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Modeling Aerosol Growth due to SOA Formation

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NEW PARTICLE FORMATION BREAKOUT SESSION, ASR FALL WORKING GROUP MEETING, ROCKVILLE, MD
NOVEMBER 5, 2013

Mechanisms of SOA Formation

No.	Mechanism	Parameters Controlling Growth Dynamics
#1	Gas-phase diffusion limited condensation of effectively non-volatile organics	Aerosol surface area
#2	Absorption of semi-volatile organic vapors according to Raoult's law or Henry's law	Aerosol volume (& composition), Solute volatility, Phase state (viscosity, diffusivity)
#3	Mechanism #2 followed by particle-phase chemical reactions to form effectively non-volatile oligomers, organic salts, organosulfates, organic acids, etc.	Particle size (& composition), Solute Volatility, Phase state (viscosity, diffusivity), Particle-phase reactivity

Viscosity of α-pinene secondary organic material and implications for particle growth and reactivity

Lindsay Renbaum-Wolff[a], James W. Grayson[a], Adam P. Bateman[b], Mikinori Kuwata[b], Mathieu Sellier[c], Benjamin J. Murray[d], John E. Shilling[e], Scot T. Martin[b,f,1], and Allan K. Bertram[a,1]

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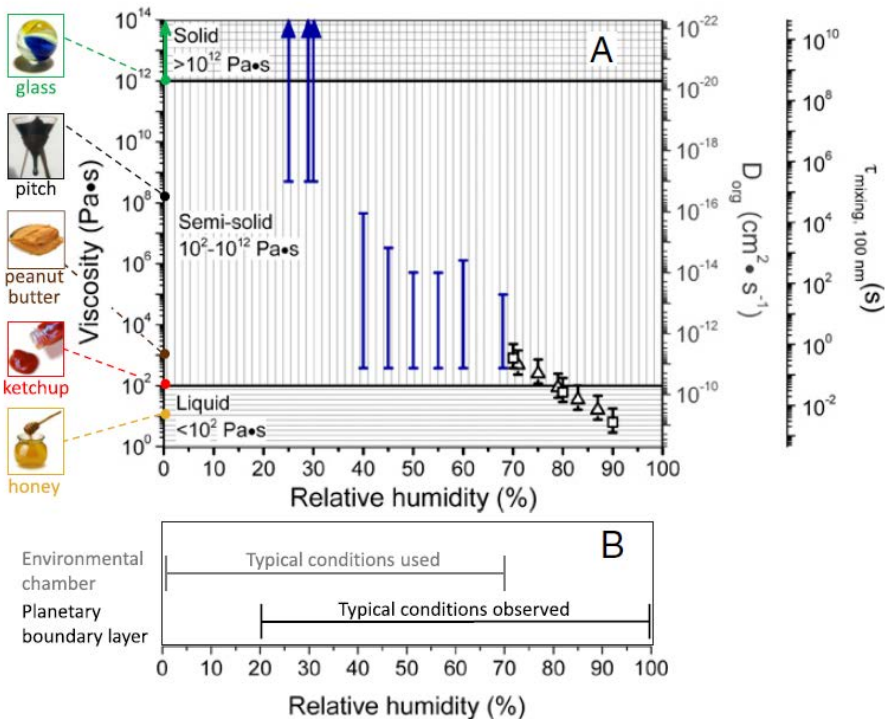
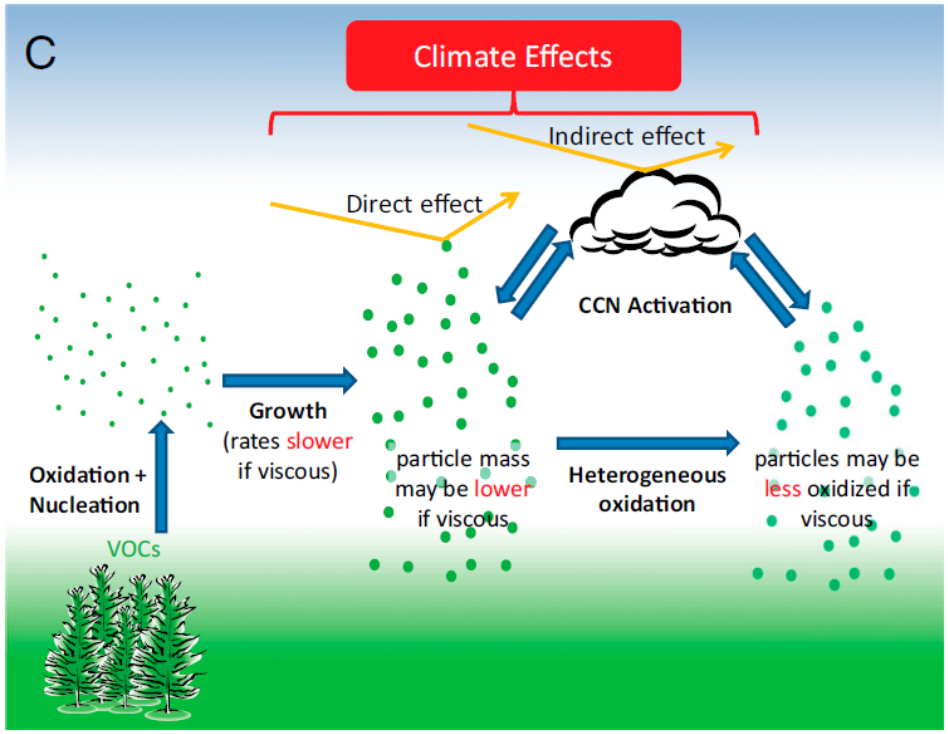




New Kinetic SOA Partitioning Model

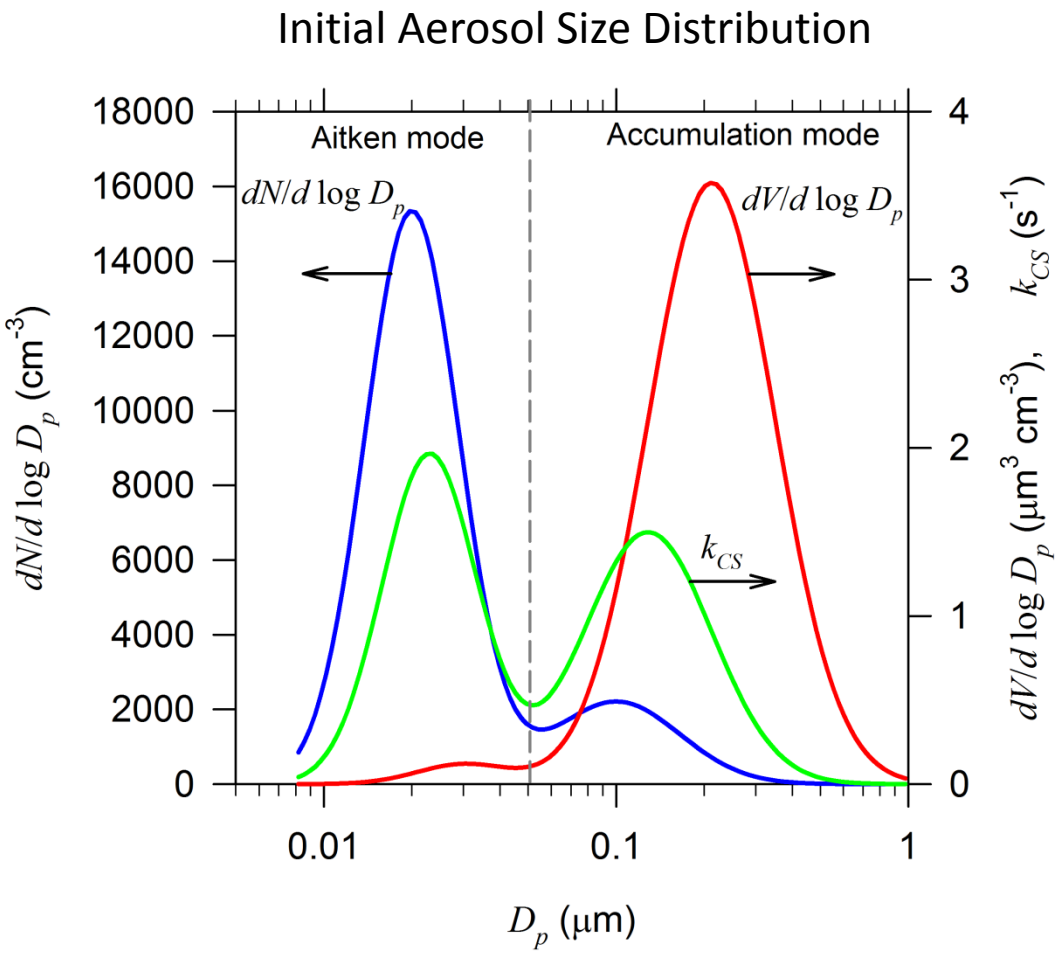
Zaveri, R. A., Easter, R. C., Shilling, J. E., and Seinfeld, J. H.: Modeling kinetic partitioning of secondary organic aerosol and size distribution dynamics: representing effects of volatility, phase state, and particle-phase reaction, Atmos. Chem. Phys. Discuss., 13, 28631-28694, doi:10.5194/acpd-13-28631-2013, 2013.

Implemented in the sectional aerosol model MOSAIC. Efficiently accounts for effects of:

- Volatility
- Phase state and viscosity (in terms of diffusivity)
- Particle-phase chemical reactivity

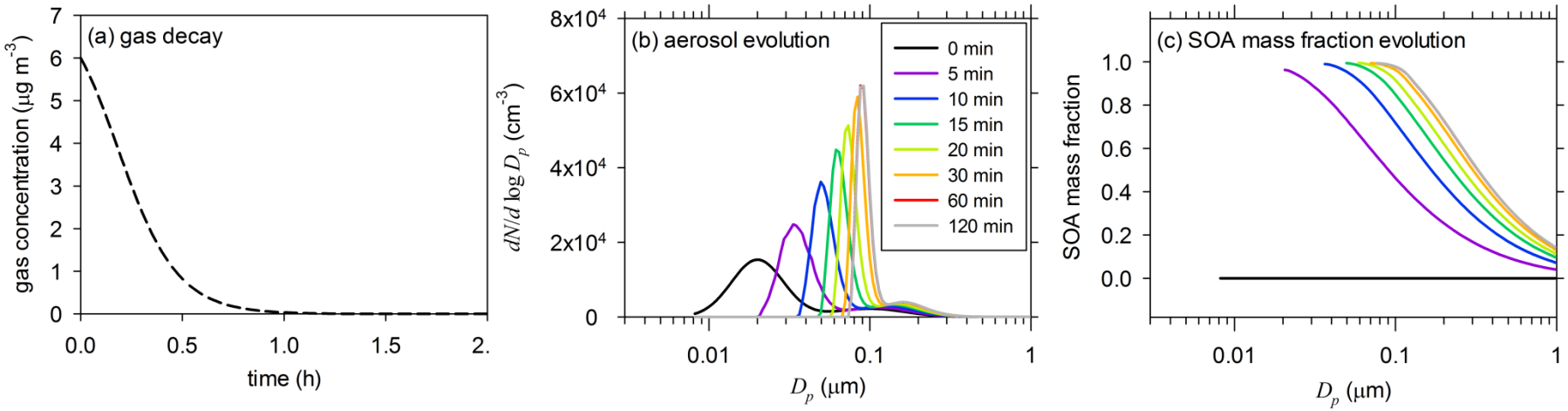
Amenable for use in regional and global model, but presently awaits specification of the actual species, reactions, and phase state properties.

Competitive Growth Dynamics



C_{OA} = 2 μg m^{-3}

Mechanism #1: $C^* = 0$

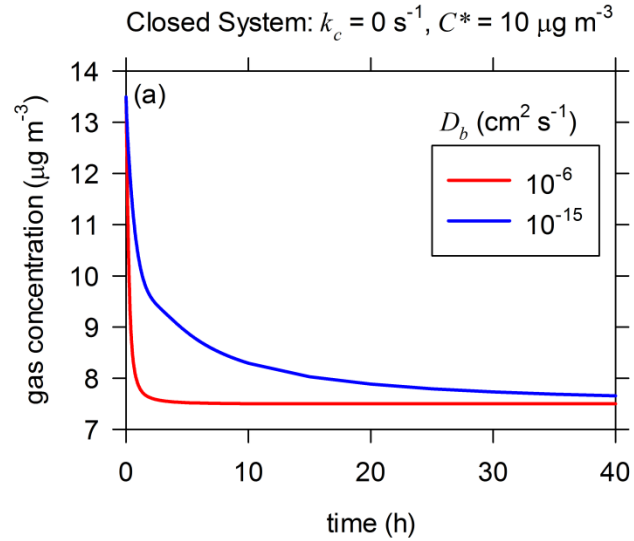


Final C_{SOA} = 6 μg m^{-3}

Final bulk SOA mass fraction = 0.75

Final C_{OA} = 8 μg m^{-3}

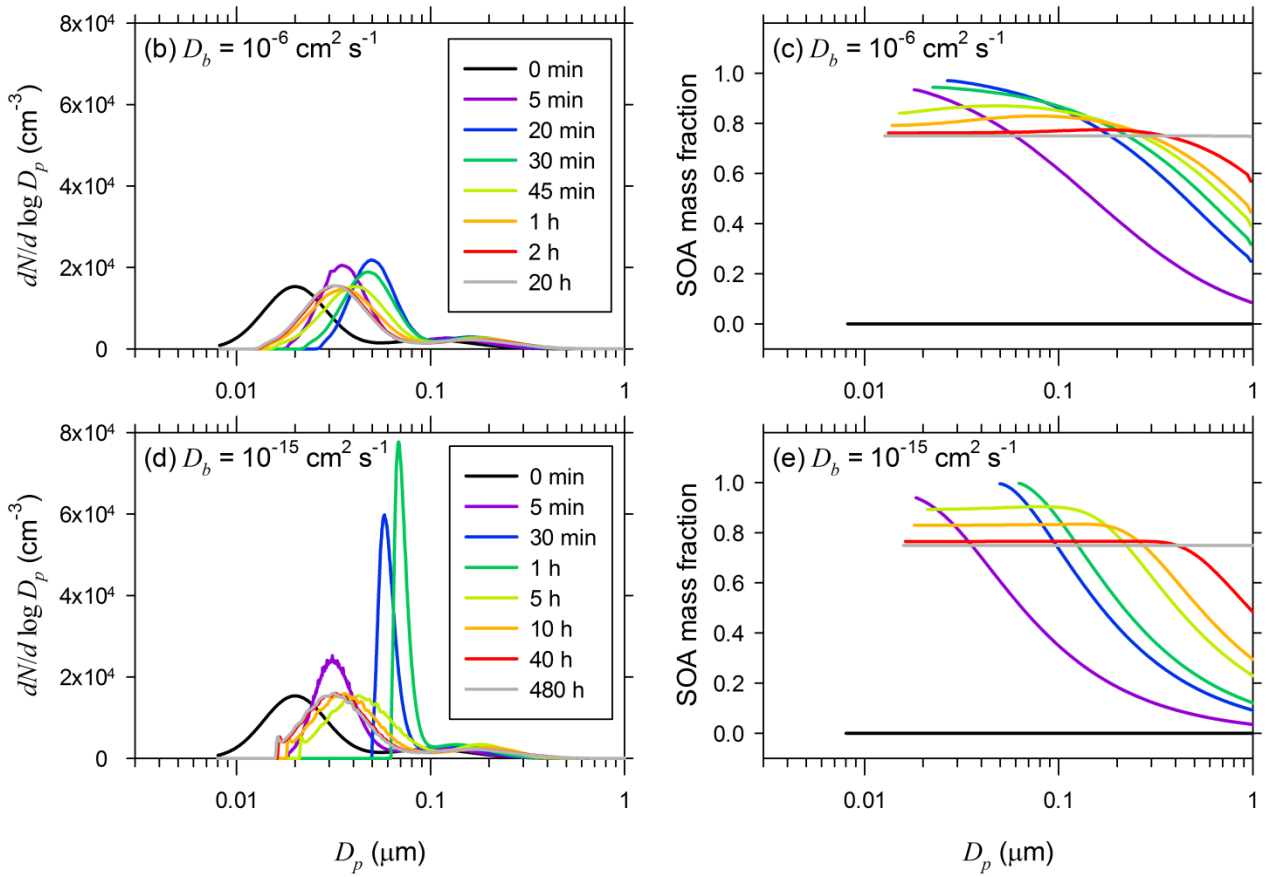
Mechanism 2:
k_c = 0, C^* = 10 µg m^{-3}



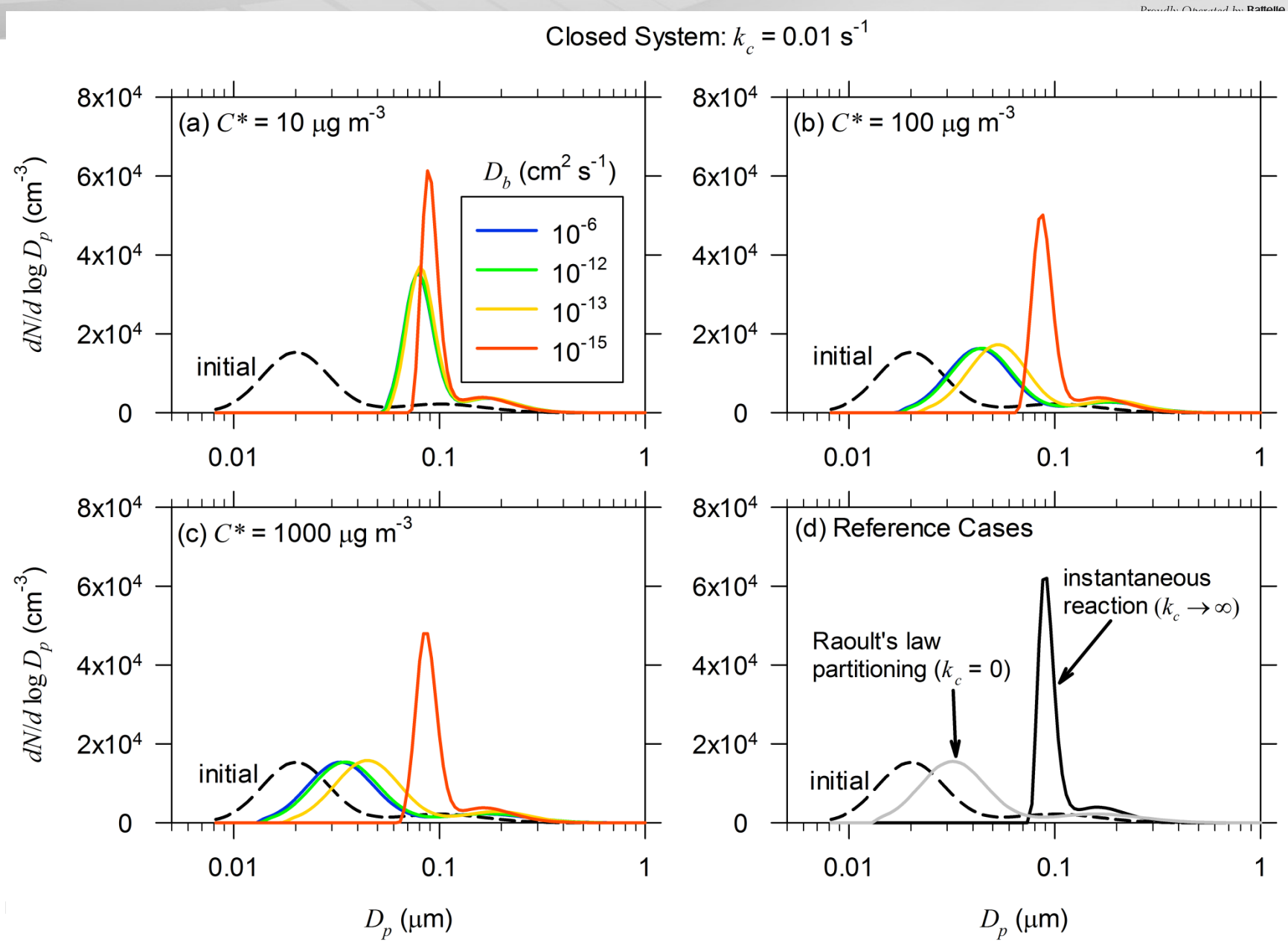
Final C_{SOA} = 6 µg m^{-3}

Final C_{OA} = 8 µg m^{-3}

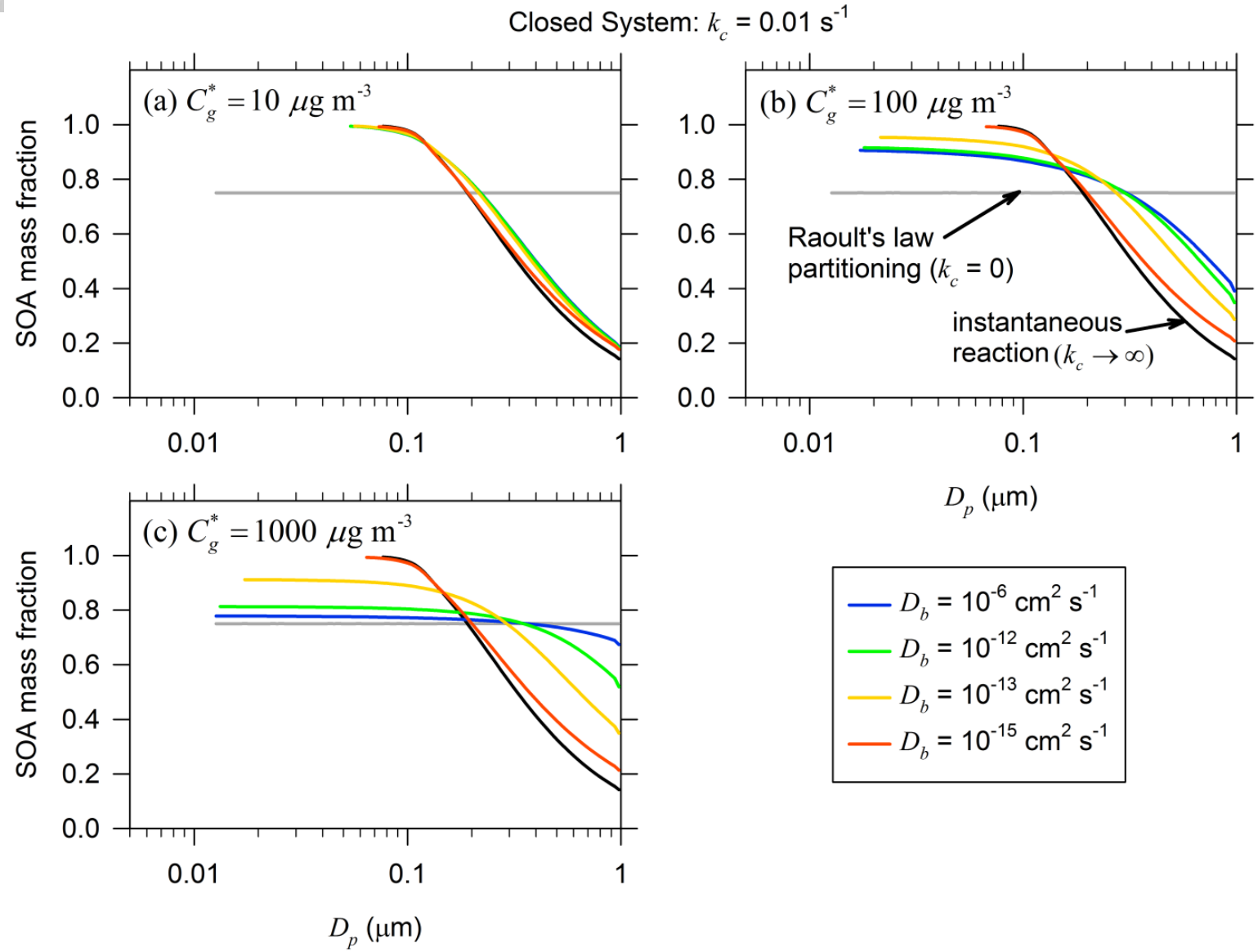
Final SOA m.f. = 0.75



Mechanism #3


Closed System: k_c = 0.01 s^{-1}
(a) C^* = 10 μg m^{-3}
(b) C^* = 100 μg m^{-3}
(c) C^* = 1000 μg m^{-3}
(d) Reference Cases
D_b (cm^2 s^{-1})
10^{-6}
10^{-12}
10^{-13}
10^{-15}
initial
Raoult's law partitioning (k_c = 0)
instantaneous reaction ($k_c \to \infty$)
$dN/d\log D_p$ (cm^{-3})
D_p (μm)
0
2x10^4
4x10^4
6x10^4
8x10^4
0.01
0.1
1

Mechanism #3: SOA Mass Fraction



Contribution to Focus Group Objectives

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1. Develop models for *nucleation rates* and *growth rates* of atmospheric nanoparticles.

- develop empirical models that accurately describe atmospheric observations (a short term objective that would be of value).
- develop first-principles models for the dependence of these rates on concentrations of participating gas phase species (a primary goal of this research).
- Use observations of the chemical species and mechanisms responsible for growth to determine climatically important physico-chemical properties of the aerosol formed by nucleation such as hygroscopicity, phase, and surface tension.

near term

2. Incorporate mechanistic models for nucleation and growth rates into regional models to assess model performance during intensive atmospheric observations in well-defined environments.

longer term

3. Incorporate these models into global climate models to quantify the effects of new particle formation on climate.