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Theory and Experimental Validation of the AAC Data Inversion

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Division A: Energy, Fluid Mechanics and Turbomachinery

Overview

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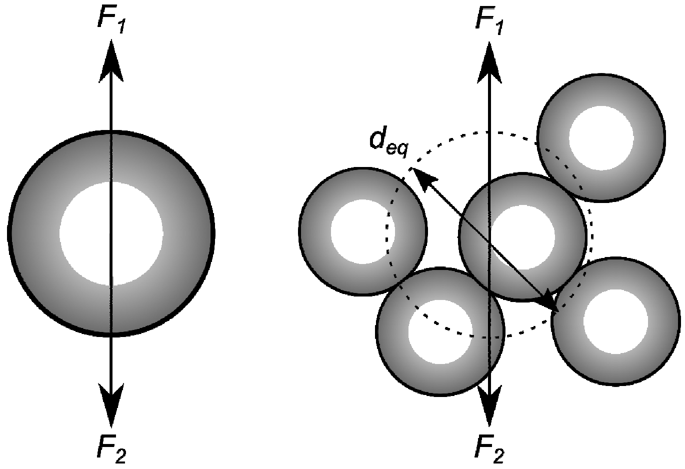
Equivalent Particle Diameters



Equivalent Diameter, d_{eq}	Force 1, F_1	Force 2, F_2
Aerodynamic Diameter, d_a	Weight/ Centrifugal	Drag
Electrical Mobility Diameter, d_m	Electrostatic	Drag

- Particle Relaxation Time (τ):

$$\tau = m \cdot B = \frac{C_c(d_a) \cdot \rho_o \cdot d_a^2}{18\mu} = \frac{C_c(d_m) \cdot \rho_{eff} \cdot d_m^2}{18\mu} = \frac{C_c(d_{ve}) \cdot \rho_p \cdot d_{ve}^2}{18\mu \cdot \chi}$$

Where m is the particle mass, B is the particle mobility, C_c is the Cunningham Slip Correction, μ is the viscosity of the surrounding gas, ρ_o is unit density (1000 kg/m^3), ρ_{eff} is the effective density of the particles, ρ_p is the particle material density, d_{ve} is the volume equivalent diameter and χ is the particle shape factor.

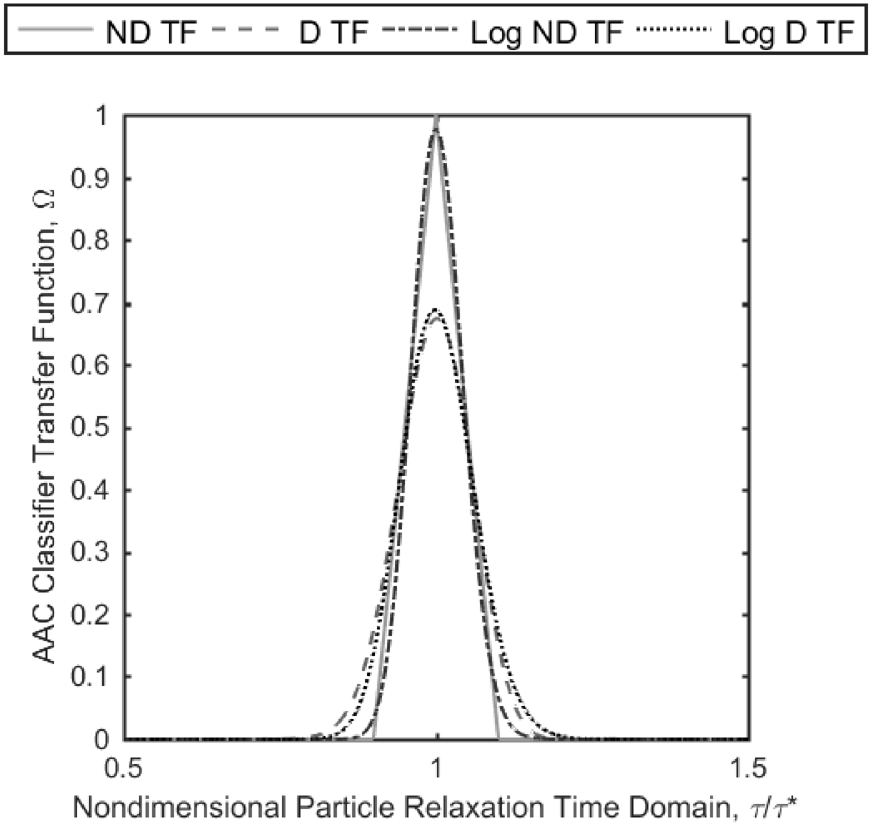
AAC Introduction and Theory

CAMBUSTION

Aerodynamic Aerosol Classifier

Animation provided by Cambustion (http://www.cambustion.com/products/aac)

AAC Transfer Function (TF) - Balanced Flows

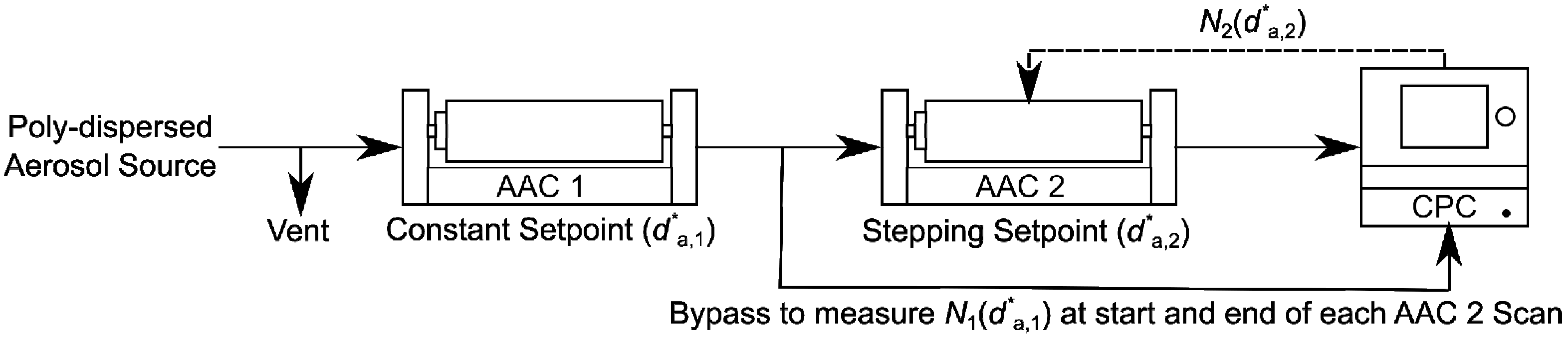


AAC Setpoint: $\tau^* = \frac{Q_{\mathrm{sh}}+Q_{\mathrm{exh}}}{\pi w^2 (r_1+r_2)^2 L}$

Non-dimensional Flow Parameter: $\beta = \frac{Q_{\mathrm{a}}}{Q_{\mathrm{sh}}}$

- Non-diffusing (ND) transfer function is based on the particle streamline model (Tavakoli and Olfert, 2013)
- Diffusing (D) transfer function assumes that diffusion spreads the particles in a Gaussian distribution about the particle streamline model (Tavakoli and Olfert, 2013)
- Lognormal (Log) approximation of the AAC transfer function was calculated following the theory developed by Stolzenburg and McMurry (2008) to represent the DMA transfer function lognormally

TF Characterization using a Tandem AAC Setup



- Upstream AAC (AAC 1) is set at a constant setpoint and selects one aerodynamic particle diameter from the poly-dispersed aerosol source.
- Downstream AAC (AAC 2) steps through the aerodynamic diameter domain of the classified particles and records the corresponding doubly classified particle concentration at each setpoint.

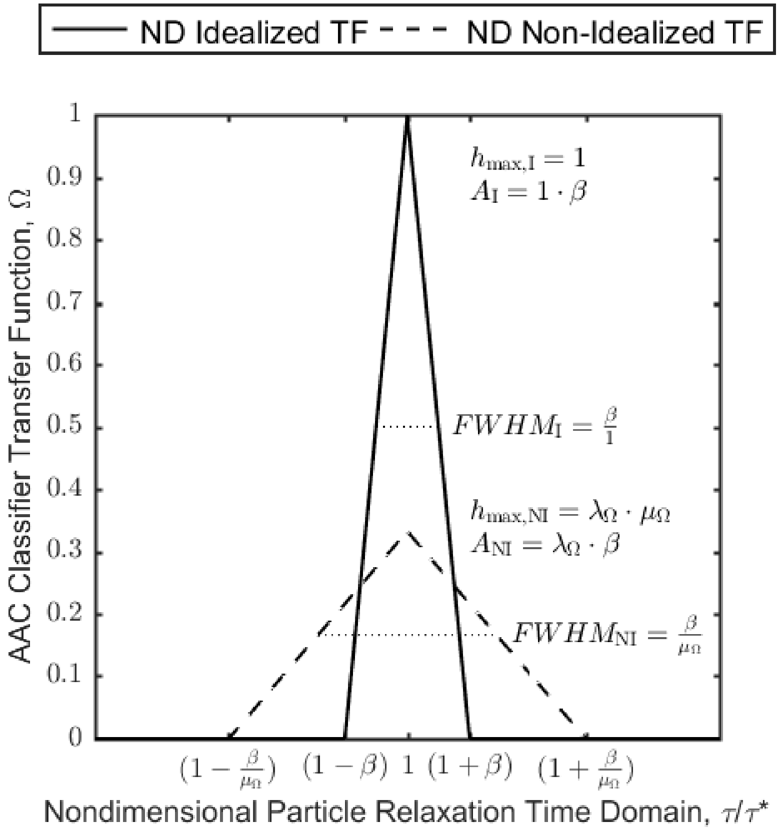
Parameterized TF for Tandem AAC Deconvolution

- Similar to Martinson et al.’s (2001) characterization of the Differential Mobility Analyzer (DMA) transfer function, the AAC transfer function was parameterized to capture non-ideal behaviour, such as particle diffusion and losses, using:
  - Transmission Efficiency (λ_Ω)

    Scales area under transfer function
  - Transfer Function Width Factor (μ_Ω)

    Scales transfer function FWHM

$$\Omega_{\mathrm{NI}}(\tau,\tau^*,\beta,\lambda_\Omega,\mu_\Omega) = \begin{cases} \lambda_\Omega \cdot \mu_\Omega \left[1+\dfrac{\mu_\Omega}{\beta}\cdot\left(\dfrac{\tau}{\tau^*}-1\right)\right] & \text{if } \left(1-\dfrac{\beta}{\mu_\Omega}\right)\cdot\tau^* \le \tau \le \tau^* \\ \lambda_\Omega \cdot \mu_\Omega \left[1+\dfrac{\mu_\Omega}{\beta}\cdot\left(1-\dfrac{\tau}{\tau^*}\right)\right] & \text{if } \tau^* < \tau \le \left(1+\dfrac{\beta}{\mu_\Omega}\right)\cdot\tau^* \\ 0 & \text{elsewhere} \end{cases}$$

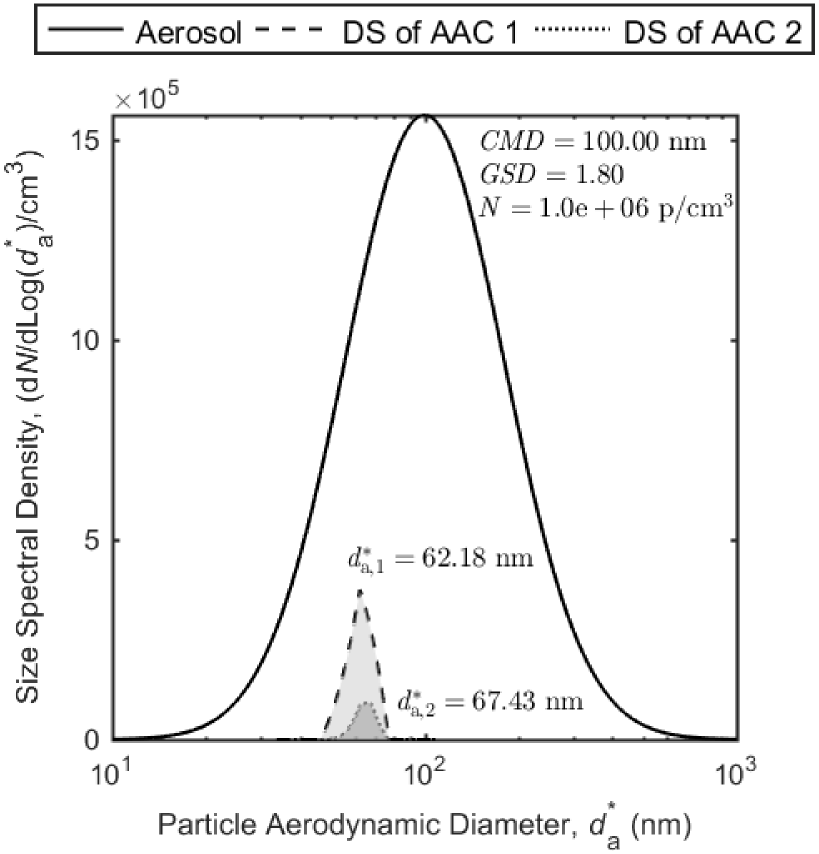


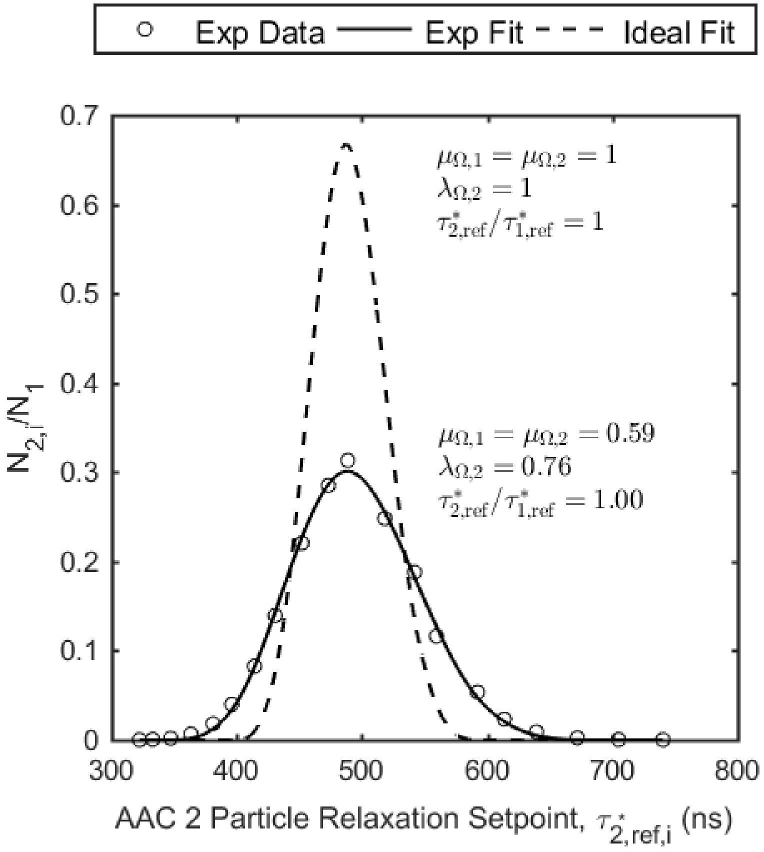
AAC Setpoint: $\tau^* = \frac{Q_{\mathrm{sh}}+Q_{\mathrm{exh}}}{\pi w^2 (r_1+r_2)^2 L}$

Non-dimensional Flow Parameter: $\beta = \frac{Q_\mathrm{a}}{Q_{\mathrm{sh}}}$

Tandem AAC Theory and Deconvolution

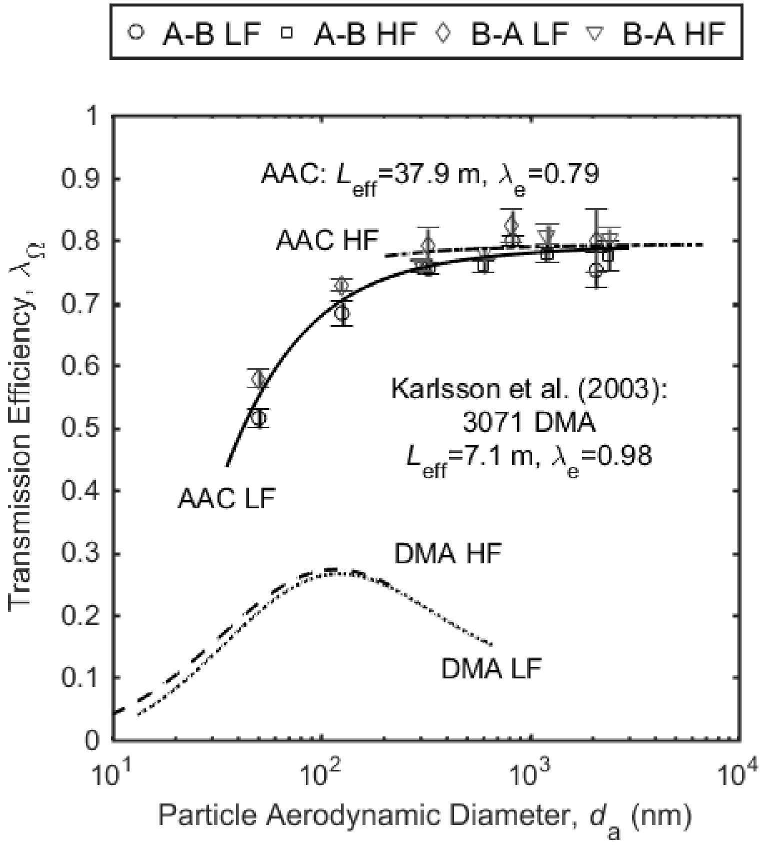
$$\frac{N_2(\tau_2^*)}{N_1} = \frac{\int \eta_i(d_{\mathrm{a},2})\cdot\Omega_{\mathrm{NI},1}(\tau_1,\tau_1^*,\beta_1,\lambda_{\Omega,1},\mu_{\Omega,1})\cdot\Omega_{\mathrm{NI},2}(\tau_2,\tau_2^*\cdot\tau_{\mathrm{agree}}^*,\beta_2,\lambda_{\Omega,2},\mu_{\Omega,2})\cdot\mathrm{d}N_i}{\int \eta_i(d_{\mathrm{a},1})\cdot\Omega_{\mathrm{NI},1}(\tau_1,\tau_1^*,\beta_1,\lambda_{\Omega,1},\mu_{\Omega,1})\cdot\mathrm{d}N_i}$$





Transmission Efficiency, λ_Ω

Scales area under AAC transfer function



LF: $Q_\mathrm{a}/Q_\mathrm{sh} = 0.3/3\ \mathrm{LPM}$, HF: $Q_\mathrm{a}/Q_\mathrm{sh} = 1.5/15\ \mathrm{LPM}$

- AAC transmission efficiency $(\lambda_{\Omega,\mathrm{AAC}})$ at aerodynamic diameter (d_a) can be estimated from:

$$\lambda_{\Omega,\mathrm{AAC}} = \lambda_\mathrm{D}(d_\mathrm{a}) \cdot \lambda_\mathrm{e}$$

- DMA transmission efficiency $(\lambda_{\Omega,\mathrm{DMA}})$ at electrical mobility diameter (d_m) can be estimated from:

$$\lambda_{\Omega,\mathrm{DMA}} = \lambda_\mathrm{D}(d_\mathrm{m}) \cdot \lambda_\mathrm{e} \cdot f_n(d_\mathrm{m})$$

Where:

- λ_e is the losses due to classifier entrance/exit effects
- λ_D is the diffusional penetration (Karlsson et al., 2003):

$$\lambda_\mathrm{D} = \begin{cases} 0.819\mathrm{e}^{-11.5\delta} + 0.0975\mathrm{e}^{-70.1\delta} + 0.0325\mathrm{e}^{-179\delta} & \delta \geq 0.007 \\ 1 - 5.50\delta^{2/3} + 3.77\delta + 0.814\delta^{4/3} & \delta < 0.007 \end{cases}$$

- f_n is the fraction of particles with mobility diameter d_m neutralized to a minus one charge state [estimated by Wiedensohler (1988) and Gunn et al. (1956)].

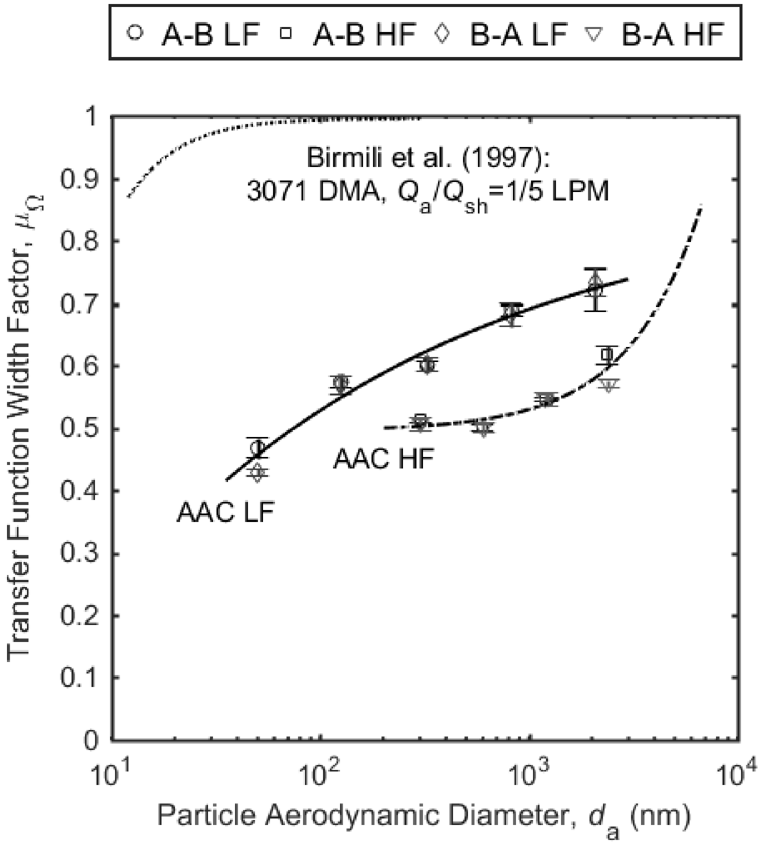
- The non-dimensional deposition parameter (δ):

$$\delta(d_\mathrm{p}) = \frac{L_\mathrm{eff} \cdot D(d_\mathrm{p})}{Q_\mathrm{a}}$$

Where L_eff is the length of a circular tube with the same diffusion deposition as the classifier, D is the diffusion coefficient of the particles with diameter d_p and Q_a is the aerosol flowrate into the classifier.

Transfer Function Width Factor, μ_Ω

Scales width of AAC transfer function



LF: $Q_a/Q_{sh} = 0.3/3$ LPM, HF: $Q_a/Q_{sh} = 1.5/15$ LPM

The transfer function width factor of the AAC $\left(\mu_{\Omega,\mathrm{AAC}}(d_\mathrm{a})\right)$ or DMA $\left(\mu_{\Omega,\mathrm{DMA}}(d_\mathrm{m})\right)$ can be estimated from:

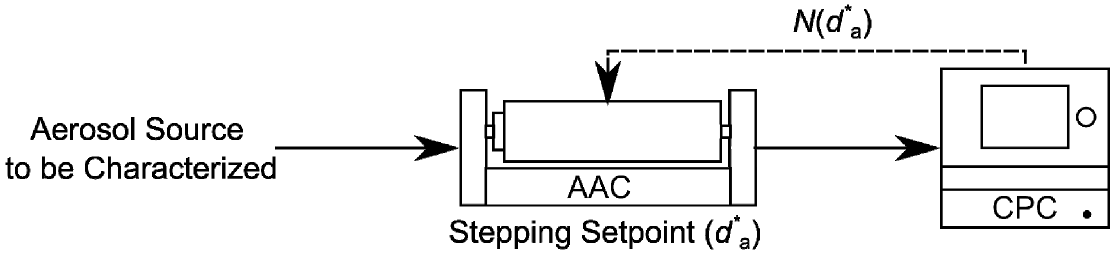
$$\mu_\Omega(d_\mathrm{p}) = a \cdot d_\mathrm{p}^b + c$$

Where d_p is the particle diameter in nm.

Instrument	*a*	*b*	*c*
DMA$^\alpha$	-11.05	-1.739	0.9956
AAC LF	-1.202	-0.2663	0.8805
AAC HF	7.144e-06	1.229	0.4947

$^\alpha$ Based on data collected by Birmili et al. (1997)

Aerodynamic Size Distribution Measurement



- This setup measures the aerodynamic size distribution $\left(\frac{\mathrm{d}N}{\mathrm{dlog}d_\mathrm{a}}\right)$ of a steady-state aerosol.
- The AAC steps through the aerodynamic diameter domain of the aerosol source and records the corresponding classified particle concentration as a function of it’s aerodynamic diameter setpoint.

AAC Inversion- Raw Measurements to d*N*/dlog*d*$_a$

- Stolzenburg and McMurry (2008) determined:

$$N_i = \int \eta_i(d_\mathrm{a}) \cdot \Omega(\tau_i) \cdot \mathrm{d}N_i$$

Where N_i is the particle concentration downstream of the classifier, η_i is the particle detector counting efficiency and Ω is the classifier transfer function at particle relaxation time setpoint τ_i.

- Applying the AAC Non-Ideal Transfer Function to this equation yields the following solution:

$$\left.\frac{\mathrm{d}N}{\mathrm{dlog}d_\mathrm{a}}\right|_{i,\mathrm{NI}} = \frac{\ln(10) \cdot N_i}{\eta_i \cdot \left.\frac{\mathrm{dlog}d_\mathrm{a}}{\mathrm{dlog}\tau}\right|_i \cdot \beta^*_{i,\mathrm{NI}}}$$

Where $\beta^*_{i,\mathrm{NI}}$ is a non-dimensional parameter that describes the transfer function resolution, and incorporates the transmission efficiency factor (λ_Ω) and width factor (μ_Ω) previously determined.

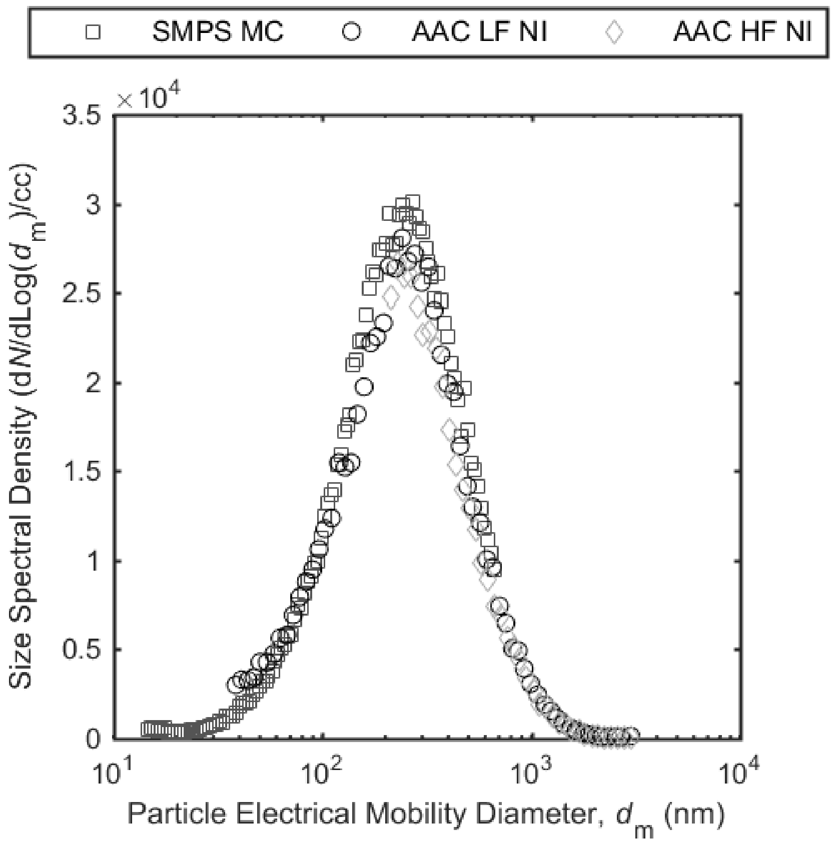
AAC Inversion Validation- AAC vs SMPS Theory

- To validate the AAC inversion, including its transfer function parameters (λ_Ω and μ_Ω), an AAC and SMPS were used in parallel to characterize the same aerosol source, however:
    - The SMPS measures the particle electrical mobility size spectral, $\frac{dN}{\mathrm{dlog}(d_\mathrm{m})}$
    - The AAC measures the particle aerodynamic size spectral, $\frac{dN}{\mathrm{dlog}(d_\mathrm{a})}$
- Therefore, the AAC's equivalent electrical mobility size distribution was calculated from its measured aerodynamic size distribution by:

$$\frac{dN}{\mathrm{dlog}(d_\mathrm{m})} = \frac{dN}{\mathrm{dlog}\left(d_\mathrm{a}\right)} \cdot \frac{k \cdot d_\mathrm{m}^{D_\mathrm{m}-1}}{\rho_\mathrm{O} \cdot d_\mathrm{a}} \cdot \frac{\left[D_\mathrm{m}-1+\frac{2.34\cdot\lambda\cdot(D_\mathrm{m}-2)}{d_\mathrm{m}}+1.05\cdot\lambda\cdot\exp\left(-0.39\cdot\frac{d_\mathrm{m}}{\lambda}\right)\cdot\left(\frac{D_\mathrm{m}-2}{d_\mathrm{m}}-\frac{0.39}{\lambda}\right)\right]}{\left[2\cdot d_\mathrm{a}+2.34\cdot\lambda+1.05\cdot\lambda\cdot\exp\left(-0.39\cdot\frac{d_\mathrm{a}}{\lambda}\right)\cdot\left(1-\frac{0.39\cdot d_\mathrm{a}}{\lambda}\right)\right]}$$

    - Derived from the definition of particle relaxation time: $\tau = \frac{C_c(d_m)\cdot\rho_{eff}\cdot d_m^2}{18\cdot\mu}$
    - Assumes fractal effective particle density: $\rho_\mathrm{eff}(d_\mathrm{m}) = k \cdot d_\mathrm{m}^{D_\mathrm{m}-3}$
    - Cunningham slip correction function was estimated following Allen and Raabe (1985)

AAC Inversion Validation- AAC vs SMPS Results



- DOS nebulized by constant output atomizer
- Both the SMPS multiple-charge correction$^\alpha$, and AAC losses/broadening correction were significant and required
- High degree of agreement between corrected AAC and SMPS/CPC measurements (*CMD*, *GSD* and N_{total} agreement of -0.8%, 1.2% and 1.4% respectively)

	CMD (nm)	*GSD*	N_{total} (p/cm^3)	Percent Difference from:	
				CPC N_{total}	SMPS MC *CMD*
SMPS Raw Data	212.90	1.82	3.12E+04	62.6%	-13.3%
AAC LF Raw Data	258.11	1.94	1.37E+04	-28.5%	5.1%
SMPS MC Corrected	245.58	1.98	2.15E+04	**11.8%**	N/A
AAC LF λ and μ Corrected	243.58	2.00	1.95E+04	**1.4%**	**-0.8%**
CPC (Direct Measurement)	N/A	N/A	1.92E+04	N/A	N/A

$^\alpha$ SMPS multiple-charge correction was applied following He et al. (2013) with the particle charging fractions estimated by Wiedensohler (1988) and Gunn et al. (1956).

Other Considerations: Varying Classifier Conditions

- Decarlo et. al (2004) determined:

$$d_{\mathrm{a}} = d_{\mathrm{ve}}\sqrt{\frac{1}{\chi}\cdot\frac{\rho_{\mathrm{p}}}{\rho_{\mathrm{o}}}\cdot\frac{Cc(d_{\mathrm{ve}})}{Cc(d_{\mathrm{a}})}}$$

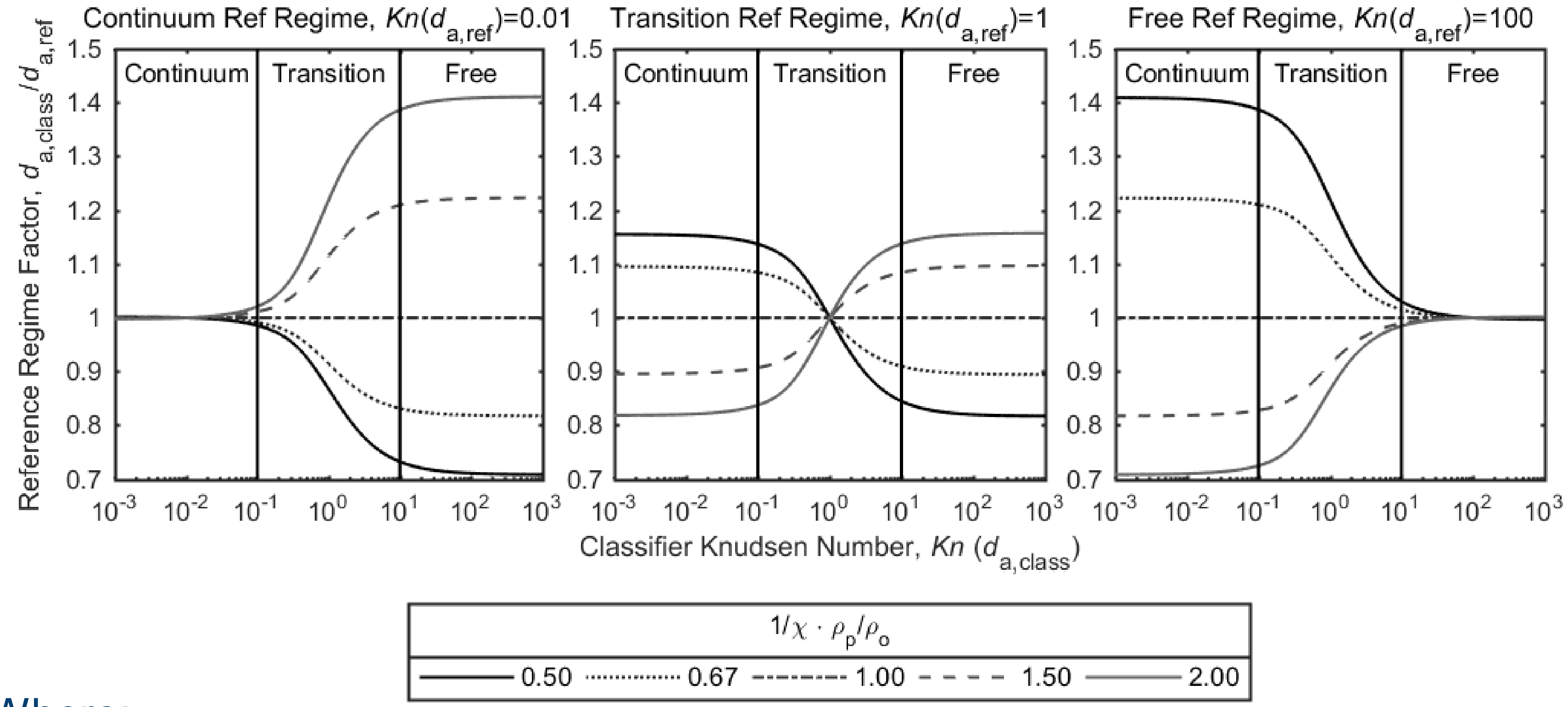
  Where d_{a} is the particle aerodynamic diameter, d_{ve} is the particle volume equivalent diameter, χ is the shape factor and Cc is the Cunningham slip correction.

- Since d_{ve} in an intrinsic particle property, it can be used to relate the change in d_{a} at different conditions (i.e. classifier versus reference):

$$\frac{d_{\mathrm{a,class}}}{d_{\mathrm{a,ref}}} = \sqrt{\frac{Cc(d_{\mathrm{ve}})_{\text{@ Classifier Conditions}}}{Cc(d_{\mathrm{ve}})_{\text{@ Reference Conditions}}}\cdot\frac{Cc\left(d_{\mathrm{a,ref}}\right)_{\text{@ Reference Conditions}}}{Cc\left(d_{\mathrm{a,class}}\right)_{\text{@ Classifier Conditions}}}}$$

Assumes χ is constant over regimes $(x_c \approx \chi_t \approx x_v)$

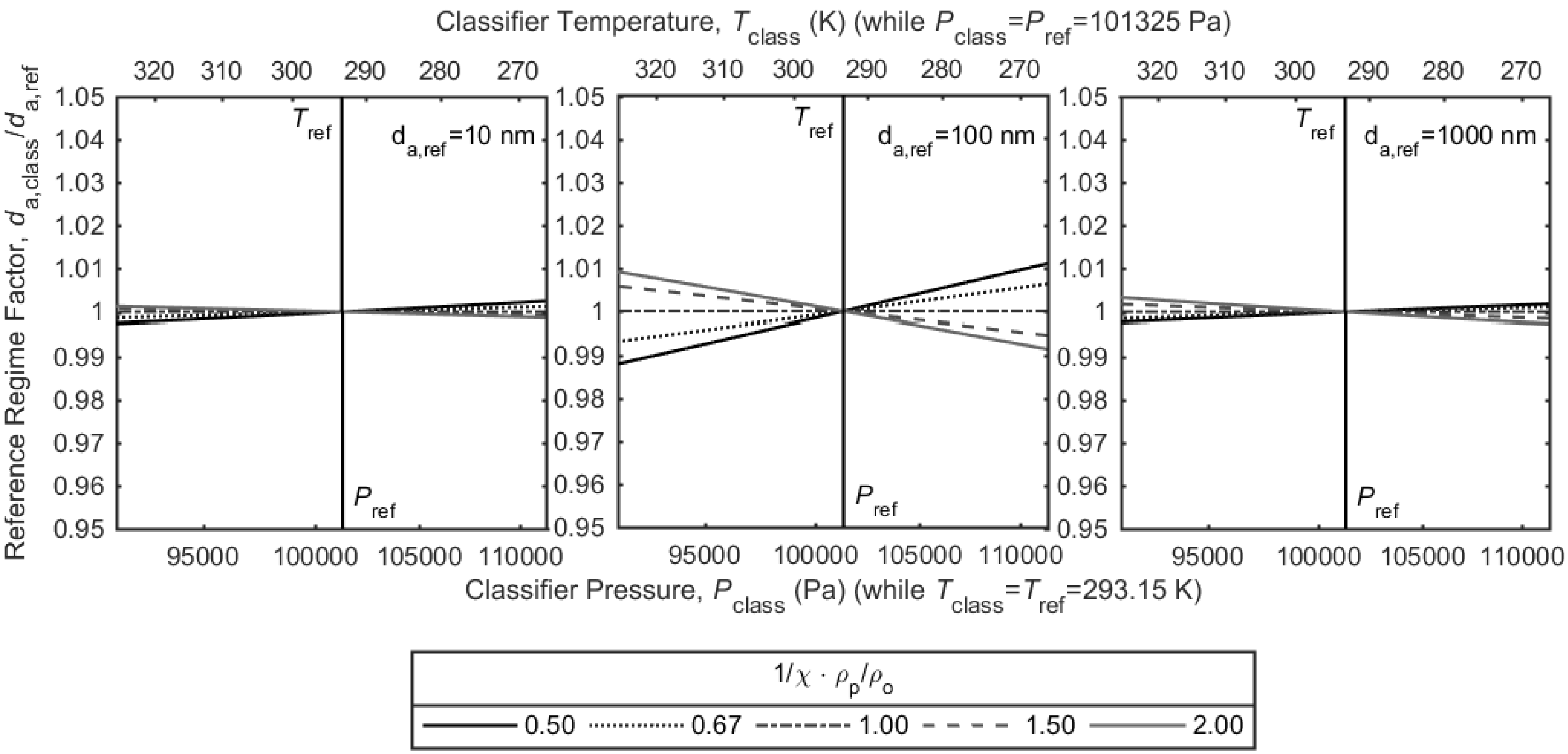
Kn at Classifier versus Reference Conditions



Where:

- Cc is only a function of Knudsen Number (Kn)
- At the same conditions: $Kn(d_{\mathrm{ve}}) = Kn(d_{\mathrm{a}})\frac{d_{\mathrm{a}}}{d_{\mathrm{ve}}} = Kn(d_{\mathrm{a}})\sqrt{\frac{1}{\chi}\cdot\frac{\rho_{\mathrm{p}}}{\rho_{\mathrm{o}}}\cdot\frac{Cc\big(Kn(d_{\mathrm{ve}})\big)}{Cc\big(Kn(d_{\mathrm{a}})\big)}}$

Considering Normal AAC Operating Conditions



Summary

- The AAC is a novel instrument that classifies particles based on their aerodynamic diameter.
- A tandem AAC setup was used to characterized the transfer function of individual AACs and experimentally determined:
  - High transmission efficiencies ($\lambda_\Omega \approx 80\%$); and
  - Transfer function broadening higher than predicted by theory ($\mu_\Omega \cong 0.45 \text{ to } 0.75$).
- The AAC transfer function inversion theory was developed and validated experimentally as shown by the high degree of agreement with SMPS measurements completed in parallel.
- The change in the selected particle aerodynamic diameter due to varying classifier temperature and pressure is negligible (<1%) within the AAC operating range.

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Questions?

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