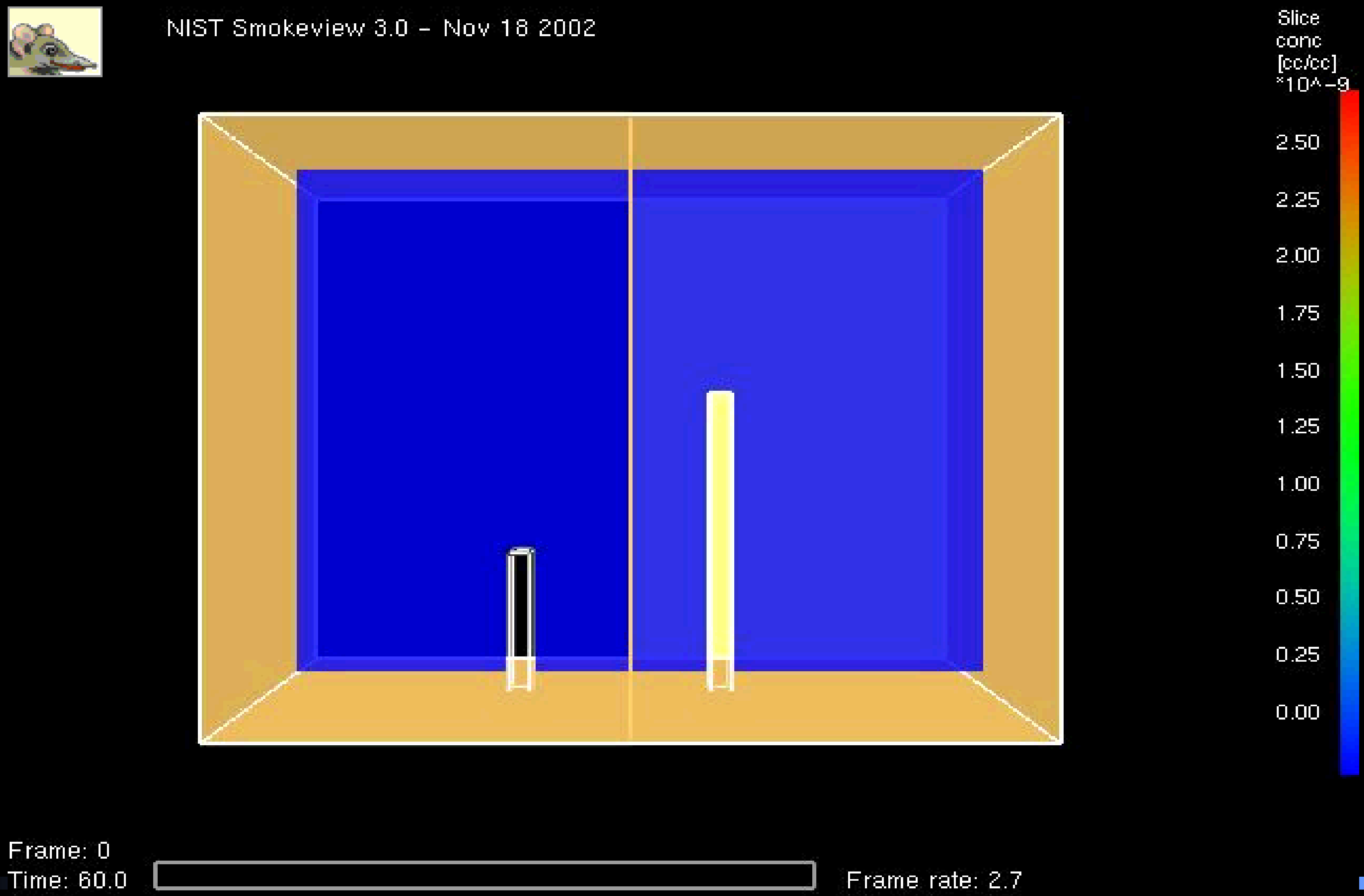
- Size: 180x60x150 cm
- Variable release and sampling locations
- Antistatic tubing
- Release via nebulizer
- NIST traceable particle standard: 0.502 μ
- Multi-channel laser aerosol spectrometer

Code Validation

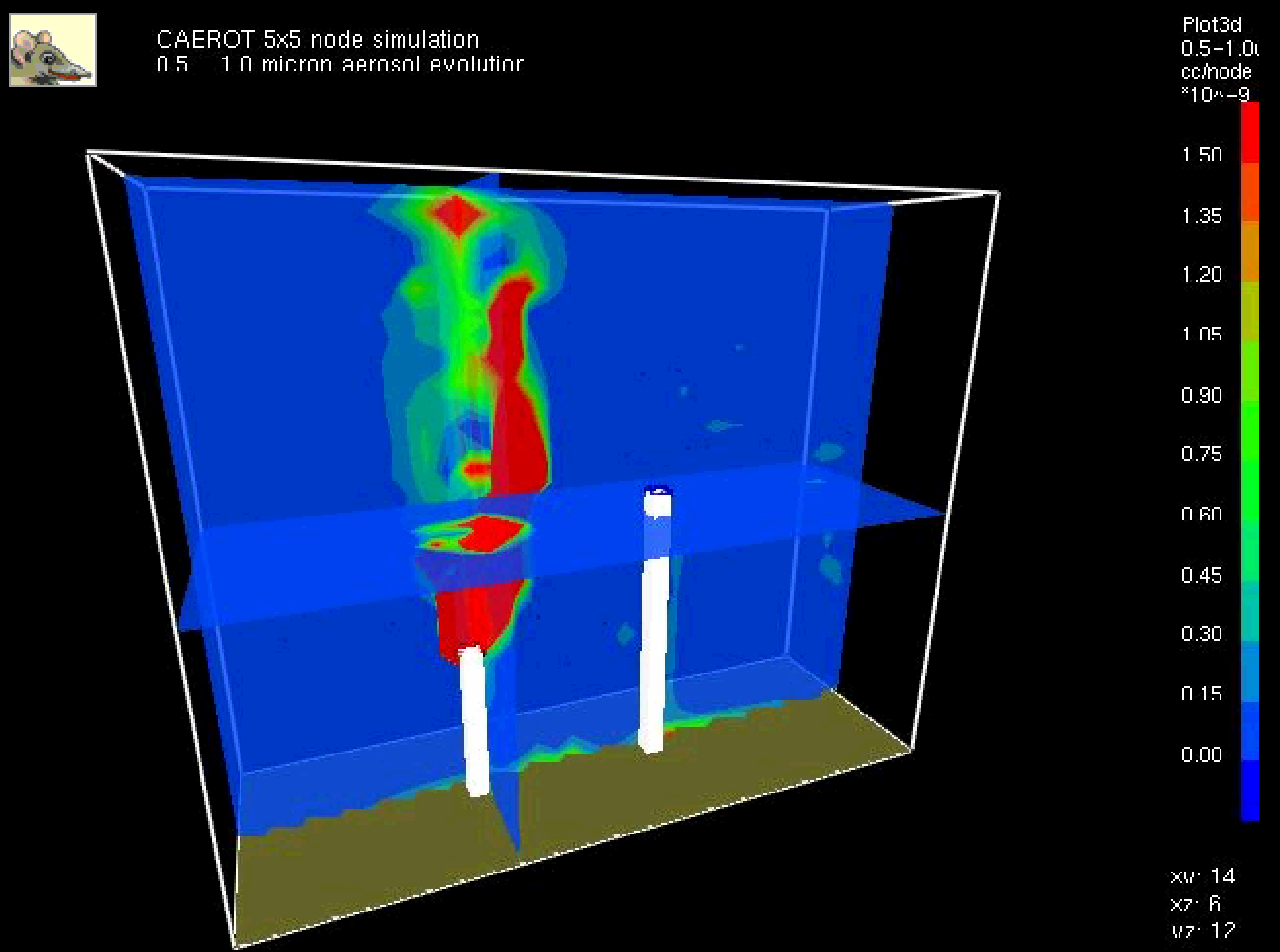
CAEROT prediction vs experiment



Visualization (total aerosol concentration)



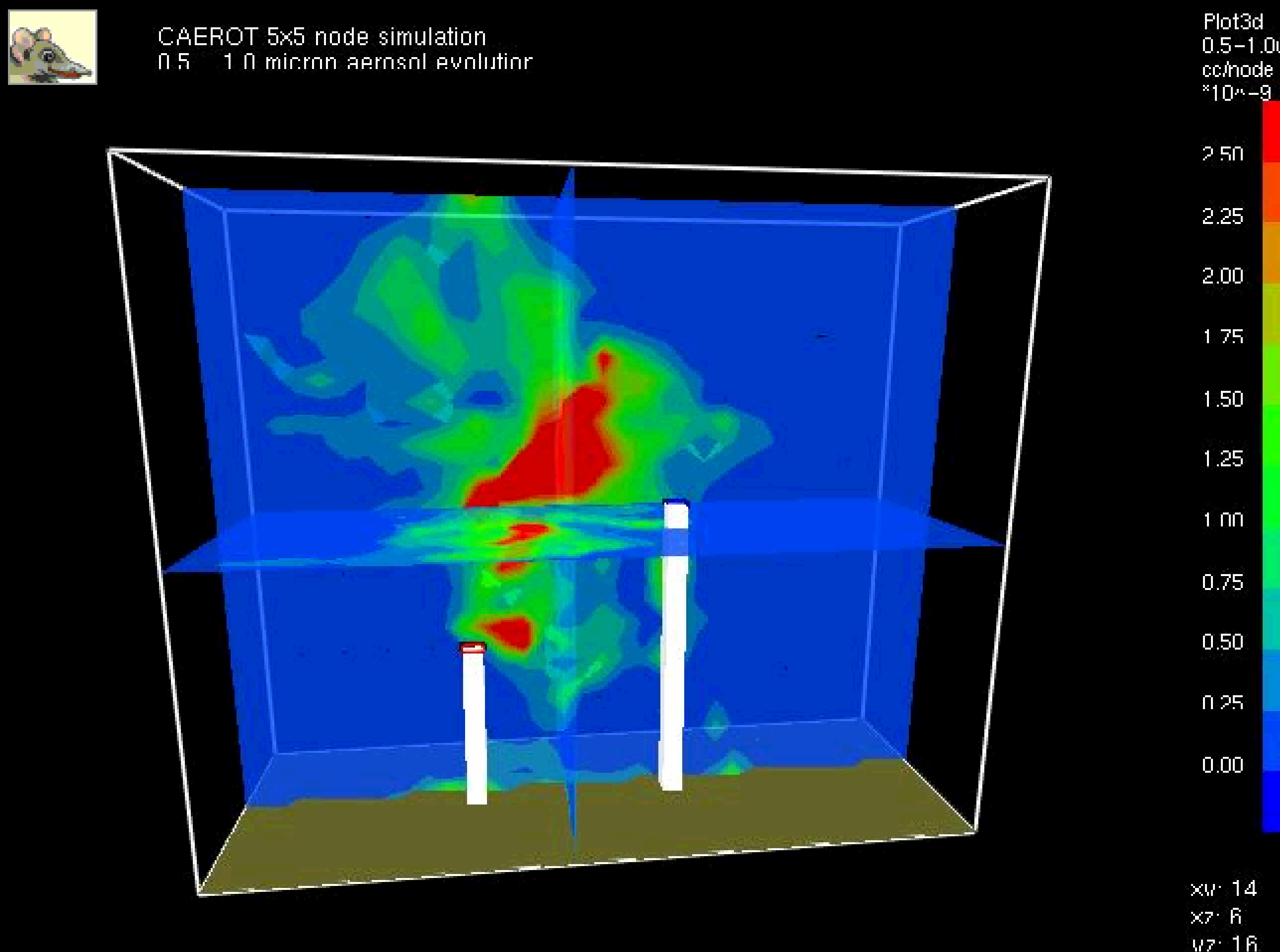
Aerosol Concentration Distribution



Particles in 0.5 to 1.0 μ, at t=100 s

Source: 60-120 s

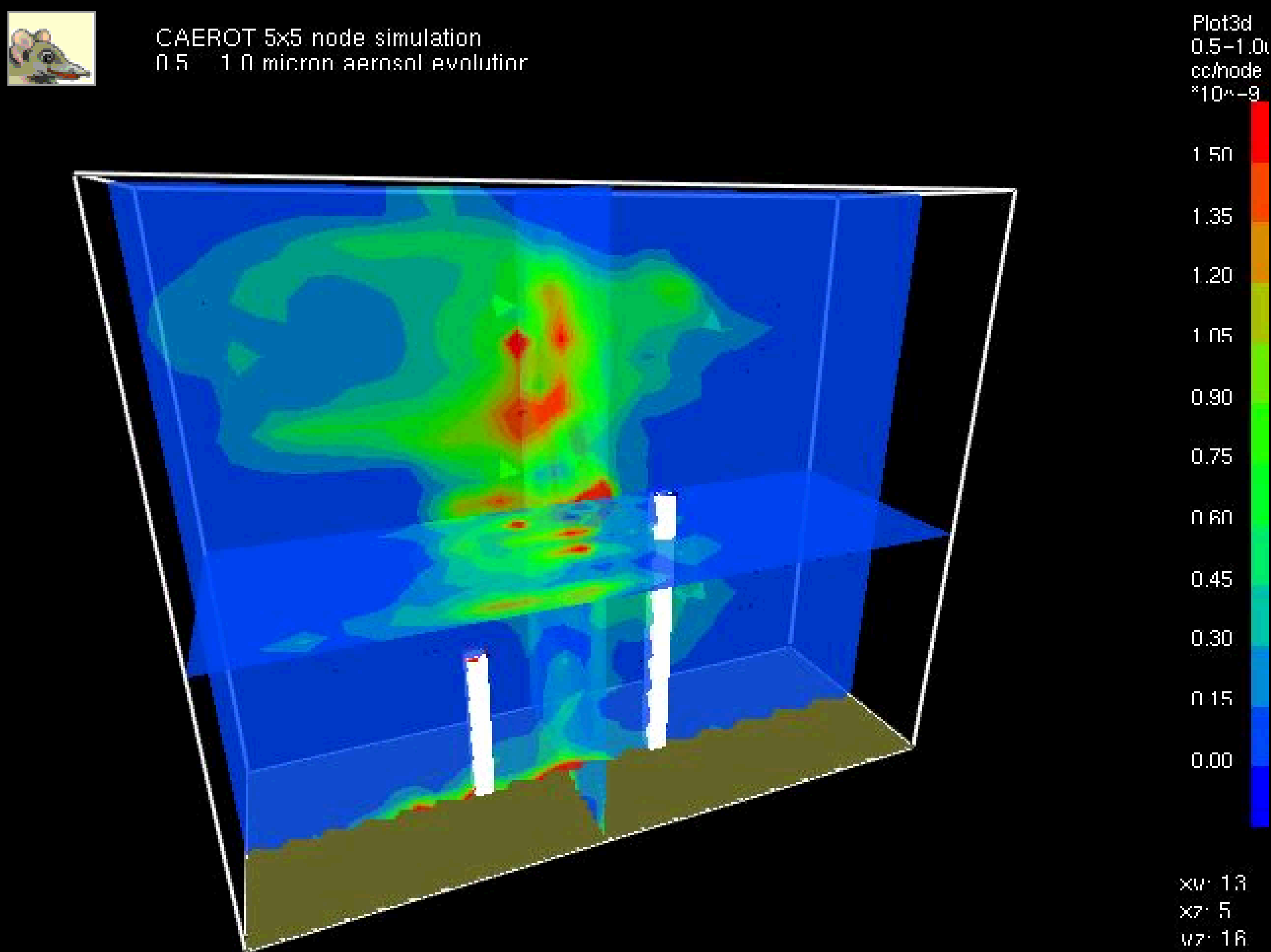
Aerosol Distribution



Particles in 0.5 to 1.0 μ, at t=150 s

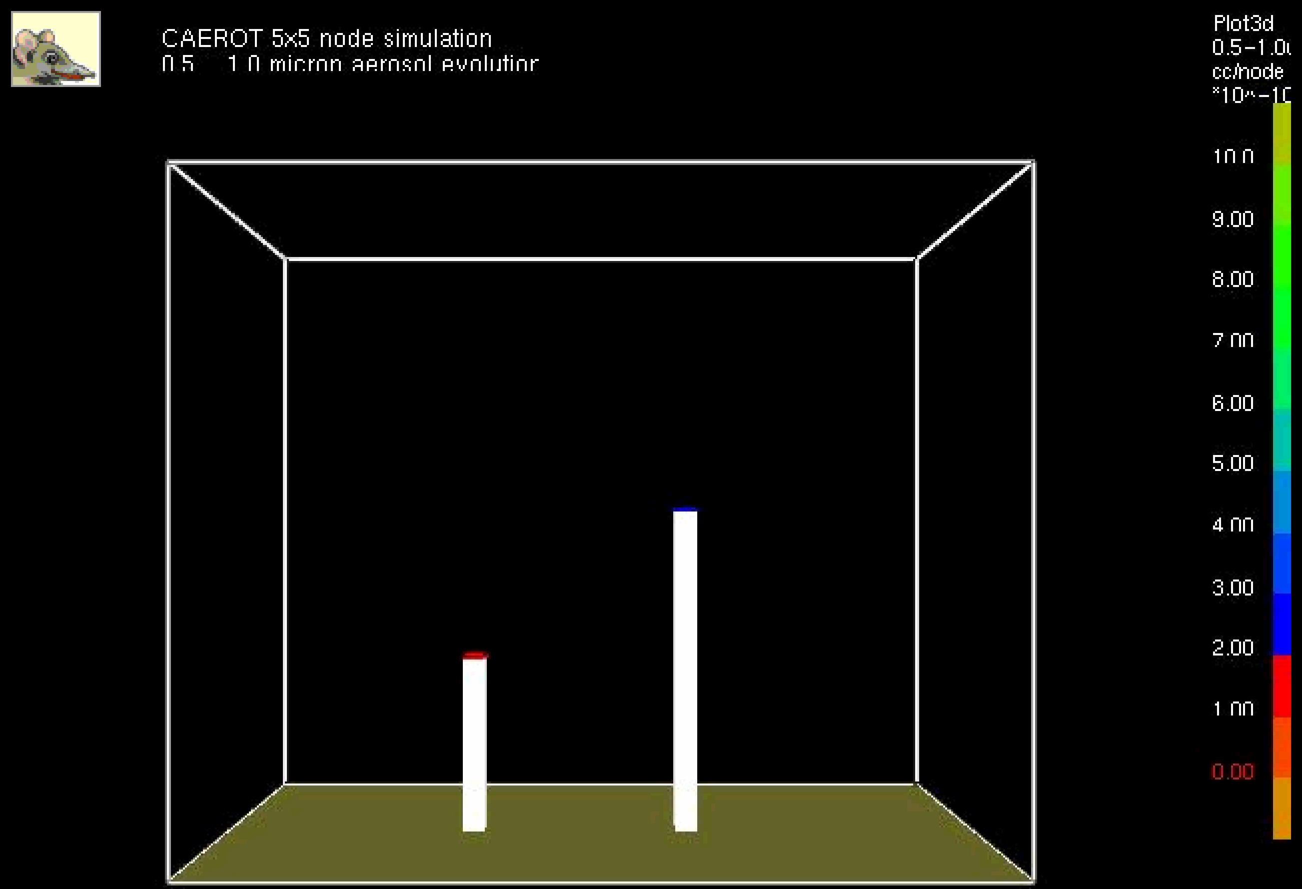
30 s after nebulizer stopped

Aerosol Distribution



Particles in 0.5 to 1.0 μ, at t=200 s

Aerosol Distribution –3D



Conclusions for the code development

- SAEROSA is stand-alone for well-mixed cases.
- CAEROT has good agreement with experiments.
- Result of simulation is sensitive to velocity field.
  – Low velocities require finer spatial mesh for CAEROT
- Further refinements:
  – Turbulent coagulation
  – Growth (condensation/evaporation)
  – Phoretic effects (thermo-, electro-)
  – Multi-species aerosol
- Availability: Planned through ORNL RSICC library.

Current/Future Work

- Sensitivity studies
  - Validity with different experiment and different geometries
- Inclusion of obstructions is coded but not validated
- Open boundaries
- Applications:
  - Transport through ducts: design a detector
  - Transport in the lung: better understanding

Design of an Aerosol Detector

Transport through micro-fabricated channels

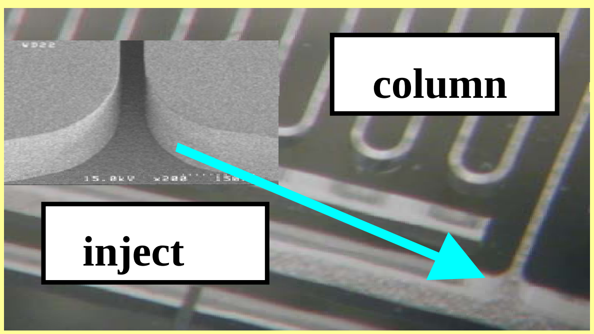
Rapid Aerosol Detection with Species Identification

- Small size detector
  - Resolves size spectrum
  - Screens organic vs inorganic species
  - Identifies organic molecules
- Rapid response
- Wireless units operated in a network
- Provides near-real-time aerosol phase space information

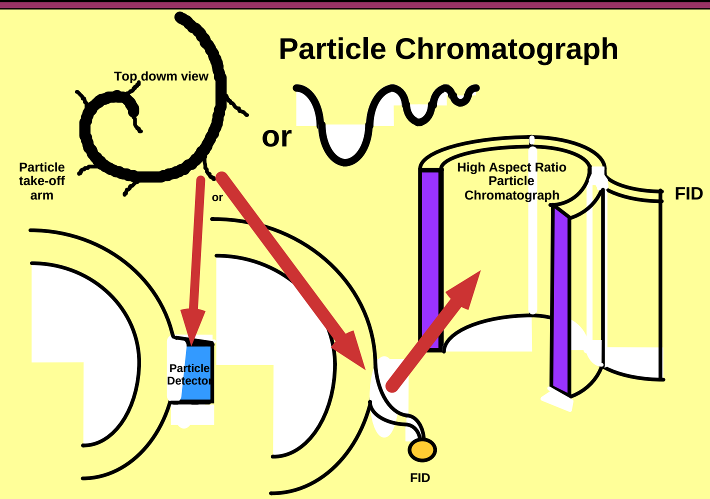
High Aspect Ratio Particle Chromatograph (HARPc)

- Momentum sorting through a micro-fabricated channel system
- Material identification via flame ionization

QuickTime™ and a Graphics decompressor are needed to see this picture.



Pictures of High Aspect Ratio GC Columns, made with LIGA microfabrication technology, of metal tubes 50µ wide and 500µ high, and 2 meters in length.



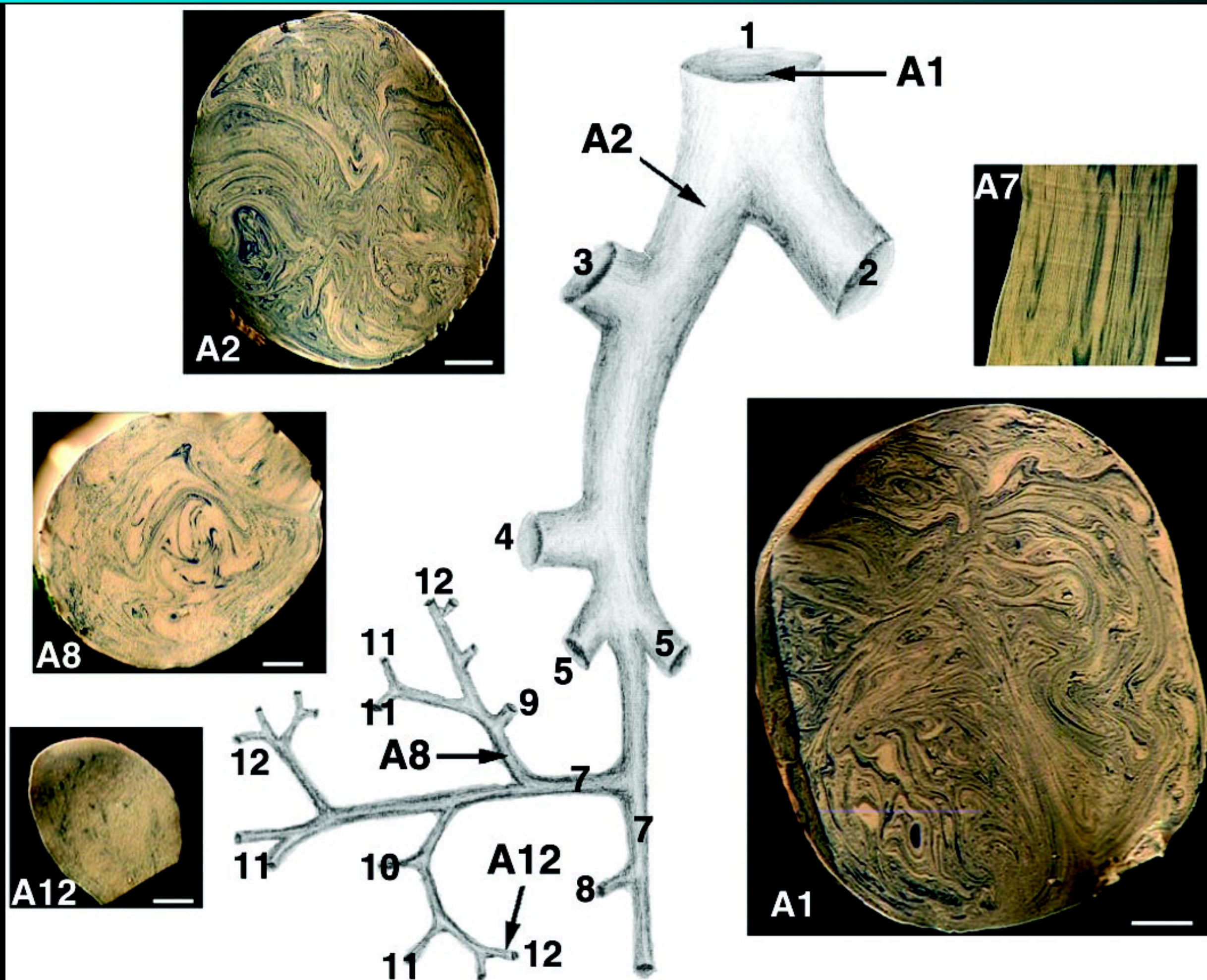
Concept drawing showing possible particle take-off arms for detection of hydrocarbon containing aerosol particles with the “Particle Chromatograph”.

Transport in the lung

Aerosol dynamics in chaotic mixing

Flow patterns in the airways

A1: Trachea (bar=500 μ)
A2: Main stem bronchus (bar =500 μ)
A7: Medium size airway (bar =100 μ)
A8: Medium size airway (bar =200 μ)
A12: Small airway (bar =100 μ)



Courtesy of A. Tsuda, Harvard U.

Critical factor in aerosol retention: kinematic interaction between inhaled and residual alveolar gas.

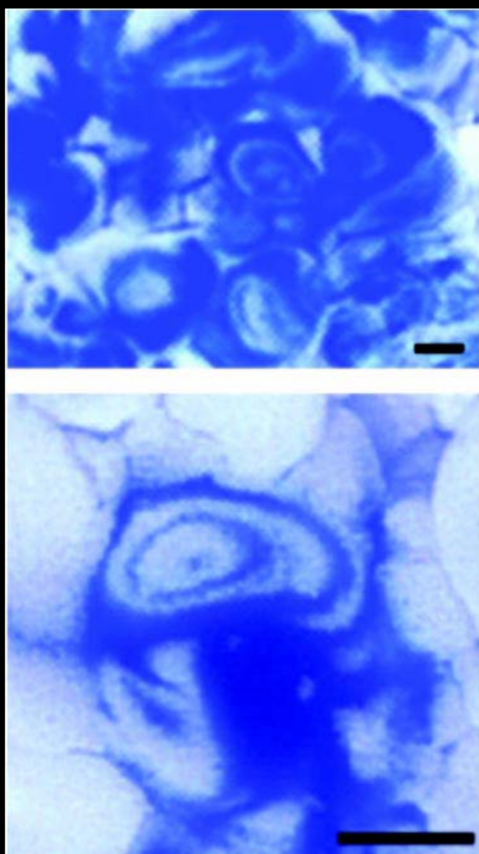
Air flow in the alveolar region

- Low Re number (~1)
- Reversible lung wall motion
- Kinematically reversible Stokes flow?
- In reality:
  - Inertial stream-line crossing, sedimentation and diffusion alone do not explain the degree of deposition seen in experiments.
  - Oscillatory Stokes flow can result in chaotic behavior
  - Stagnation saddle points in the alveolar openings
  - Lagrangian simulation shows irreversible stretched and folded flow patterns

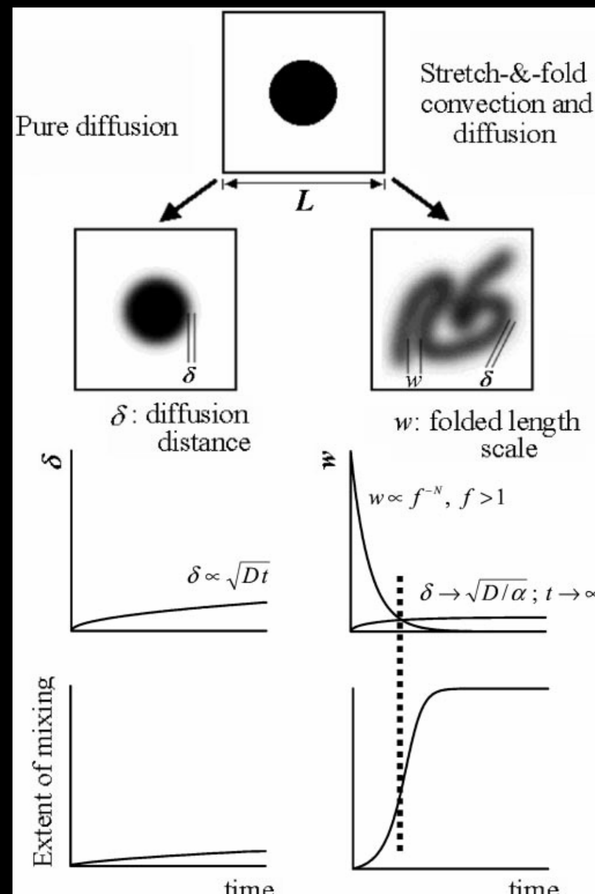
Stretch and fold patterns

interaction of diffusion and convection

Alveolar recirculation (bar = 100 μ)



Brownian mixing vs strech & fold convection + diffusion



α= stretching rate
f = cycle-by-cycle folding factor

When length scales of *w* and δ are comparable, an entropy "burst" occurs characteristic to chaotic mixing

Courtesy of A. Tsuda, Harvard U.

Thank You