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Soot Deposition and Gravitational Settling Modeling and the Impact of Particle Size and Agglomeration

Fire & Evacuation Modeling Technical Conference
Gaithersburg, MD
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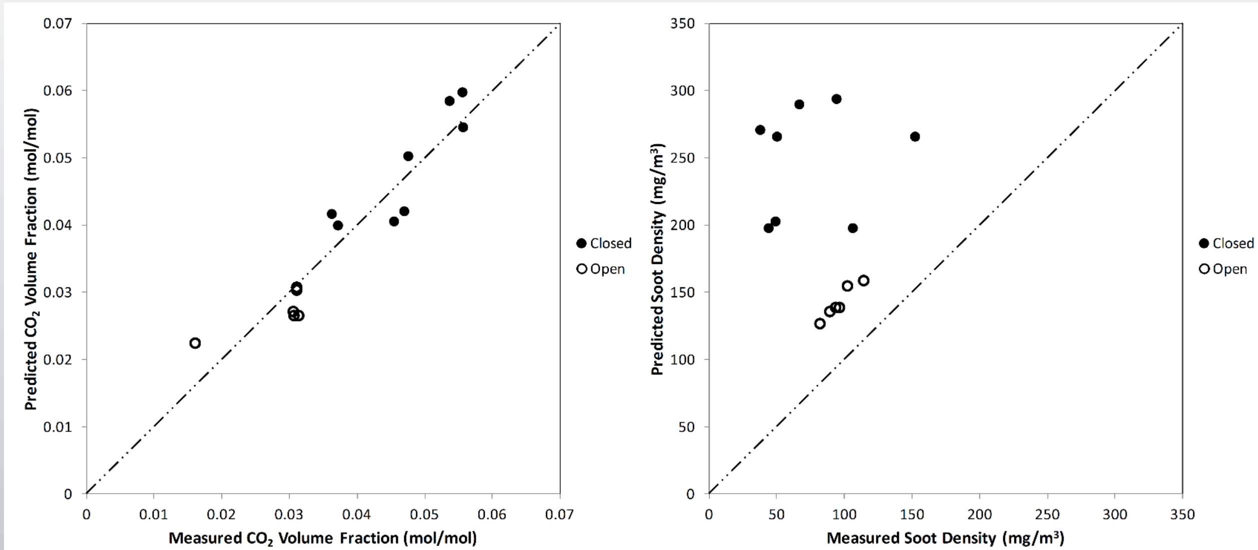
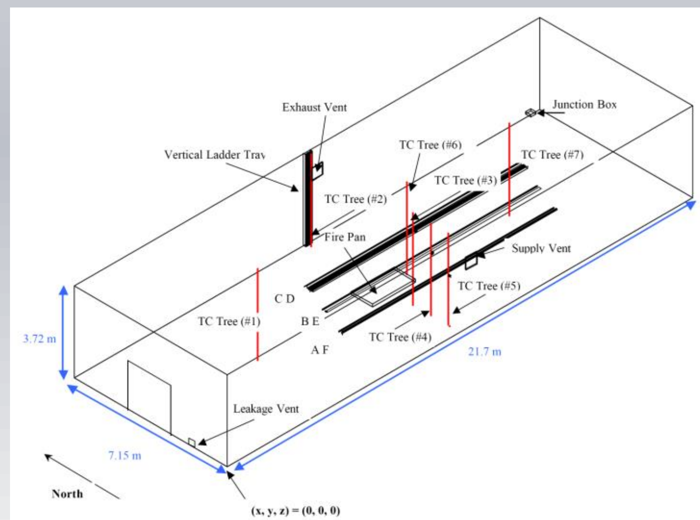
NIST/NRC Benchmark Series 3





Possible Causes

Burners were characterized in the open

Burner have to be more efficient in room

Soot oxidation

Temperatures remain well below 500 °C

Soot density derived from extinction measurements assuming 8700 m^2/kg

Would need different values for closed and open

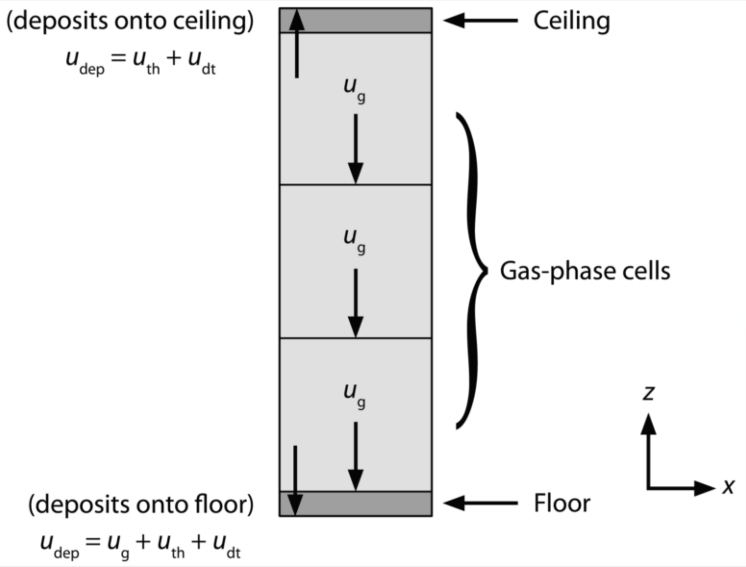
Deposition of soot on surface

Would impact closed more than open

Deposition to FDS 6

Gravitational

$$u_g = g m_a \frac{\mathrm{Cn}}{6\pi\chi_d \mu r_a}$$



Thermophoretic

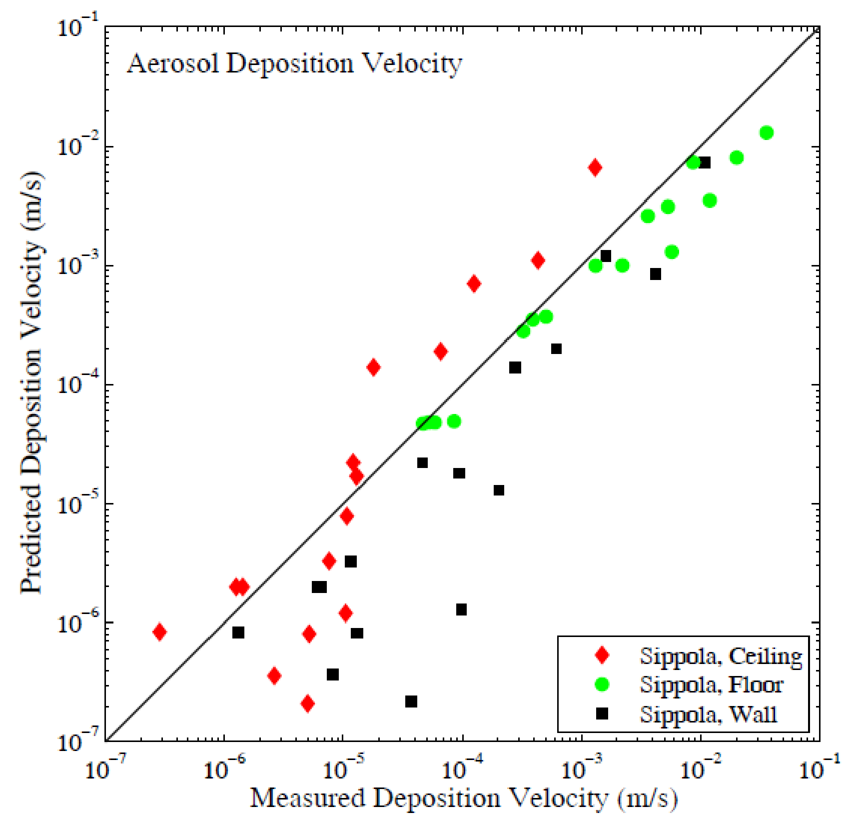
$$u_{th} = \frac{K_{th}}{T_g}\frac{\mathrm{d}T}{\mathrm{d}x} \qquad \frac{\mathrm{d}T}{\mathrm{d}x} = \frac{h\left(T_g - T_w\right)}{k_g}$$

Turbulent

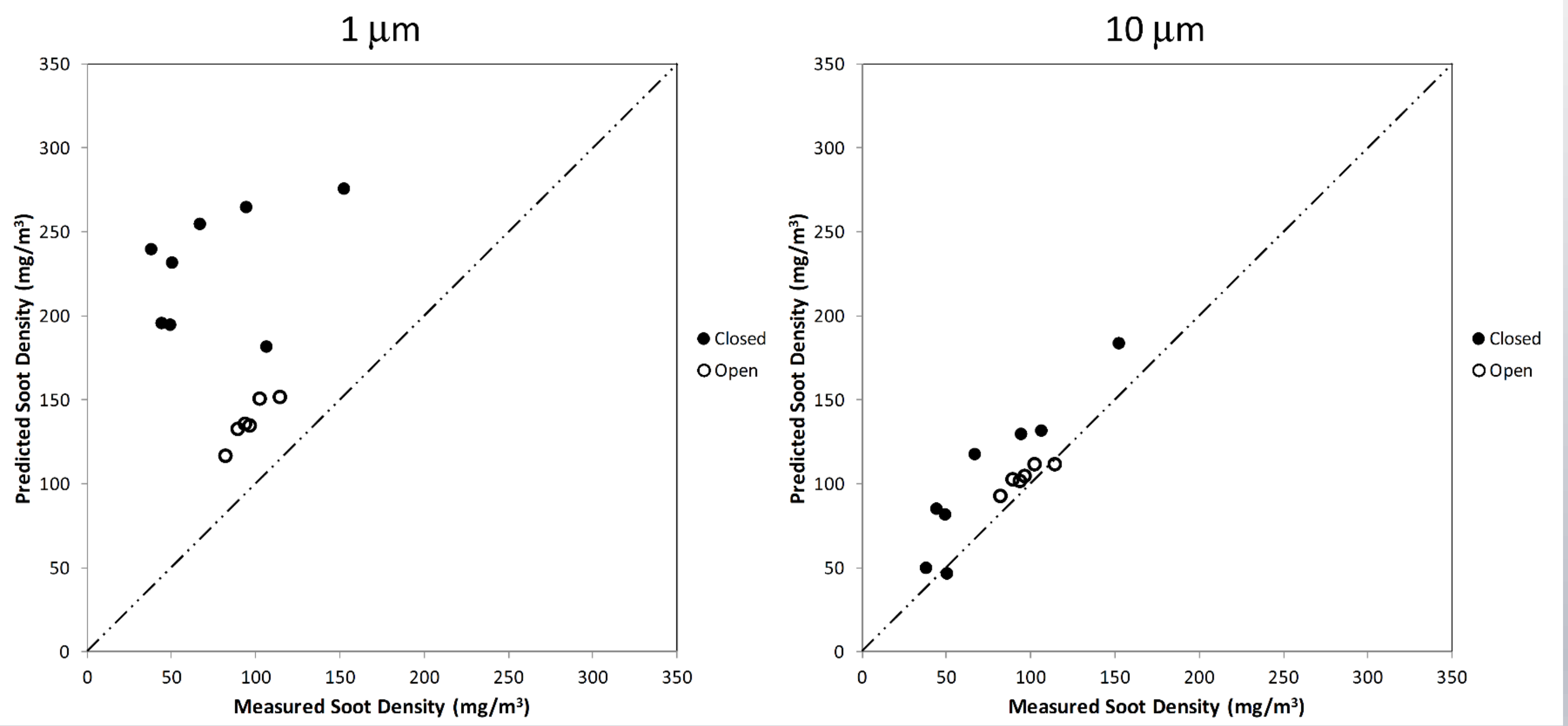
$$u_{dt} = \begin{cases} 0.086\mathrm{Sc}^{-0.7} u_\tau & \tau^+ \le 0.2 \\ 3.5\times10^{-4}\tau^{+2} u_\tau & 0.2 < \tau^+ \le 22.9 \\ 0.17 u_\tau & \tau^+ > 22.9 \end{cases} \qquad \tau^+ = \frac{\rho_a \left(2r_a\right)^2}{18\mu^2} u_t^2 \rho_g$$

Deposition in a Duct (u_t and u_g)

Test No.	Air Speed (m/s)	Particle Diameter (μm)	Particle Density (kg/m³)
1	2.2	1.0	1350
2	2.2	2.8	1170
3	2.1	5.2	1210
4	2.2	9.1	1030
5	2.2	16	950
6	5.3	1.0	1350
7	5.2	1.0	1350
8	5.2	3.1	1170
9	5.4	5.2	1210
10	5.3	9.8	1030
11	5.3	16	950
12	9.0	1.0	1350
13	9.0	3.1	1170
14	8.8	5.4	1210
15	9.2	8.7	1030
16	9.1	15	950



Effect of Particle Size



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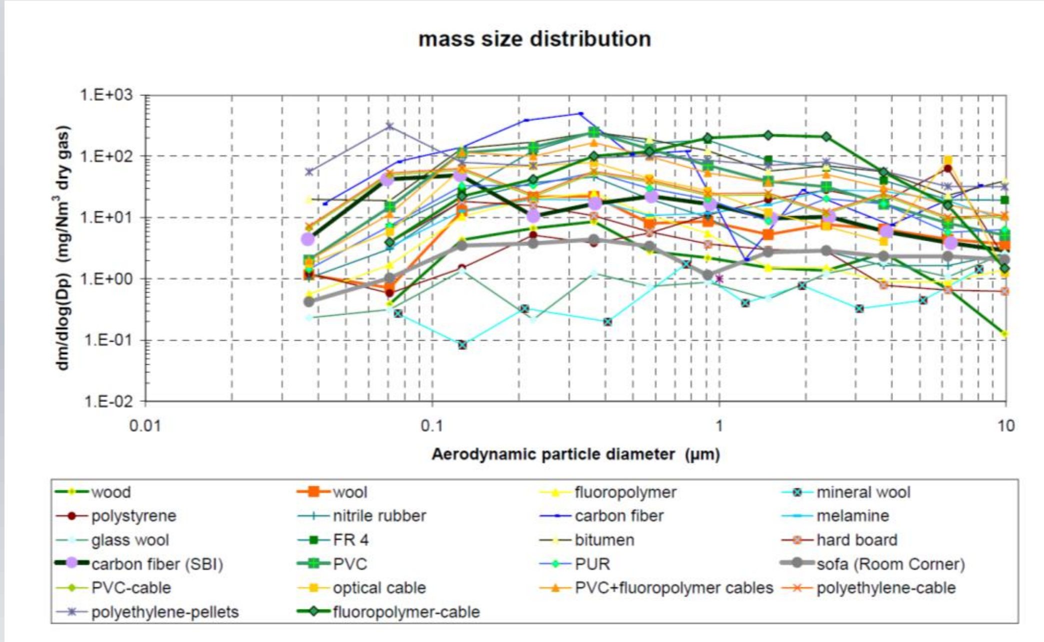
Particle Size

K_{th}, Cn, τ^+ all = f(r_a)

High-sooting fuels (toluene, acetylene) have particle diameters of 10 to 100 μm

Typical combustibles are 70 % at or below 1 μm with 5 % over 5 μm



Hertzberg, Blomqvist, Dalene, and Skarping, SP (2003)

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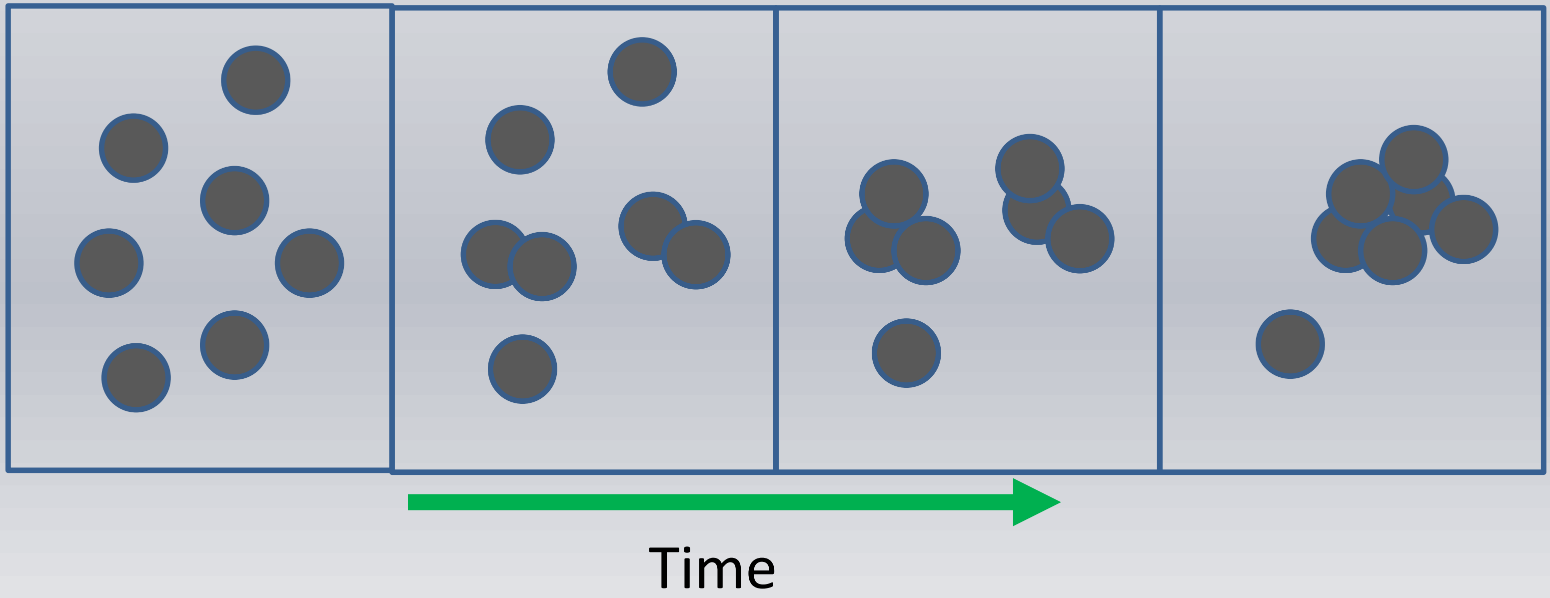
Agglomeration

Matching results requires large particles

For closed door gravitational likely dominates over time

Can get large particles by agglomeration – particles sticking together after collisions



Agglomeration

$$\frac{\partial N(m)}{\partial t} = \frac{1}{2}\int_0^m \Phi(\omega, m-\omega)N(\omega)N(m-\omega)\mathrm{d}\omega - N(m)\int_0^\infty \Phi(\omega, m)N(\omega)\mathrm{d}\omega - R(m) + S(m)$$

N=number density

Φ=agglomeration kernel

R=removal

S=source

m, ω=particle sizes

Discretized Form

Logarithmic particle bins

$$s = \left(\frac{m_{\max}}{m_{\min}} \right)^{1/M}, \quad m_i = s m_{i-1}, \quad x_i = \frac{2m_i}{1+s}$$

$$\frac{\partial N_i}{\partial t} = \sum_{j,k}^{j \geq k} \left(1 - \frac{1}{2}\delta_{j,k} \right) \eta \Phi(j,k) N_j N_k - N_i \sum_{k=1}^{M} \Phi(j,k) N_k - R_i + S_i, \quad \eta = \begin{cases} \dfrac{x_{i+1} - m}{x_{i+1} - x_i} & x_i \leq m \leq x_{i+1} \\ \dfrac{m - x_i}{x_i - x_{i-1}} & x_{i-1} \leq m \leq x_i \end{cases}$$

Agglomeration Kernel

VICTORIA kernel (USNRC)

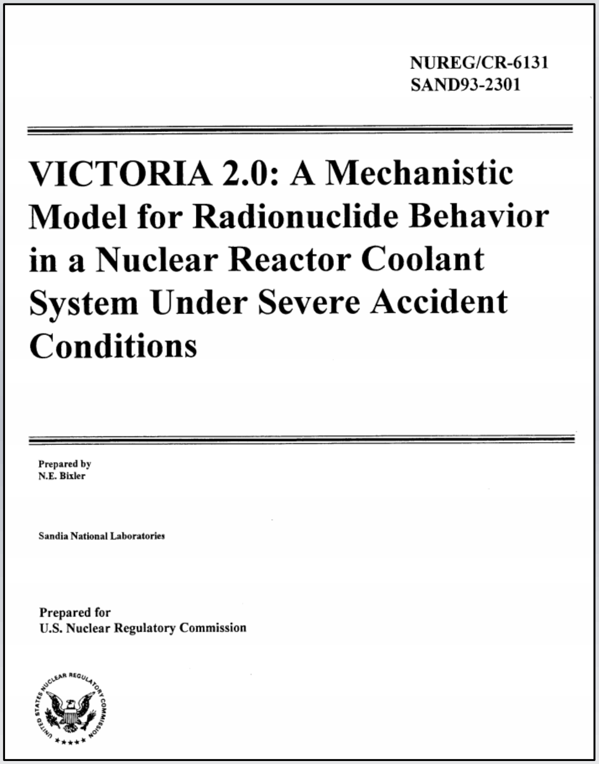
$$\Phi(m,\omega) = \Phi_B(m,\omega) + \Phi_G(m,\omega) + \sqrt{\Phi_S^2(m,\omega) + \Phi_I^2(m,\omega)}$$

***B*=Brownian**

***G*=Gravitational**

***S*=Shear**

***I*=Inertial**



NUREG/CR-6131
SAND93-2301

VICTORIA 2.0: A Mechanistic Model for Radionuclide Behavior in a Nuclear Reactor Coolant System Under Severe Accident Conditions

Prepared by
N.E. Bixler

Sandia National Laboratories

Prepared for
U.S. Nuclear Regulatory Commission

Brownian

$$\Phi_B(m,\omega) = 4\pi k_B T\left(B(m)+B(\omega)\right)\left(r_m + r_\omega\right)\mathrm{Fu}(m,\omega)$$

$$B(m) = \frac{\mathrm{Cn}}{6\pi\mu r_m}$$

$$\frac{1}{\mathrm{Fu}(m,\omega)} = \frac{1}{\mathrm{Fu}_1(m,\omega)} + \frac{1}{\mathrm{Fu}_2(m,\omega)};$$

$$\mathrm{Fu}_1(m,\omega) = \varepsilon_S \frac{r_m + r_\omega}{k_B T\left(B(m)+B(\omega)\right)}\sqrt{\frac{8k_BT}{\pi}\left(\frac{1}{m}-\frac{1}{\omega}\right)}$$

$$\mathrm{Fu}_2(m,\omega) = 1 + \frac{2\sqrt{\tilde{a}_m^2 + \tilde{a}_\omega}}{r_m + r_\omega}$$

B(m) **= mobility factor**

Fu = Fuchs factor

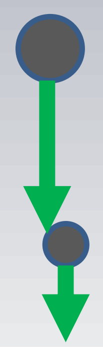
Gravitational

$$\Phi_G(m,\omega) = \varepsilon_S \varepsilon_{PK}(m,\omega)(r_m + r_\omega)^2 \left| u_g(m) + u_g(\omega) \right|$$

$$\varepsilon_{PK} = \frac{\min^2(r_m, r_\omega)}{2(r_m^2 + r_\omega^2)}$$

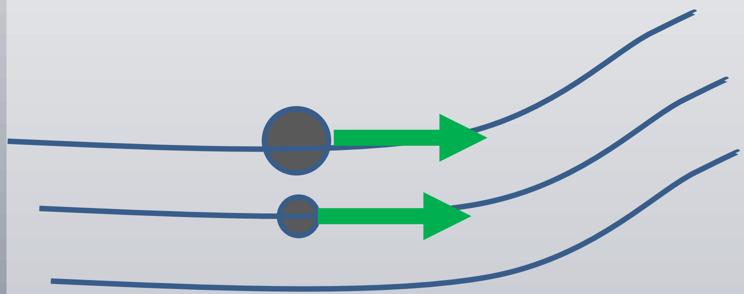
ε_S = sticking factor (assumed = 1)

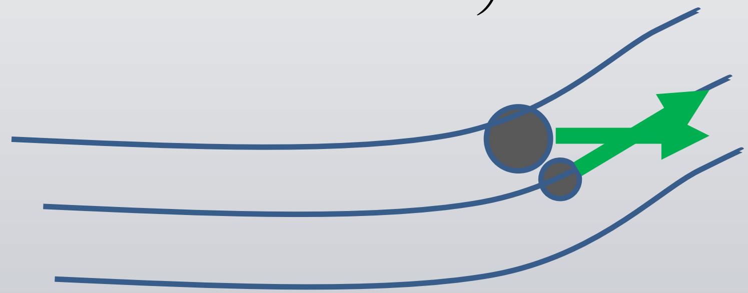
ε_{PK} = collision efficiency



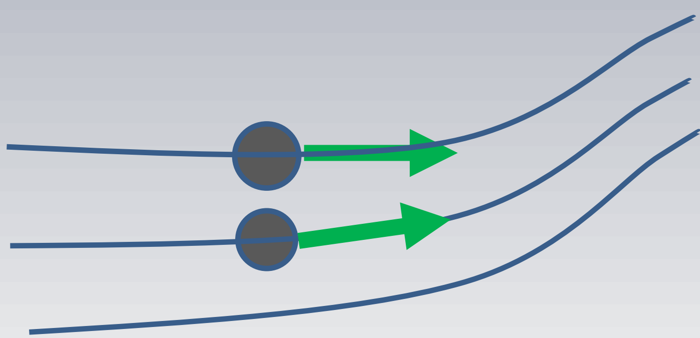
Shear and Inertial

$$\Phi_I(m,\omega) = \varepsilon_S \varepsilon_{PK}(m,\omega)(r_m + r_\omega)^2 \left(\frac{512\rho\pi^3}{15\mu} \left(\frac{0.03146 v^2}{2r \,\mathrm{Re}^{3/8}} \right)^3 \right)^{1/4} \frac{\left| u_g(m) - u_g(\omega) \right|}{g}$$





$$\Phi_S(m,\omega) = \varepsilon_S \varepsilon_{PK}(m,\omega)(r_m + r_\omega)^3 \sqrt{\frac{8\rho\pi}{15\mu} \frac{0.03146 v^2}{d \,\mathrm{Re}^{3/8}}}$$



Agglomeration Modeling

Compute agglomeration for NIST/NRC series 3

Source term is soot yield from fire

Polyethylene distribution from SP report

150 particle size bins

Ignore deposition

Volume for number density

- Open Door - upper layer volume
- Closed Door – entire volume

Removal based on door/HVAC flows

Agglomeration Modeling

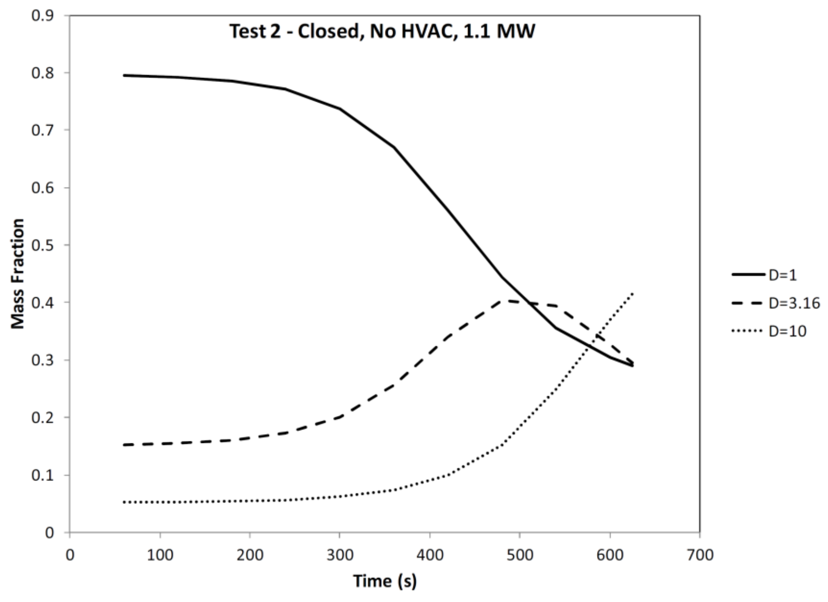
Collapse 150 bins into 3: 1, 3.6, 10 μm

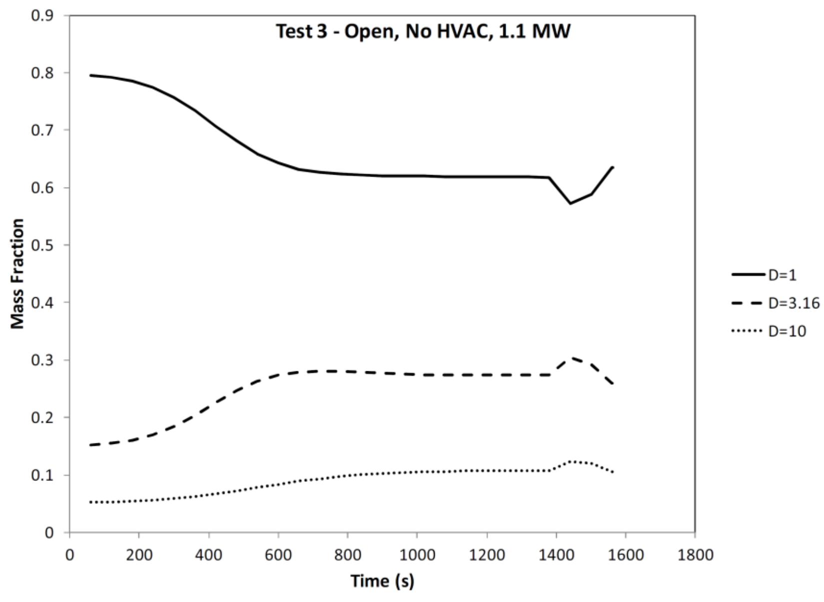
Modeled FM Global 1 m^3 settling chamber PVC test with 1, 3, and 6 bins.

1 bin to 3 bins had a large reduction in error

3 bins to 6 bins had a small reduction in error

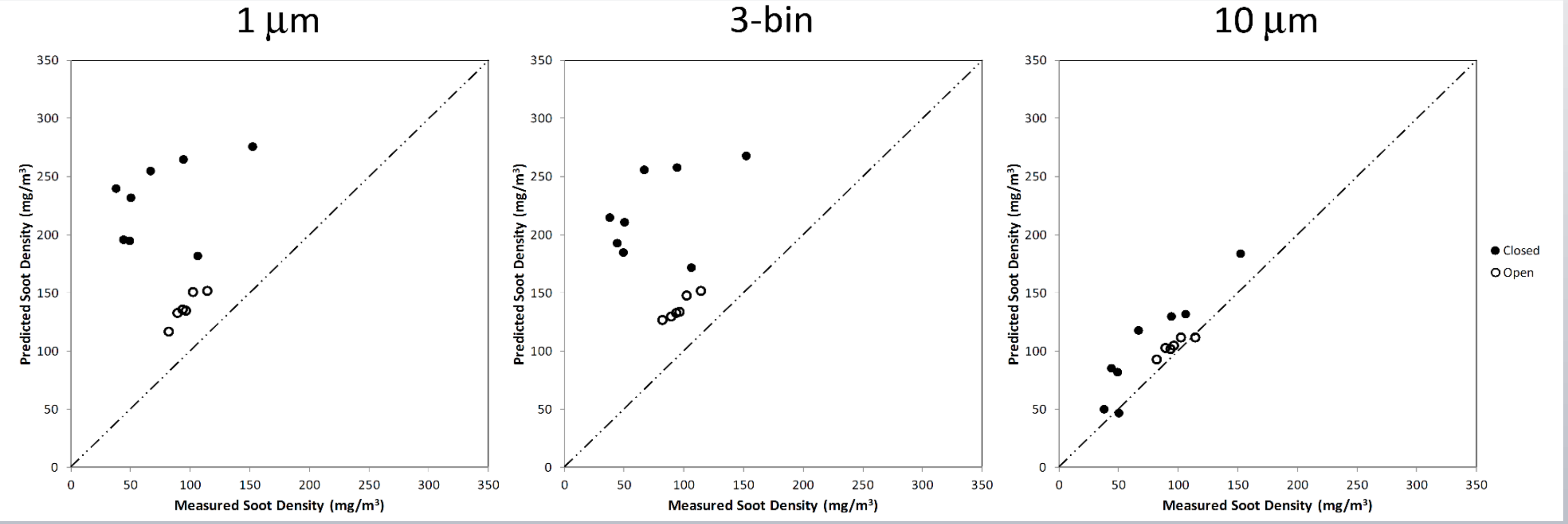
Typical Results





Results

Particle size distributions were averaged over the steady-state fire portion for each test to create test specific 3-bin distributions



Simulation Set	Error	Bias
No Deposition	0.60	3.1
1 μm particles	0.56	2.9
3-bin, post agglomeration particles	0.50	2.6
10 μm particles	0.35	1.4

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Discussion

The use of single average distribution will bias closed door to smaller size.

Some soot will be re-entrained into the flame

Agglomeration calculation did not account for higher number densities in the plume vs. post-mixing into the layer

8700 m^2/kg may not be appropriate for larger particle sizes

Initial particle size distribution from measurements on small-scale fires

Potential Research

Impact of particle size + distribution on the mass extinction coefficient.

Characterize size distributions for fuels over a range of fire sizes including smoldering sources.

During tests make gravimetric measurements of soot in addition to light extinction measurements.

Measure deposition during fire tests.

Measure of agglomeration during fire tests.

Add agglomeration to FDS in addition to deposition mechanisms

Acknowledgement/Disclaimer

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QUESTIONS

THANK YOU

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