Modelling Diffusion in Aerosol Particle Mass (APM) Analyzer

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The aerosol particle mass (APM) analyzer classifies particles by balancing centripetal and electrostatic forces. This concept was first conceived by Ehara et al. [1, 2]. Ehara's APM consists of two rotating coaxial electrodes. Charged particles pass between the two cylindrical electrodes that are rotating at an equal angular velocity. A voltage is applied between the two cylindrical electrodes creating an electrostatic field. As the particles flow through the device, they will experience an centripetal and electrostatic force acting in opposite directions. Particles of a certain mass-to-charge ratio will pass through the APM. Other particles will either be forced to the outer electrode if the centripetal force is stronger than the electrostatic force or they will be forced to the inner electrode if the electrostatic force is dominant. It is assumed that particles that impact the inner or outer electrode adhere to the surface and will not pass through the APM. By adjusting the voltage and angular velocity, particles of different mass-to-charge ratios will pass through the device. If the charge on the particles is known, then the mass of the particle passing through the APM is known. The particle's mass can be combined with aerosol size data to determine mass distributions or a particle's effective density and fractal dimension.

Ehara's original work on the APM included a theoretical model of the APM, but it neglected the effect of diffusion [2]. Later work by Hagwood et al. used a stochastic differential equation model, solved with the Monte Carlo method, to determine the effect of diffusion in the APM [3]. We have developed another diffusion model of the APM using the convective diffusion equation. This model was developed so that we could study the affect of changing the external forces in the APM. However, this presentation only includes results for the performance of the APM.

A comparison of the convective diffusion model and Ehara's non-diffusion model of the APM showed that the transfer function is dependent on the size of the particle being classified. For large particles the effect of diffusion is negligible so both models give the same result. For small particles the effect of diffusion has a strong influence on the transfer function and the transfer function is reduced. The effect of diffusion is noticeable in the APM for particle sizes less than $\sim$100 nm.

A comparison with Hagwood's diffusion model showed that the models gave identical results for small particles ($\sim$20 nm). However, for larger particle sizes ($\sim$100 nm) the convective-diffusion model gave a transfer function approximately 8% higher than Hagwood's.

To summarize; a convective diffusion model of the APM was developed. The model agreed well with Ehara's non-diffusion model for large particle sizes. It was also shown that diffusion lowers the amplitude of the transfer function when small particles are classified (particles less than $\sim$100 nm). In general, the convective diffusion model agreed well with Hagwood's diffusion model.

References

[1] K. Ehara, "Aerosol mass spectrometer and method of classifying aerosol particles according to specific mass," 1995. U.S. Patent No. 5,428,220.

[2] K. Ehara, C. Hagwood, and K. J. Coakley, "Novel method to classify aerosol particles according to their mass-to-charge ratio - aerosol particle mass analyser," *Journal of Aerosol Science*, vol. 27, no. 2, pp. 217–234, 1996.

[3] C. Hagwood, K. Coakley, A. Negiz, and K. Ehara, "Stochastic modeling of a new spectrometer," *Aerosol Science & Technology*, vol. 23, pp. 611–627, 1995.

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Outline

- Introduction
  - Description and operation of Aerosol Particle Mass (APM) analyzer
  - Motivation for using particle mass classifiers
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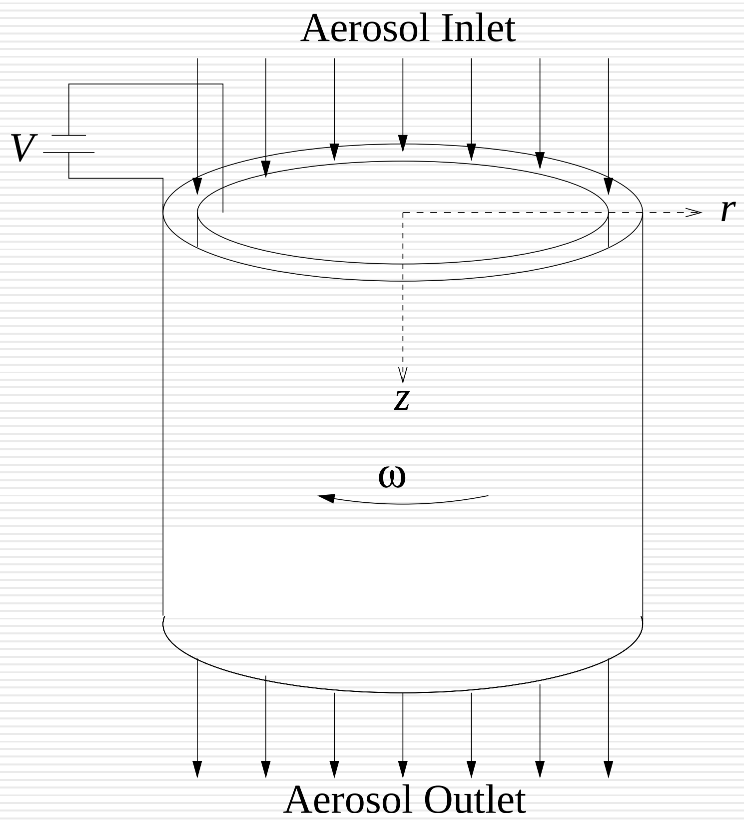
- Theory of Convective Diffusion APM Model
- Comparing the APM Models
  - Ehara's Non-Diffusion Model
  - Hagwood's Stochastic Diffusion Model
  - Convective Diffusion Model
- Summary

Operation of the Aerosol Particle Mass Analyzer (APM)

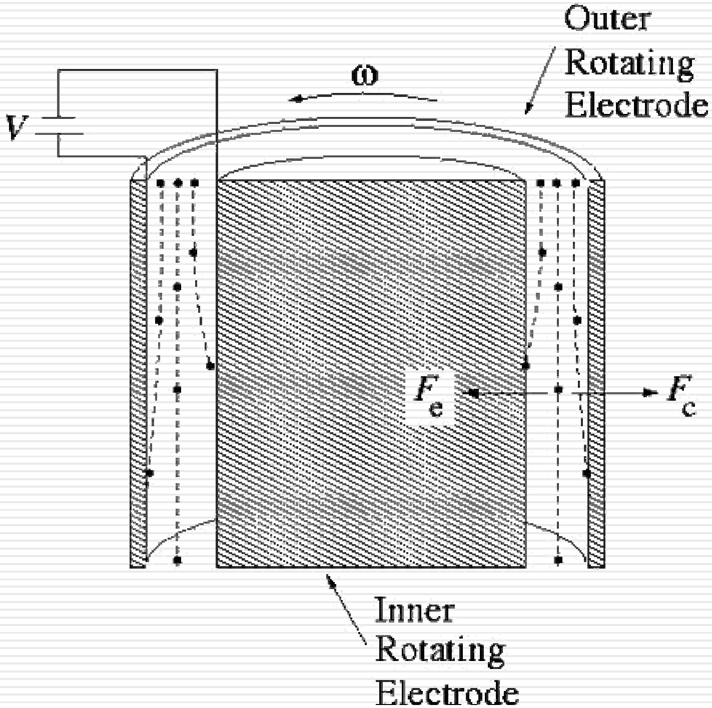
- Developed by Ehara *et al.*
- Charged particles pass through two cylindrical electrodes.
- The cylindrical electrodes rotate - creating a centripetal force on the particles. In Ehara's APM both cylinders rotate at constant ω.
- Voltage is applied between the cylindrical electrodes – creating an electrostatic force on the particles.



- Particles of a certain mass-to-charge ratio will pass through the APM.

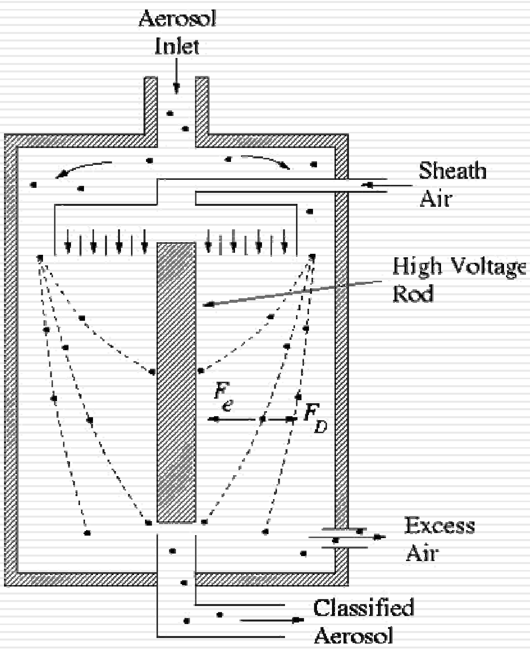
APM & DMA

Aerosol Particle Mass Analyzer



- Particles are classified by balancing electrostatic and centripetal forces.
- Particles are classified by mass.

Differential Mobility Analyzer



- Particles are classified using electrostatic and drag forces.
- Particles are classified by size.

Motivation for Classifying Particles by Mass

- Classification with purely intrinsic properties
  - Other devices classify with a drag force (drag force depends on the particles' interaction with surroundings)
- Measure particle density and fractal dimension
  - Using the DMA-APM technique (McMurry *et al*., 2002)
  - For spherical particles – the true particle density is found
  - For non-spherical particles – the effective density is found
- Measure particle mass distributions
  - Using the DMA-APM technique (Park *et al*., 2003)
  - APM is not affected by volatilization or adsorption (unlike filter measurements)

Motivation for a Convective Diffusion (C-D) APM Model

- Previous models:
  - Non-diffusion model (Ehara *et al*)
  - Stochastic diffusion model (Monte-Carlo) (Hagwood *et al*)
- For future work a model is required that has a generalized external force function
  - Such a model can be used to determine the transfer function of the APM when external forces are modified.

Theory of the Convective Diffusion APM Model

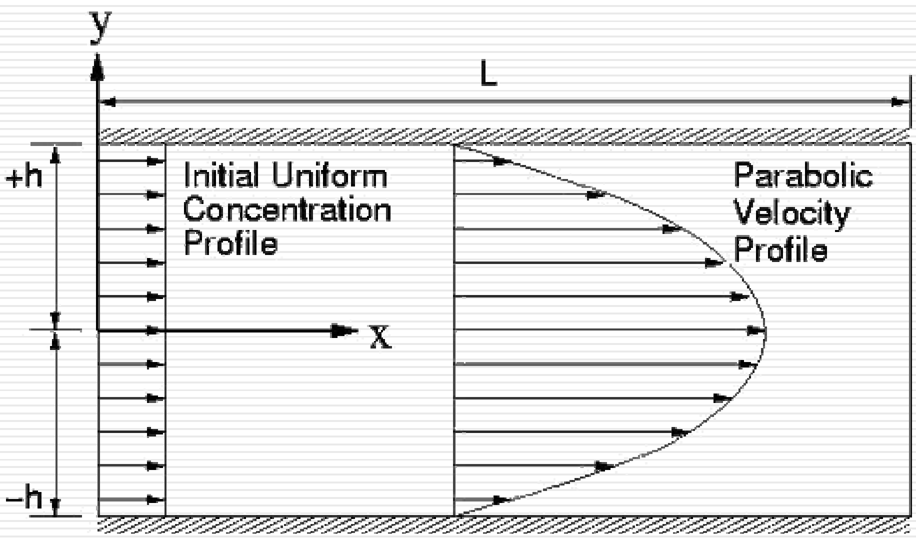
- The convective diffusion equation (Friedlander, 2000):

$$\underbrace{\frac{\partial n}{\partial t}}_{\text{transient term}} + \underbrace{\mathbf{v} \cdot \nabla n}_{\text{convection}} = \underbrace{D \nabla^2 n}_{\text{diffusion}} - \underbrace{\nabla \cdot \mathbf{c} n}_{\text{external forces}}$$

- where,
  - n - particle concentration (number per unit volume)
  - $\mathbf{v}$ – gas velocity distribution
  - D – diffusion coefficient
  - $\mathbf{c}$ – particle migration velocity resulting from external forces

Convective Diffusion APM Model

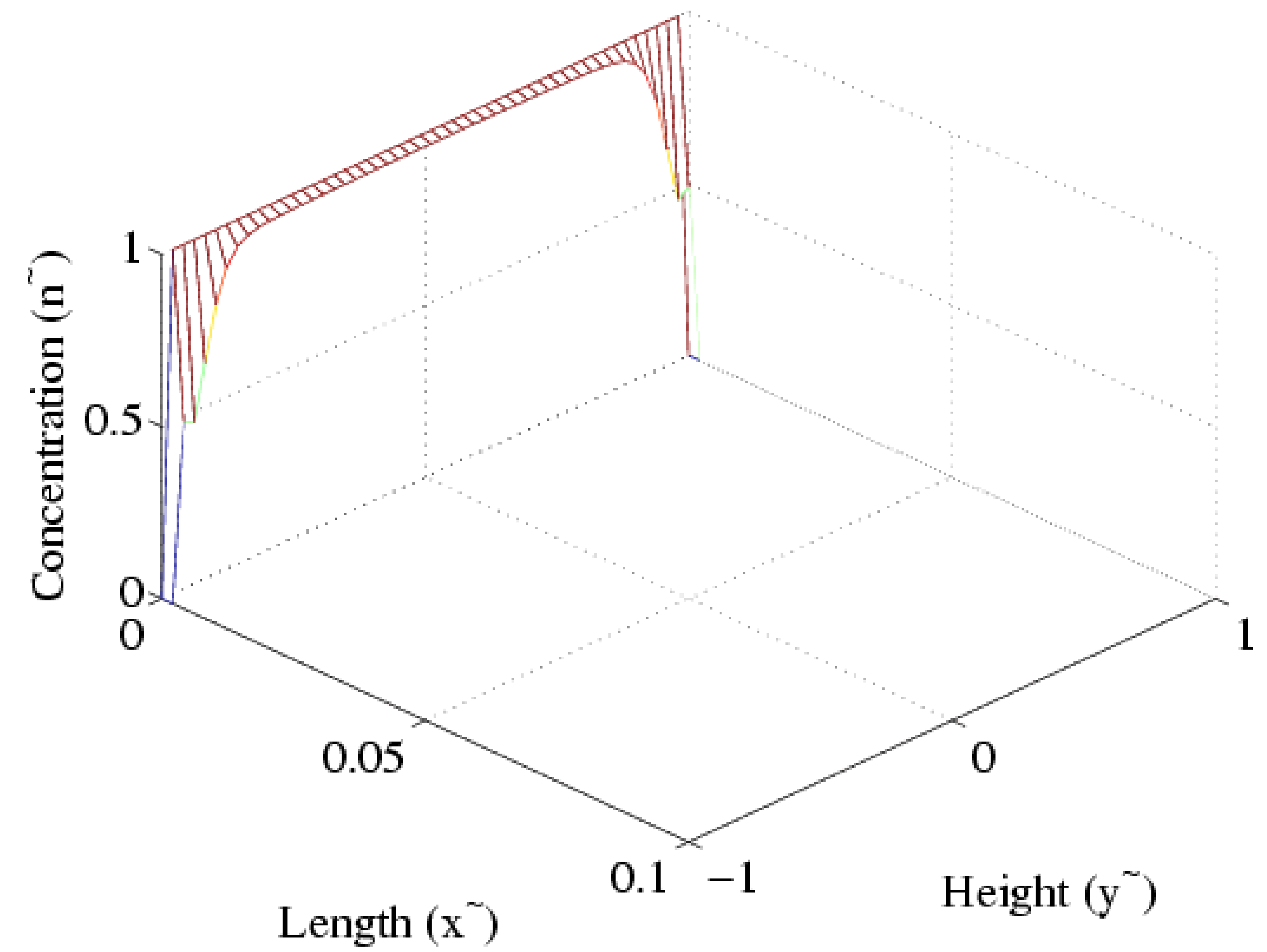
- Model the APM as two parallel plates (where, gap << radius)
- Initial particle concentration is uniform at inlet, n_o
- Flow is laminar & parabolic
- Assume no diffusion in ‘x’ direction
- Assume steady-state conditions



Convective Diffusion APM Model - Solution

- The equation is non-dimensionalized, and represented in terms of:
  - non-dimensional concentration: $\tilde{n}$
  - non-dimensional height: $\tilde{y}$
  - non-dimensional length: $\tilde{x}$
  - non-dimensional force constants: $\tilde{a}_2, \tilde{a}_1, \tilde{a}_0$
- The parabolic partial differential equation is solved with the implicit Crank-Nicolson numerical method.
- Crank-Nicolson method is convergent and stable for all finite step sizes.

Solution Results – Balanced External Forces

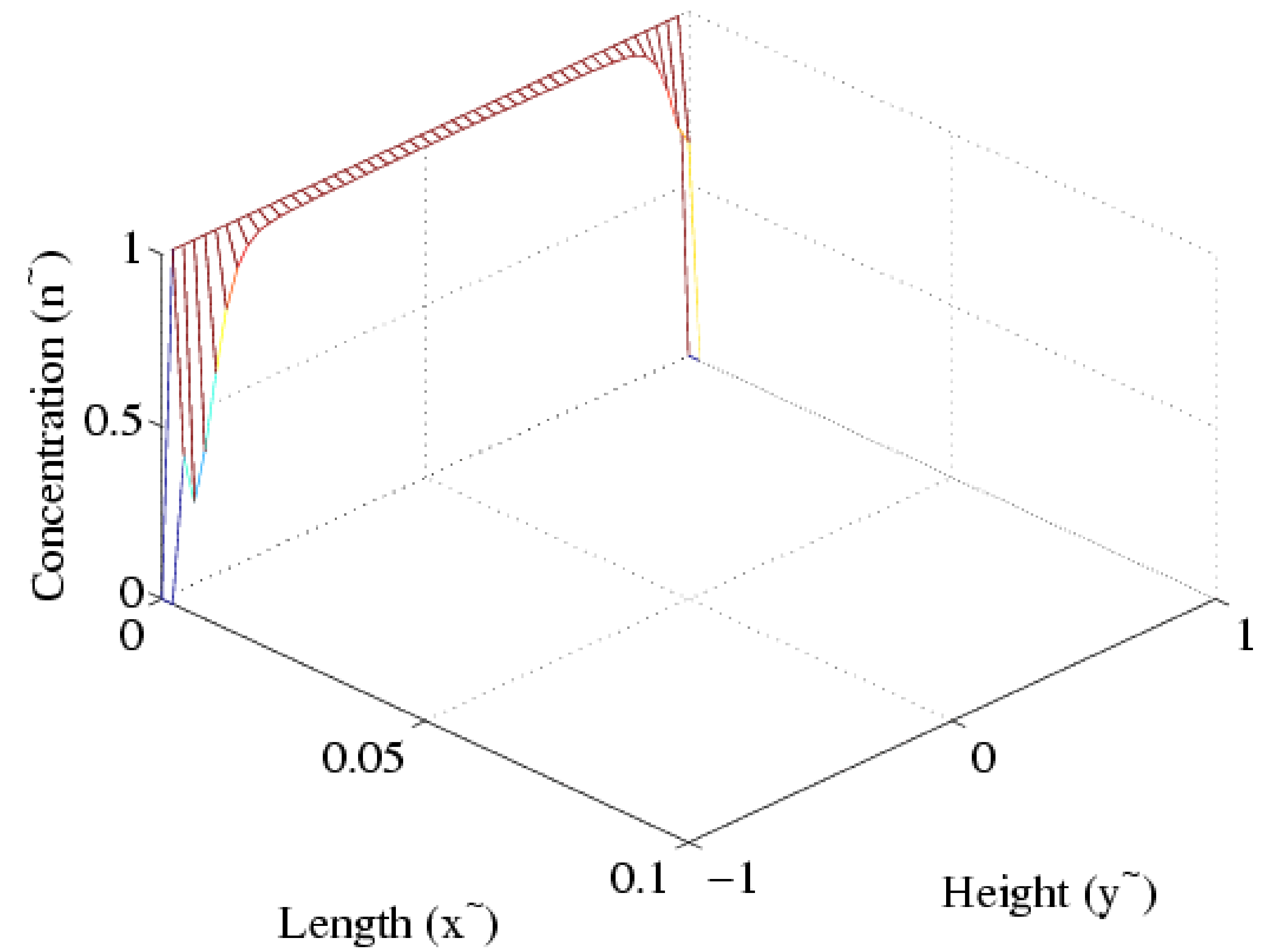


$$\tilde{a}_2 = 0$$

$$\tilde{a}_1 = 5$$

$$\tilde{a}_0 = 0$$

Solution Results – Strong Centripetal Force

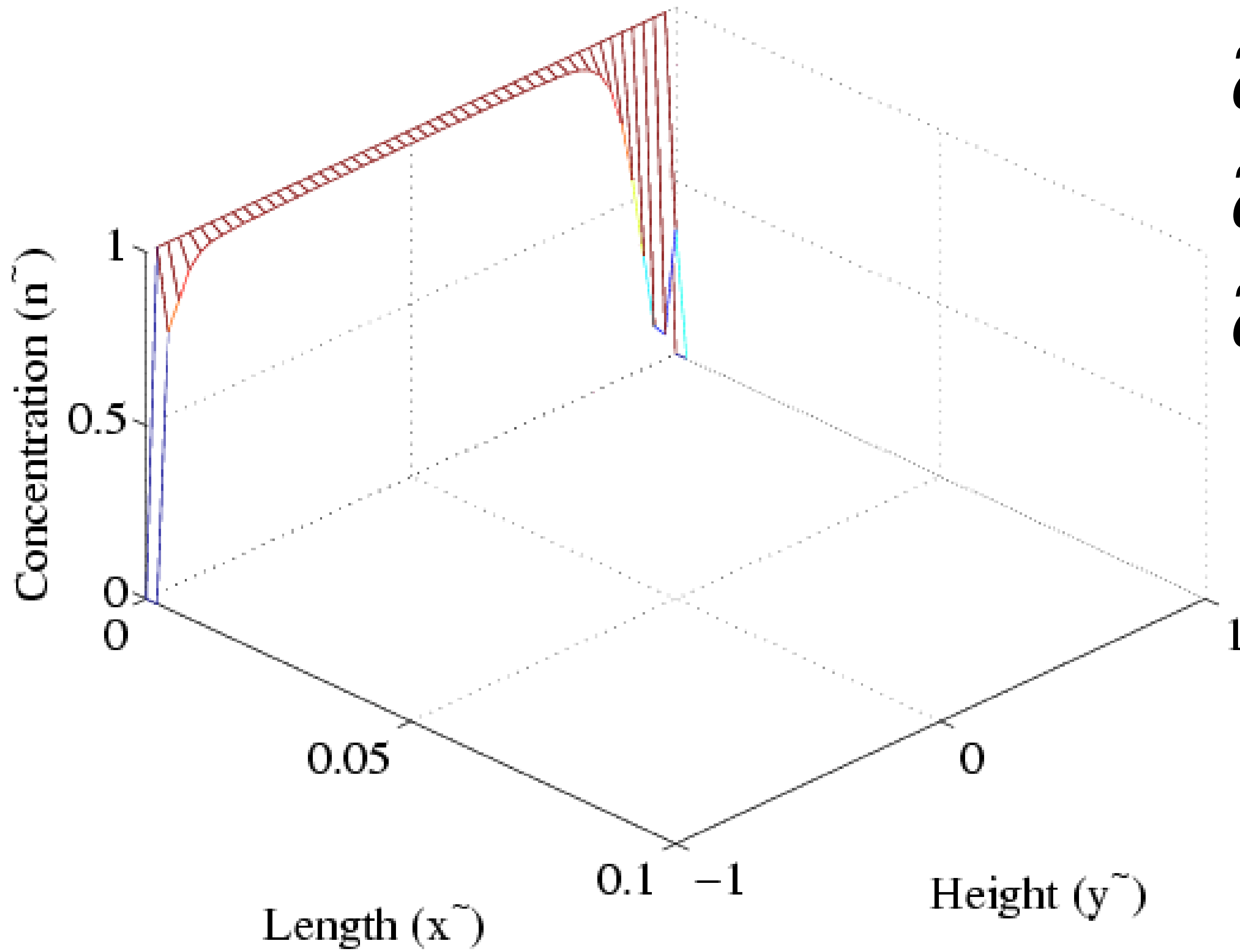


$$\tilde{a}_2 = 0$$

$$\tilde{a}_1 = 5$$

$$\tilde{a}_0 = 10$$

Solution Results – Strong Electrostatic Force



$$\tilde{a}_2 = 0$$

$$\tilde{a}_1 = 5$$

$$\tilde{a}_0 = -20$$

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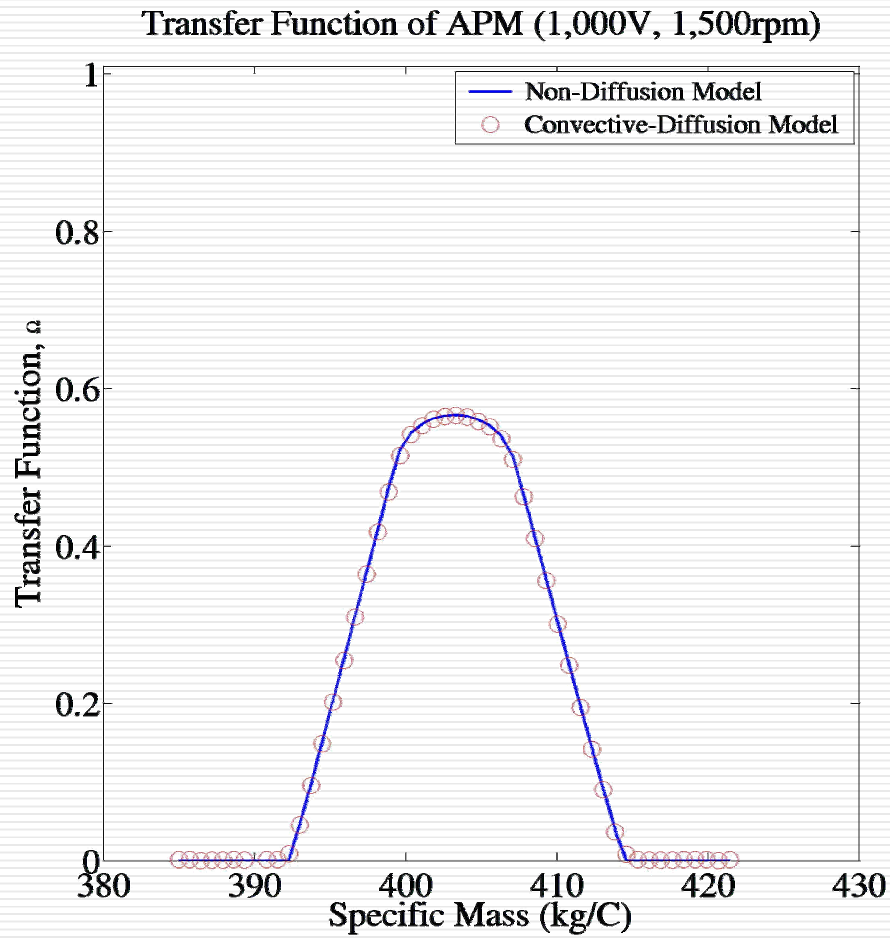
Comparing Results to Non-Diffusion Model

- Comparisons between models can be made by looking at transfer functions.

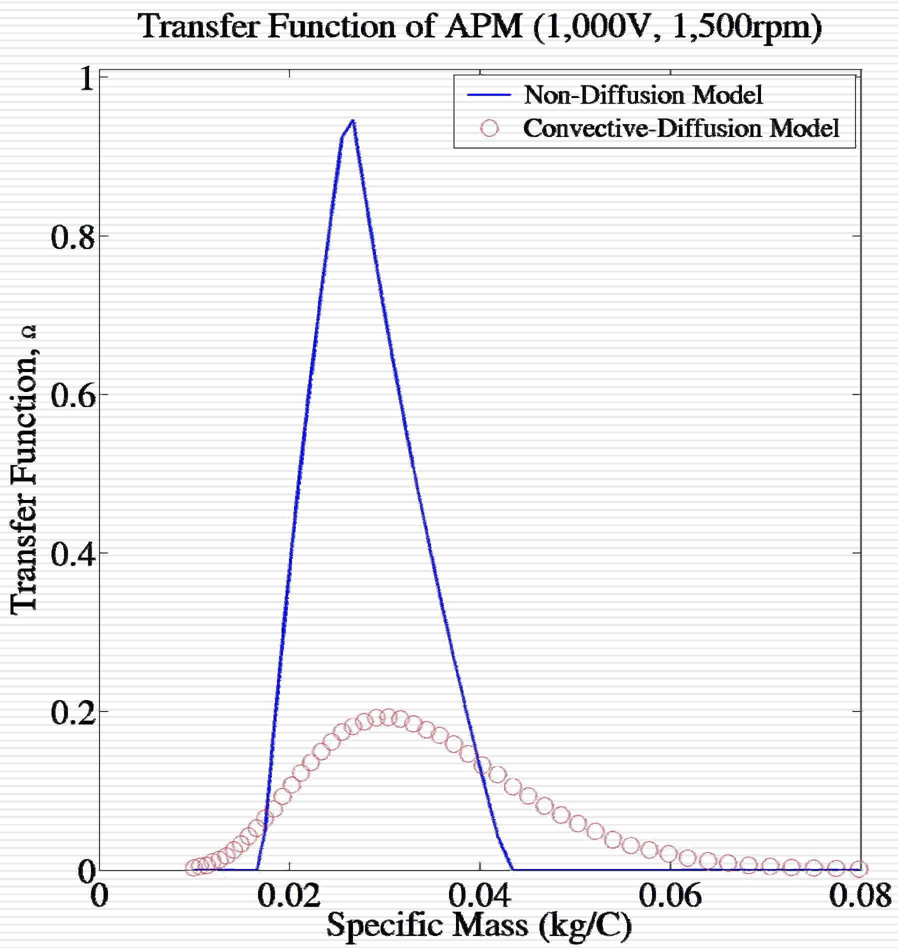
$$\text{Transfer Func., } \Omega = \frac{\text{Flux of Exiting Particles}}{\text{Flux of Entering Particles}}$$

- For large particles (where diffusion effects are small), non-diffusion model and Convective Diffusion model give matching results.



400 kg/C specific mass ≈ 500 nm diameter for single-charged particle of unit density

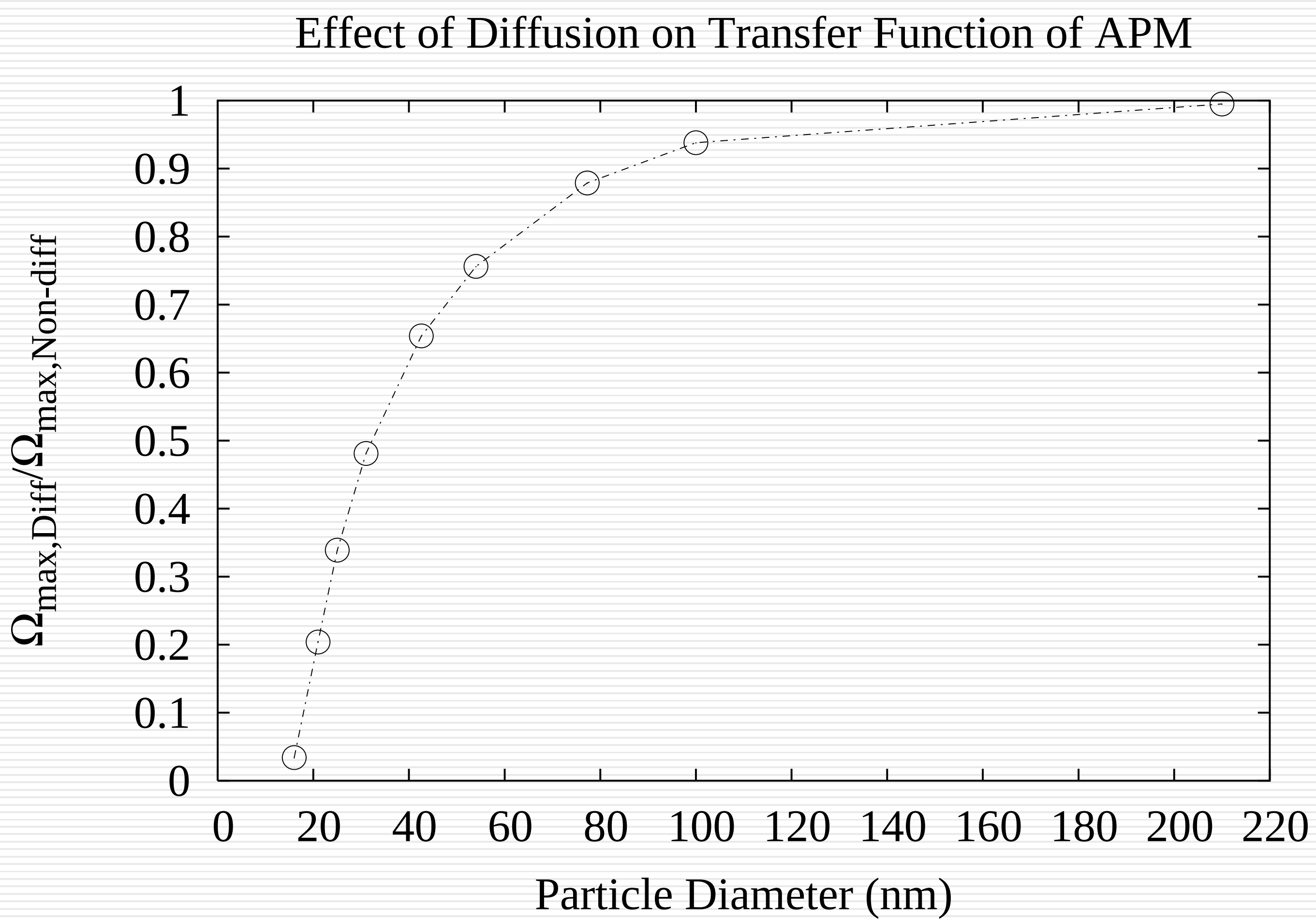
Comparing Results to Non-Diffusion Model



0.03 kg/C specific mass ≈ 20 nm diameter for single-charged particle of unit density

- For small particles (where diffusion effects are large), the transfer function broadens and reduces in height

Effect of Diffusion on APM

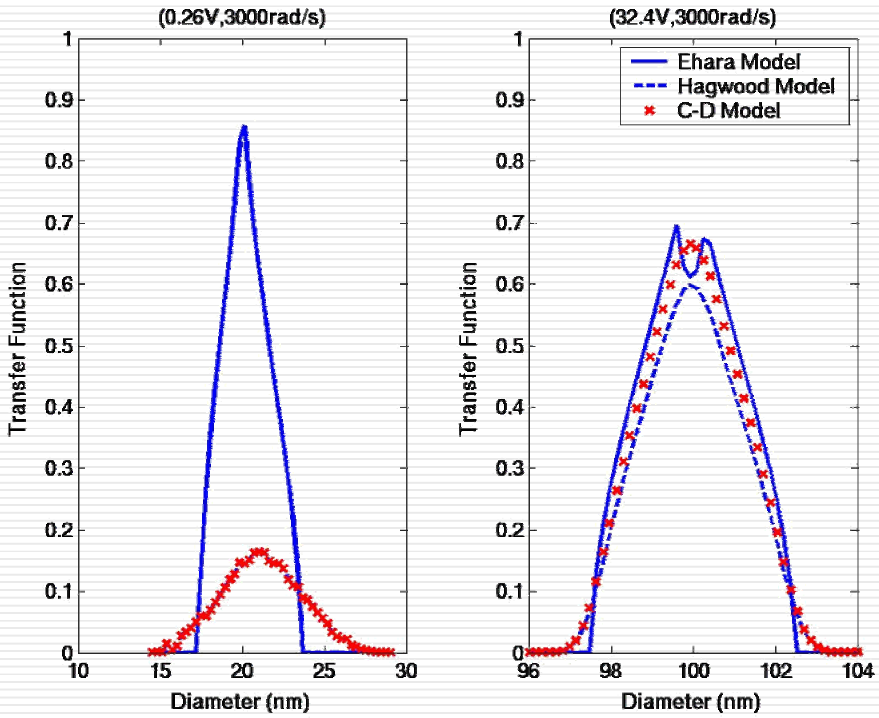


Comparing Results to Monte-Carlo Diffusion Model

- Hagwood used a different definition of the transfer function, Ω.

$\Omega =$ Probability particle will exit APM

- Results agree for small particles. For larger particles the C-D model gives a slightly higher transfer function.



Summary

- A Convective Diffusion model of the APM has been developed.
- The C-D model agrees well with Ehara's non-diffusion model when diffusion effects are small.
- Diffusion effects are significant for small particles (broadens and reduces transfer function).
- Results agree fairly well with Hagwood's Monte-Carlo diffusion model.

Questions/Comments?