Modelling aerosol dynamic processes

HANNELE KORHONEN

SUMMER SCHOOL ON

"INTEGRATED MODELLING OF METEOROLOGICAL AND CHEMICAL TRANSPORT PROCESSES / IMPACT OF CHEMICAL WEATHER ON NUMERICAL WEATHER PREDICTION AND CLIMATE MODELLING"

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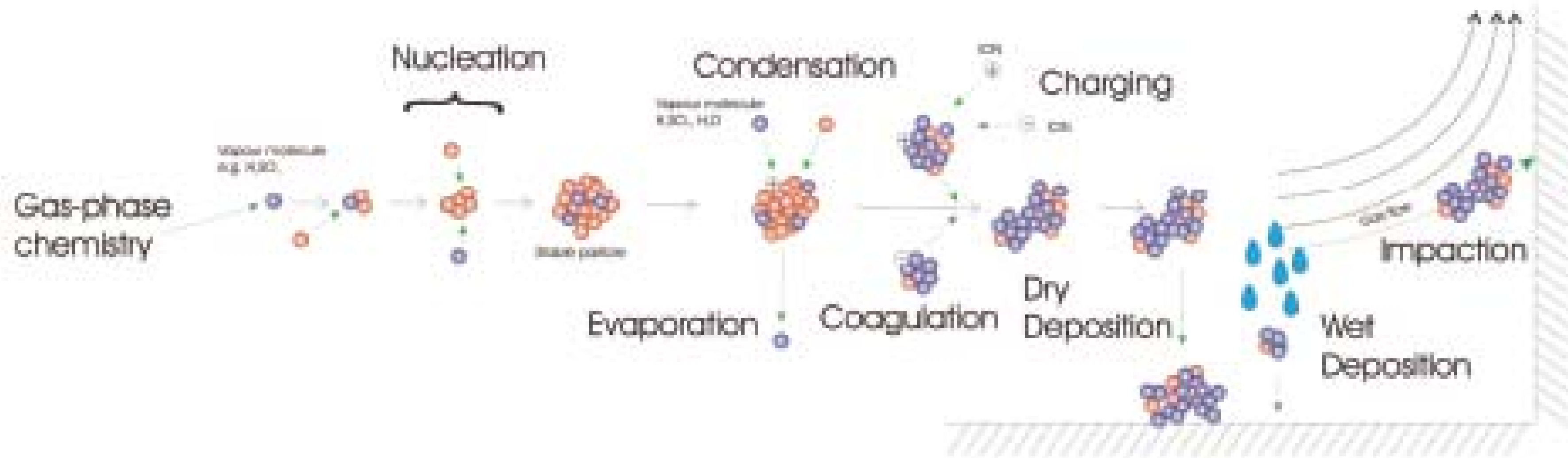
Why would we want to simulate aerosol in an atmospheric model?

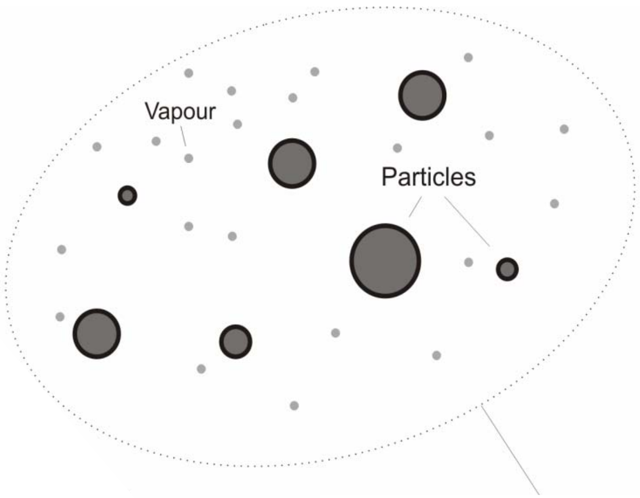
What aerosol properties would we be interested in?

Describing changes in aerosol population in a model



General dynamic equation (GDE)

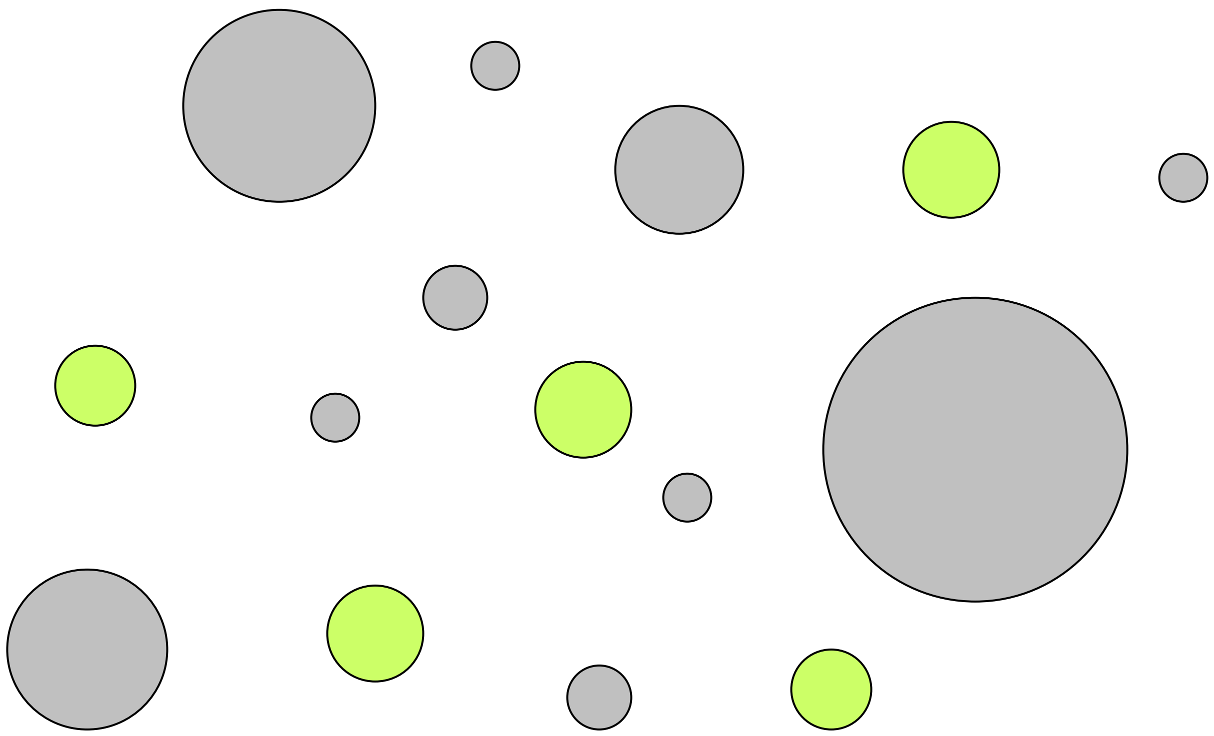
For particles with volumes *v*...*v*+*dv* the number concentration at time *t* is *n(v,t)dv*



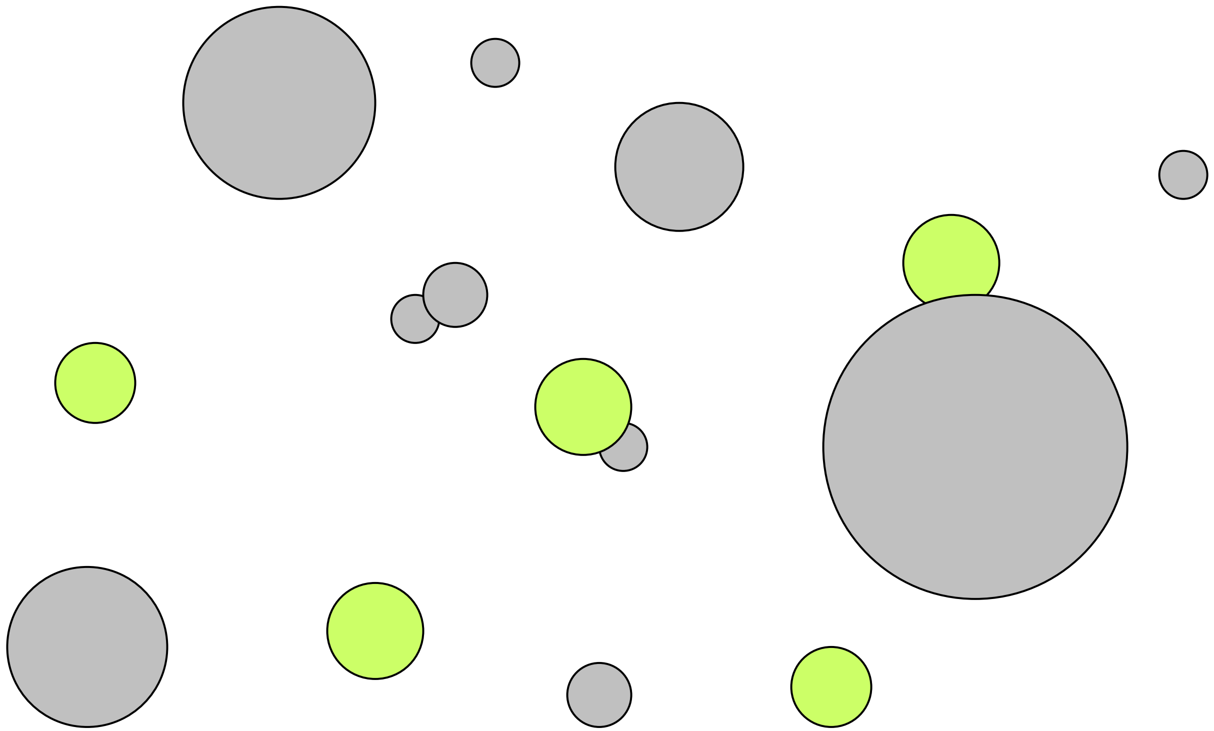
Let's look at a spatially homogeneous volume of air

$$\frac{dn(v,t)}{dt} = \left(\frac{dn(v,t)}{dt}\right)_{nucl} + \left(\frac{dn(v,t)}{dt}\right)_{cond} + \left(\frac{dn(v,t)}{dt}\right)_{coag} + \underset{(source)}{S} - \underset{(removal)}{R}$$

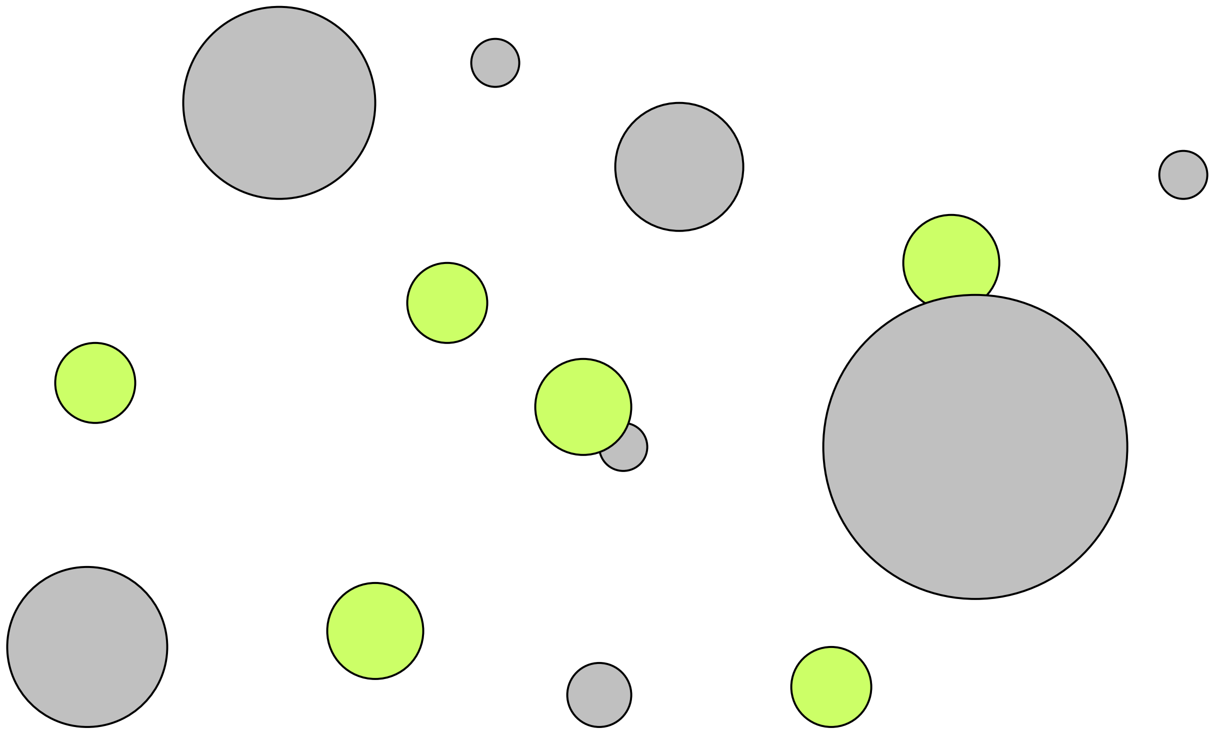
Consider particles in volume range $v \ldots v+dv$



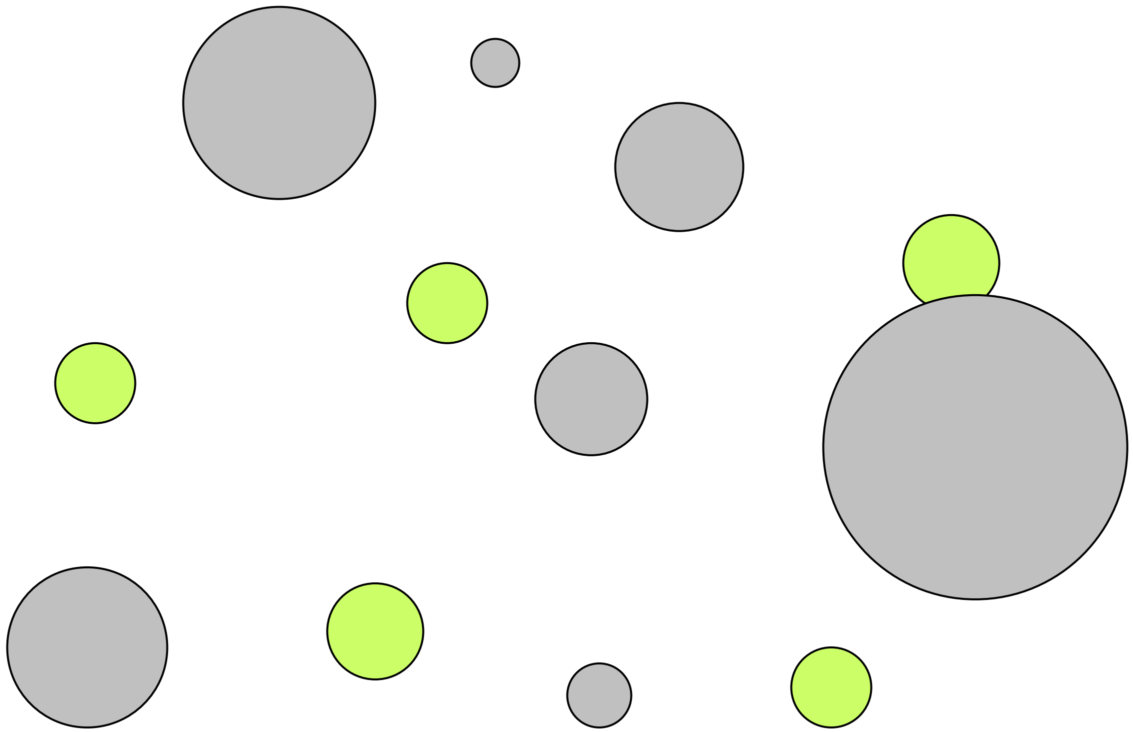
Coagulation



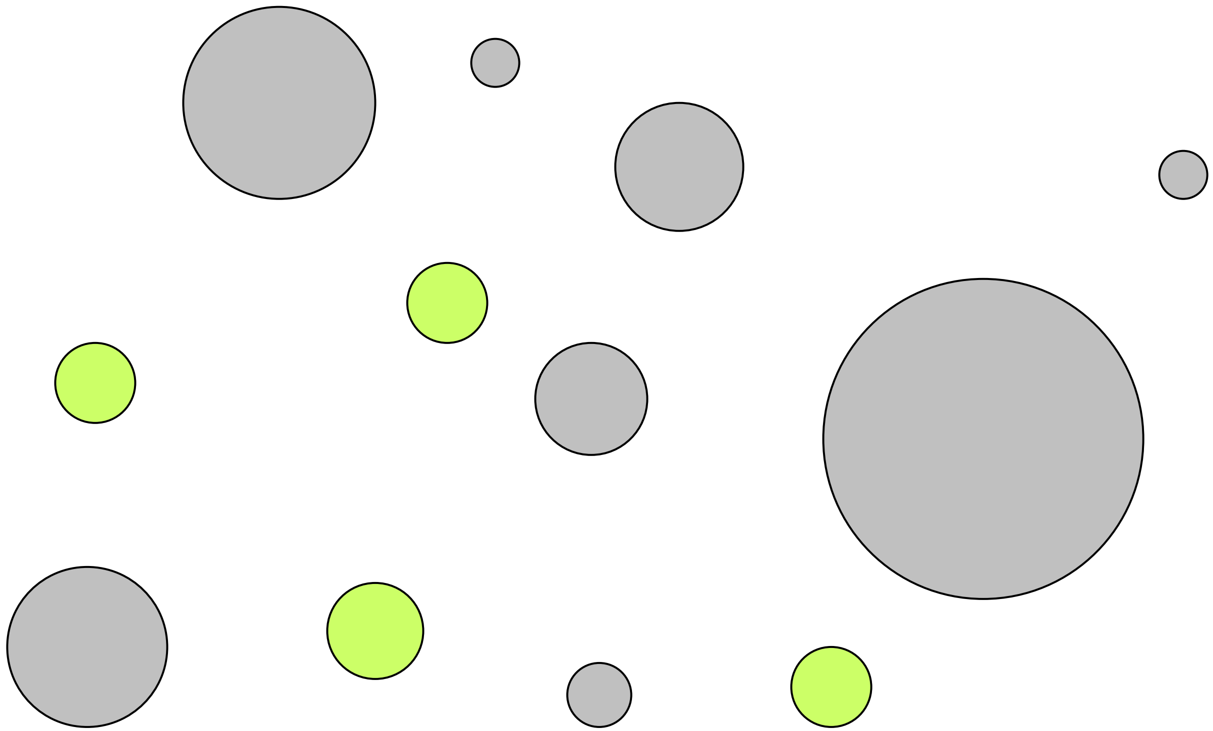
Coagulation



Coagulation



Coagulation



Coagulation in GDE

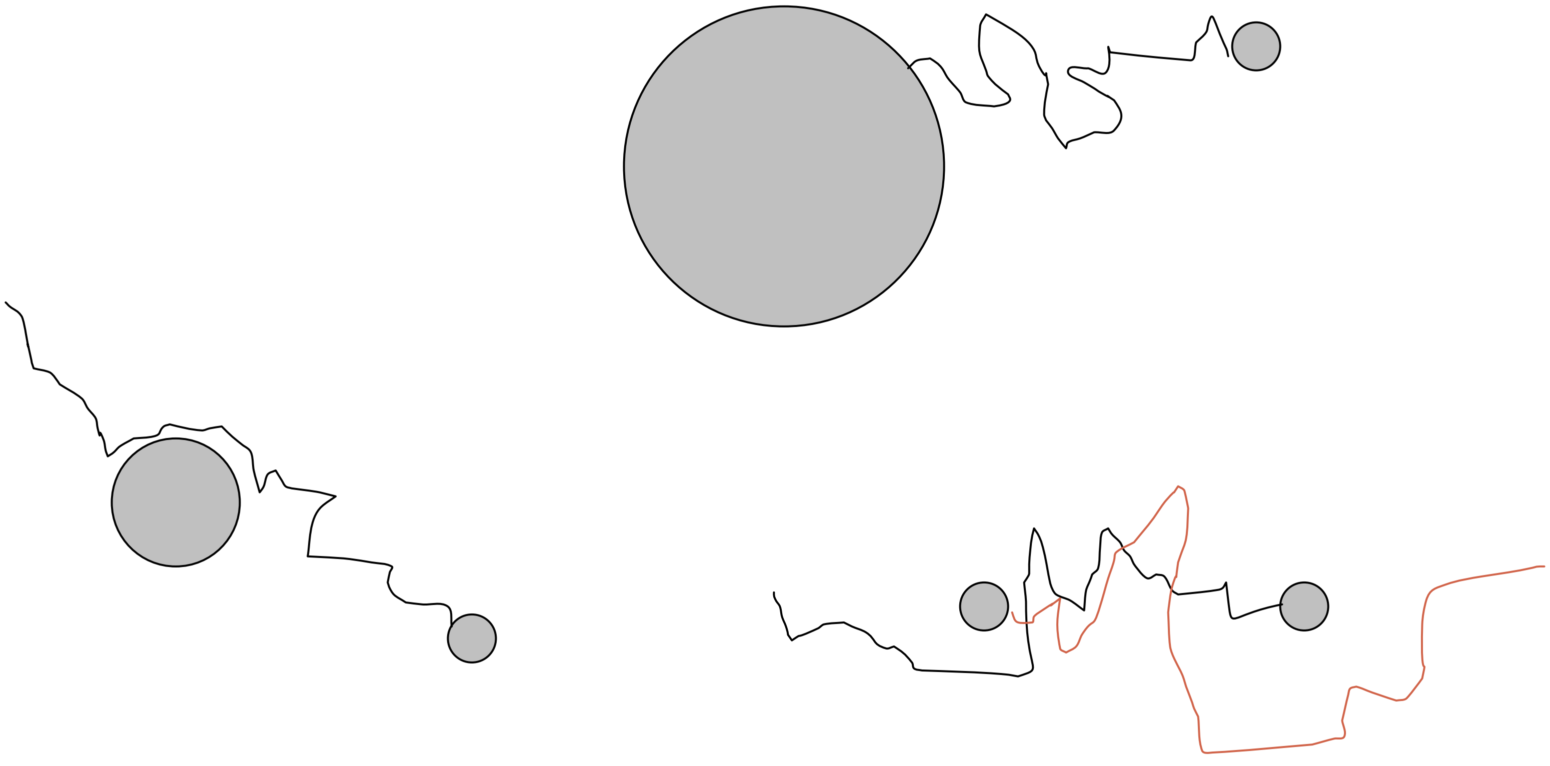
Particles of volume *v* are produced by collision of two particles whose <u>combined</u> volume is *v* (we denote them *u* and *v*-*u*).

Particles of volume *v* are lost by collision with all sized particles.

$$\left(\frac{dn}{dt}\right)_{coag} = \frac{1}{2}\int_0^v \beta(u, v-u)n(u)n(v-u)du$$

$$-\int_0^\infty \beta(u, v)n(u)n(v)du$$

Coagulation coefficient



Coagulation coefficient

$$K_{12} = 2\pi(D_1 + D_2)(D_{p1} + D_{p2})\left(\frac{D_{p1} + D_{p2}}{D_{p1} + D_{p2} + 2(g_1^2 + g_2^2)^{1/2}} + \frac{8(D_1 + D_2)}{(\bar{c}_1^2 + \bar{c}_2^2)^{1/2}(D_{p1} + D_{p2})}\right)^{-1}$$

where

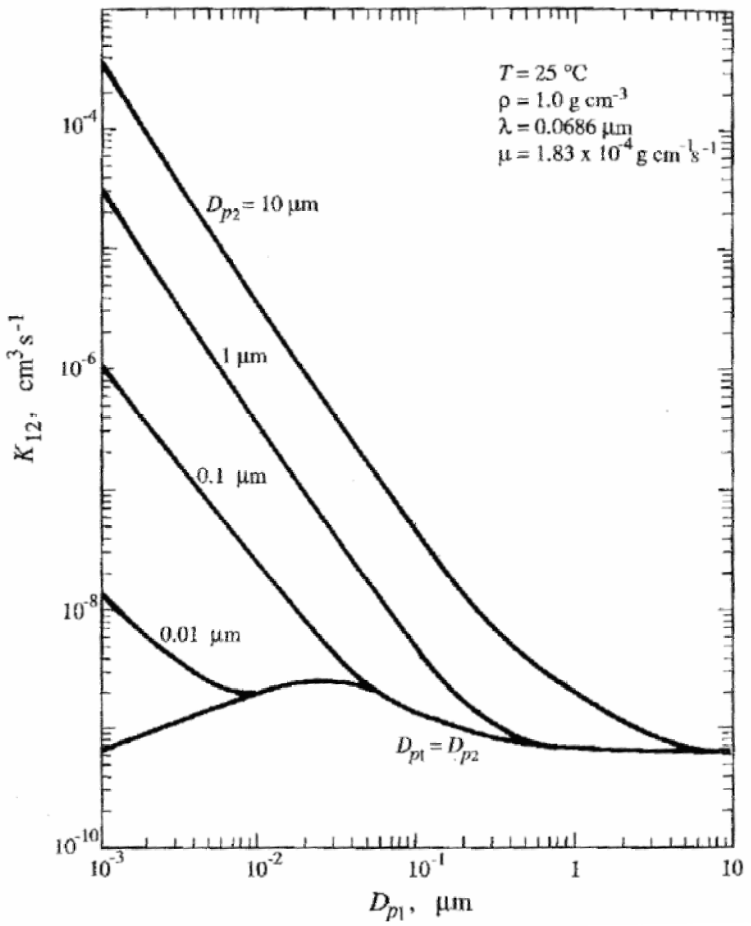
$$D_i = \frac{kT}{3\pi\mu D_{pi}}\left(\frac{5 + 4Kn_i + 6Kn_i^2 + 18Kn_i^3}{5 - Kn_i + (8+\pi)Kn_i^2}\right)$$

$$Kn_i = \frac{2\lambda_{air}}{D_{pi}}$$

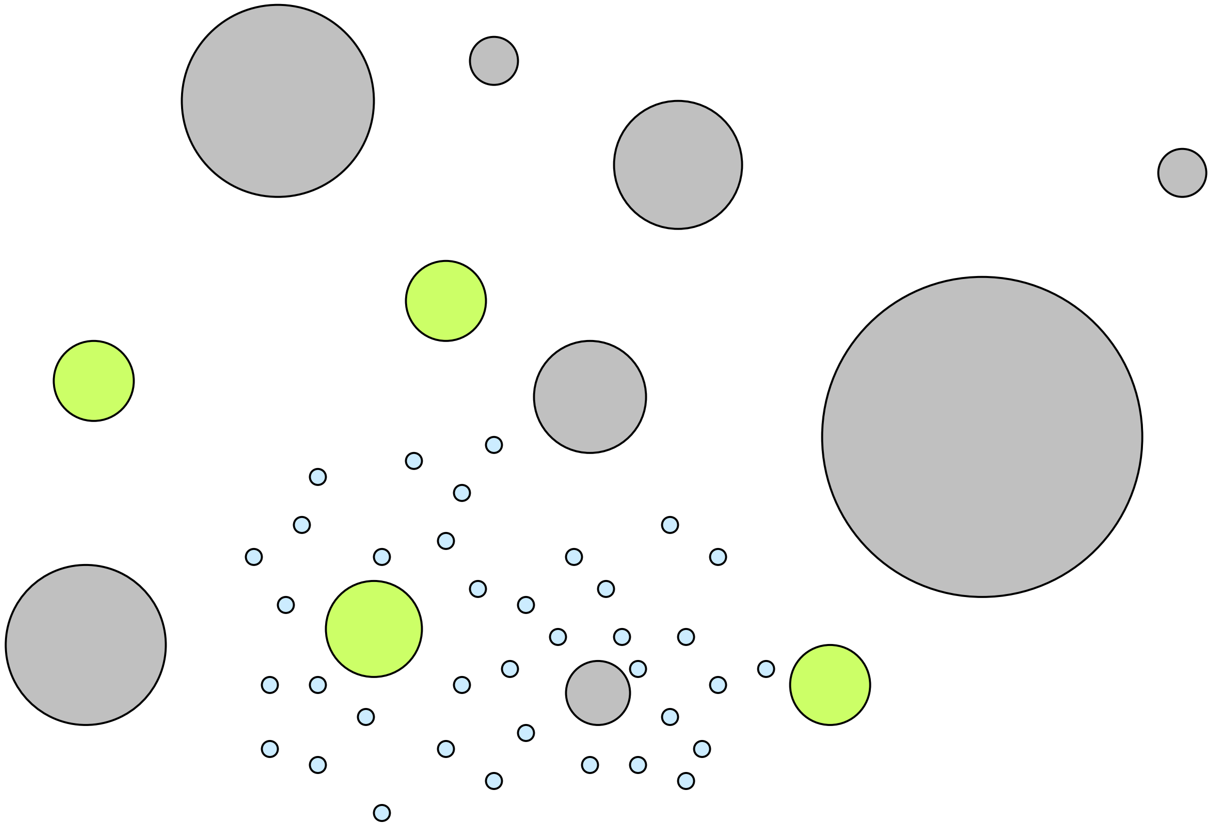
$$g_i = \frac{1}{3D_{pi}\ell_i}\left[(D_{pi} + \ell_i)^3 - (D_{pi}^2 + \ell_i^2)^{3/2}\right] - D_{pi}$$

$$\ell_i = \frac{8D_i}{\pi\bar{c}_i}$$

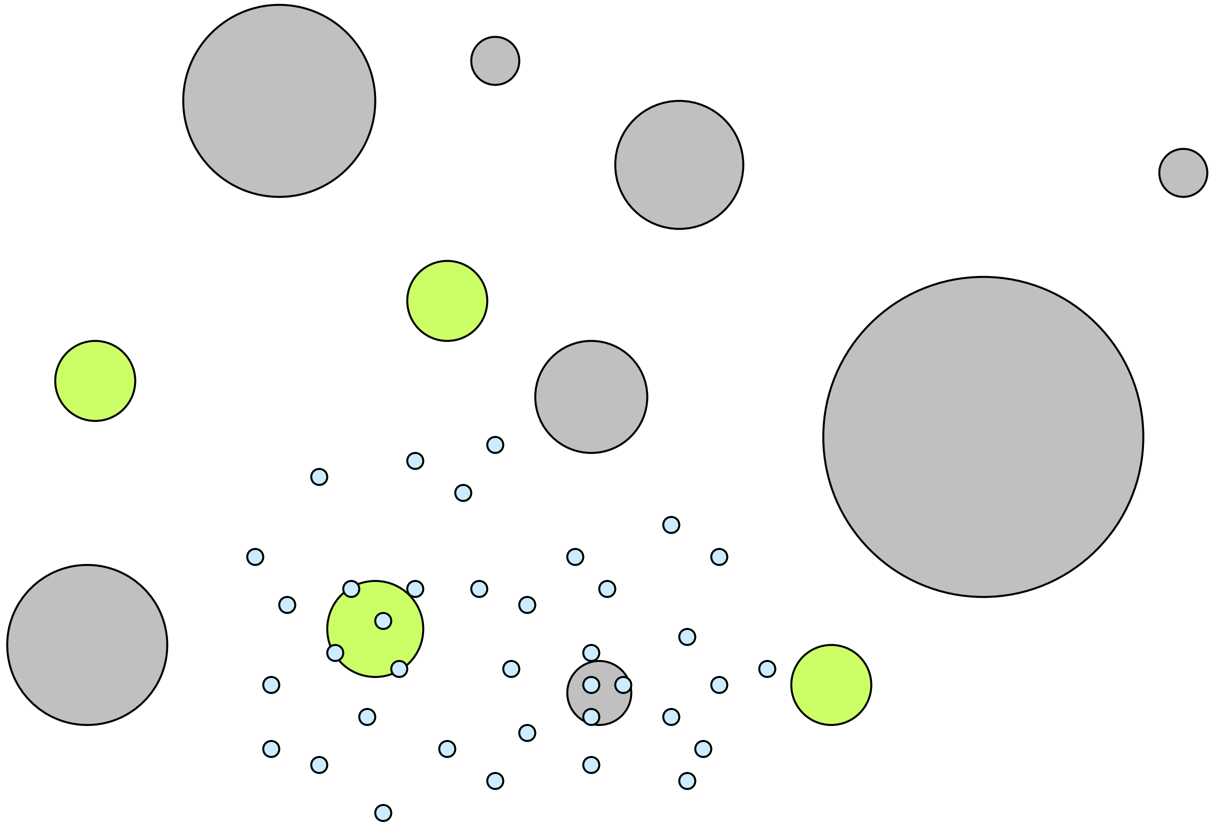
$$\bar{c}_i = \left(\frac{8kT}{\pi m_i}\right)^{1/2}$$



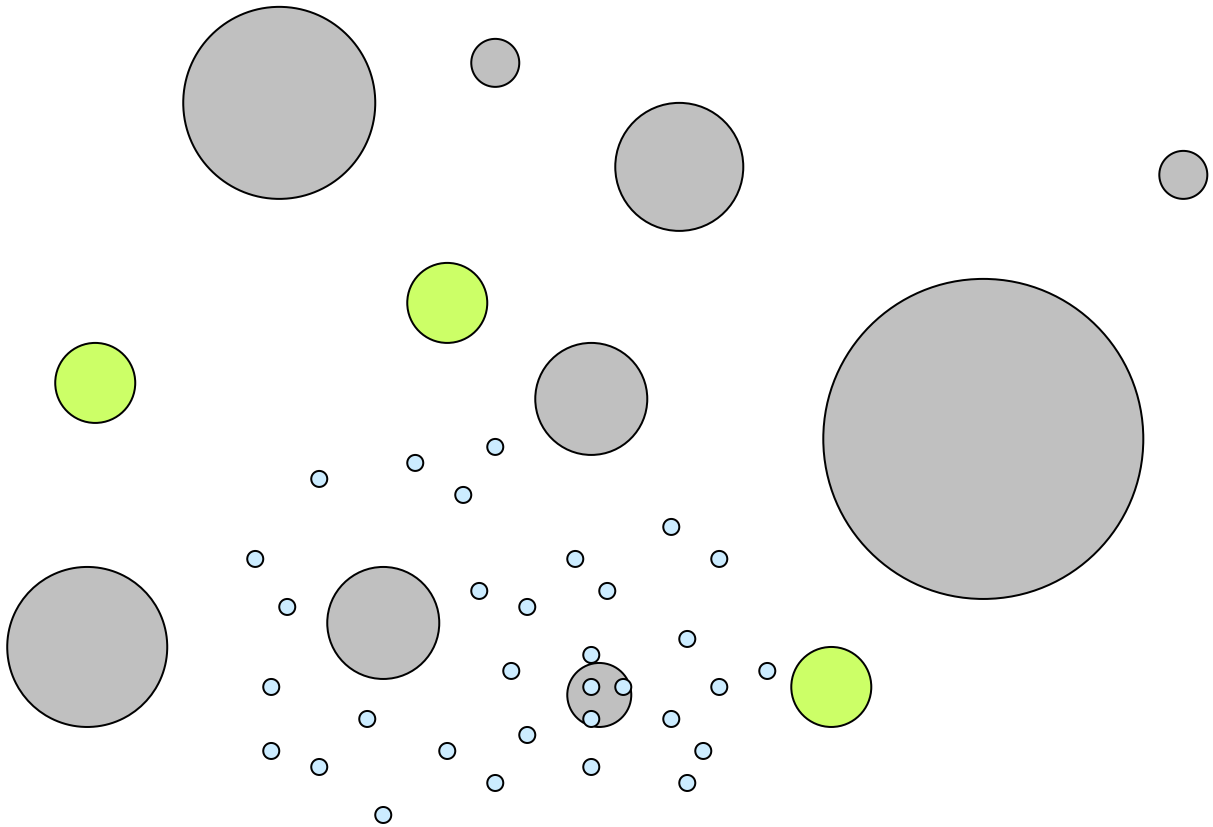
Condensation



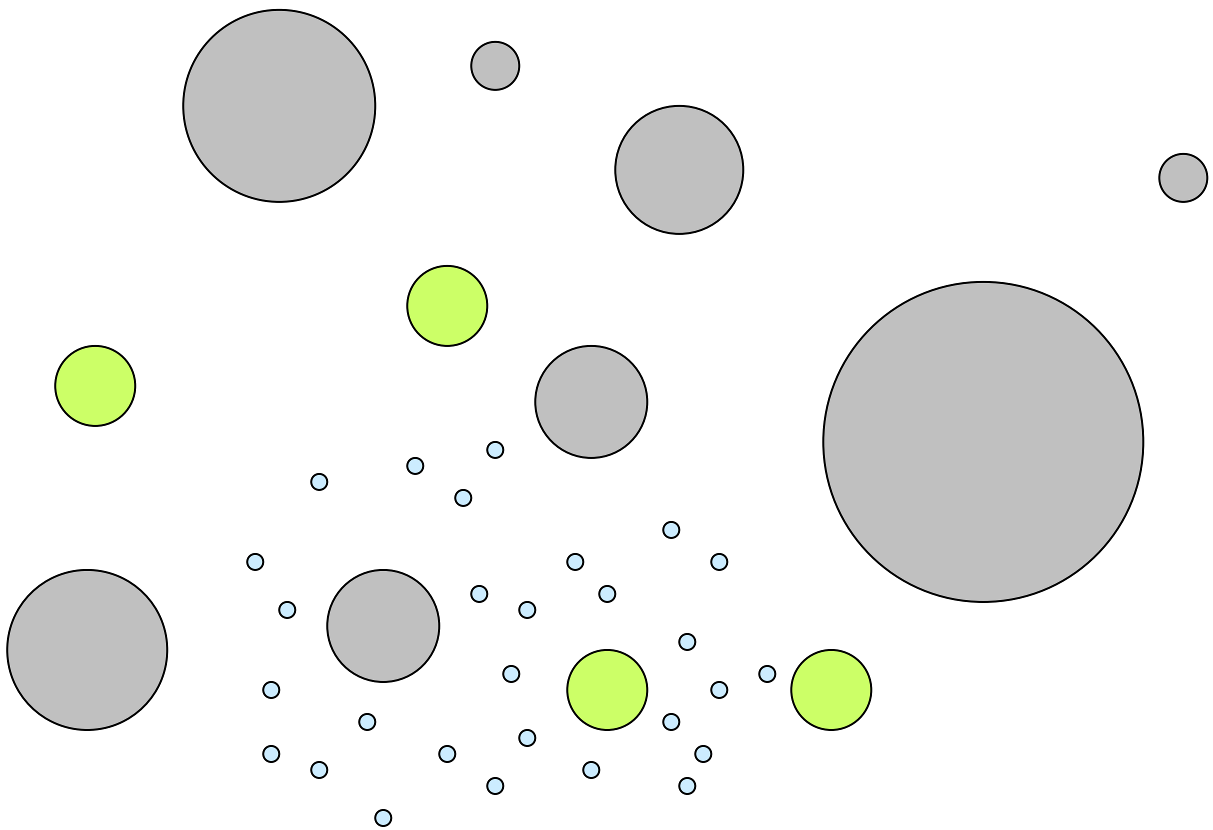
Condensation



Condensation



Condensation



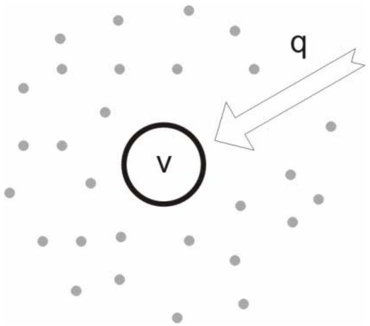
Condensation in GDE

Particles of volume *v* can form when smaller particles grow or larger particles shrink to size *v*.

Particles of volume *v* are lost when condensation grows them to larger sizes or evaporation shrinks them to smaller sizes.

Let us denote $\frac{dv}{dt} = q(v)$

Then $\left[\frac{\partial n(v,t)}{\partial t}\right]_{cond} = -\frac{\partial}{\partial v}\left[q(v,t)n(v,t)\right]$



Condensation flux

Condensation flux of gas phase compound *i* onto a particle with diameter d_p

$$\frac{dv}{dt} = 2\pi d_p D_i v_i \beta(d_p, \alpha_i)(c_i - c_{eq,i}(d_p))$$

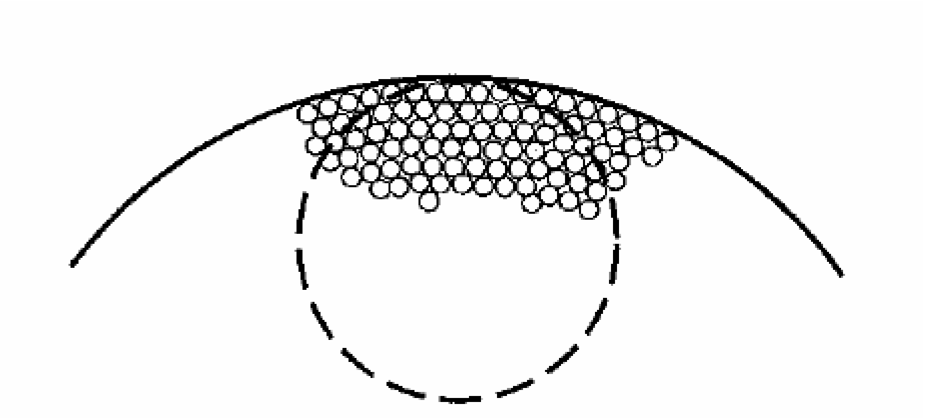
As $\lim_{d_p \to 0} \beta \to \frac{3d_p}{8\lambda}$ and $\lim_{d_p \to \infty} \beta \to 1$

$$\frac{dv}{dt} \propto d_p^2$$ for small particles

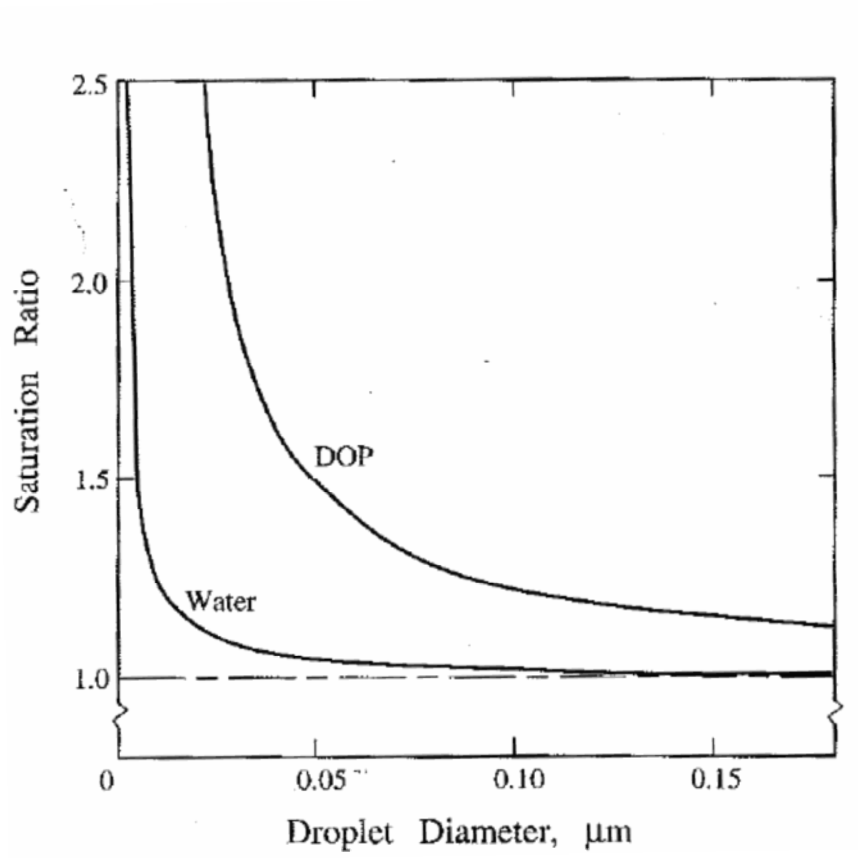
$$\frac{dv}{dt} \propto d_p$$ for large particles

Kelvin effect

$$\frac{dv}{dt} = 2\pi d_p D_i v_i \beta(d_p, \alpha)(c_i - c_{eq,i}(d_p))$$



$$Ke = \exp\left(\frac{2\sigma M}{RT\rho R_p}\right)$$



Nucleation in GDE

Nucleation forms new particles (typically) at only one size $v*$ and at formation rate $J(v,t)$.

$$\left[\frac{\partial n(v,t)}{\partial t}\right]_{nucl} = J(v)\delta(v-v^*)$$

where

$$\delta(v-v^*) = \begin{cases} 1, v = v^* \\ 0, \text{ otherwise} \end{cases}$$

(Dirac delta function)

Possible forms for $J(v)$ discussed qualitatively in Antti Lauri's lectures.

Continuous form of GDE

$$\frac{\partial n}{\partial t} = \frac{1}{2}\int_0^v \beta(u, v-u)n(u)n(v-u)du - \int_0^\infty \beta(u,v)n(u)n(v)du$$ coagulation

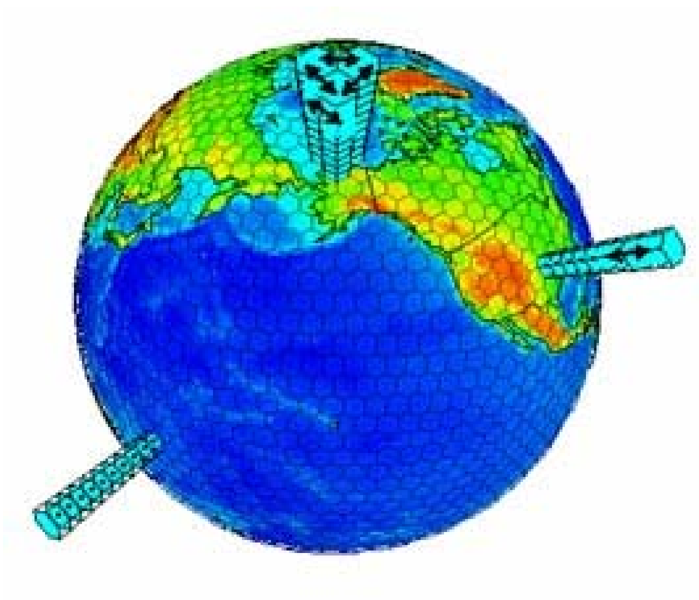
$$- \frac{\partial}{\partial v}\left[q(v)n(v)\right]$$ condensation

$$+ J(v)\delta(v - v^*)$$ nucleation

$$+ S$$ other sources

$$- R$$ removal

Transport between grid boxes

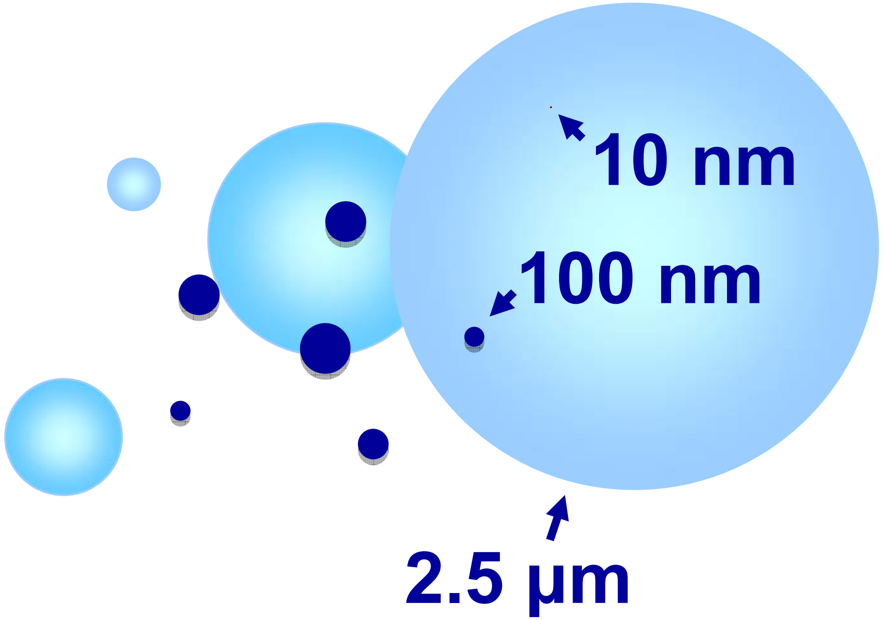


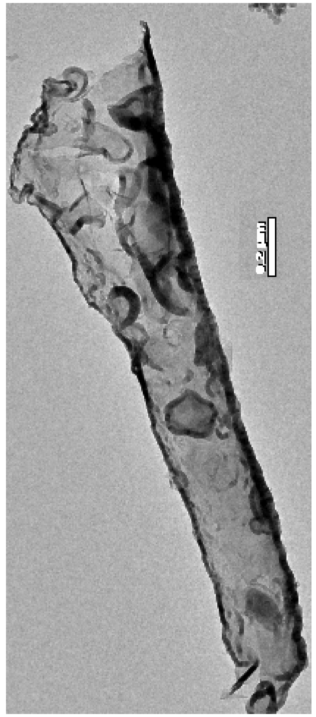
Transport can be either a source (often in remote regions) or a removal mechanism (often in aerosol source regions)

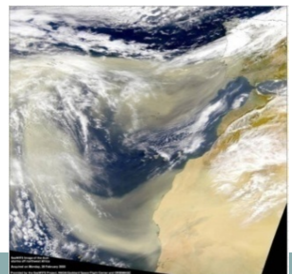
Calculated using model advection equations

Primary sources





Primary sources

Emission inventories for sulphate, OC, BC (natural and anthropogenic)

– e.g. GEIA, AEROCOM, EMEP

– emissions typically given as kg/grid/month (or year)

– often based on economic reports rather than measurements

– size distribution of emitted particles very uncertain

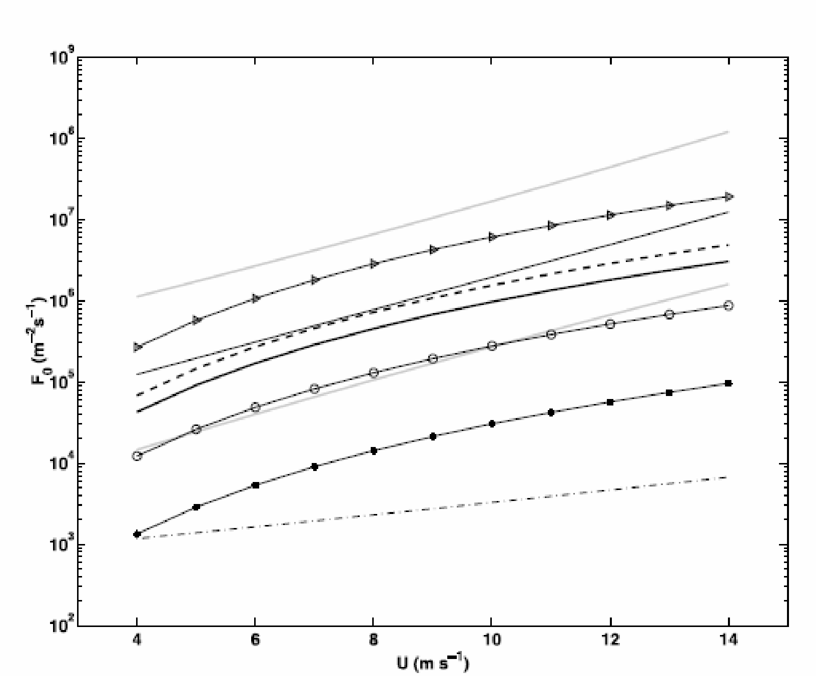
Emission parameterisations for sea salt and mineral dust

– may take into account wind speed, SST, type of dust

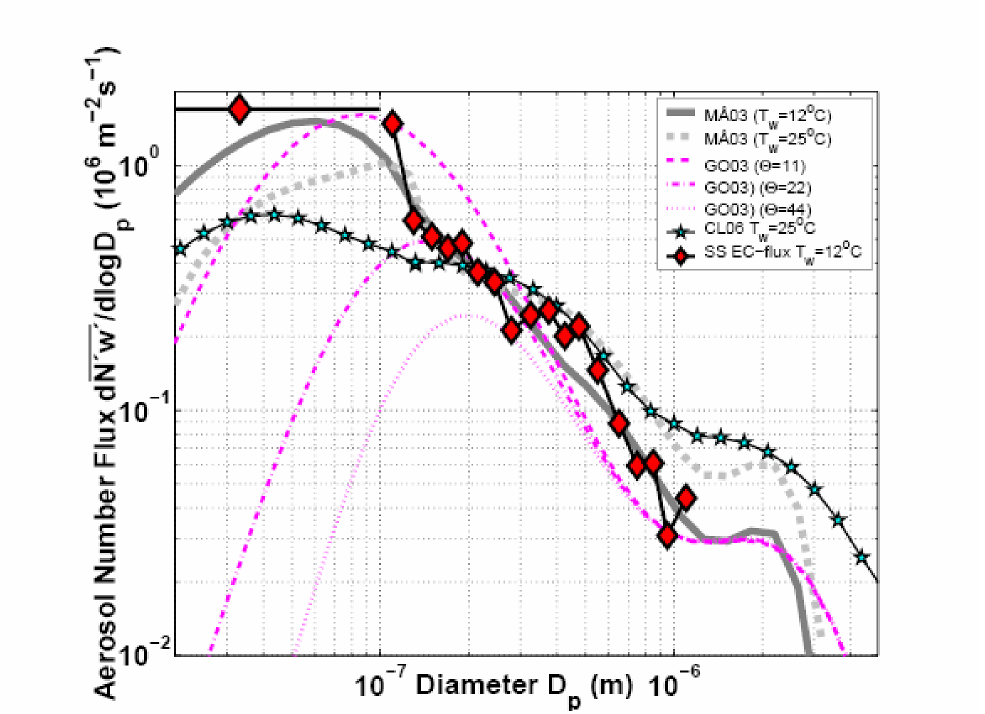
–different parameterisations may disagree by an order of magnitude

(choose the one with best experimental validation!)

Comparison of sea spray parameterisations

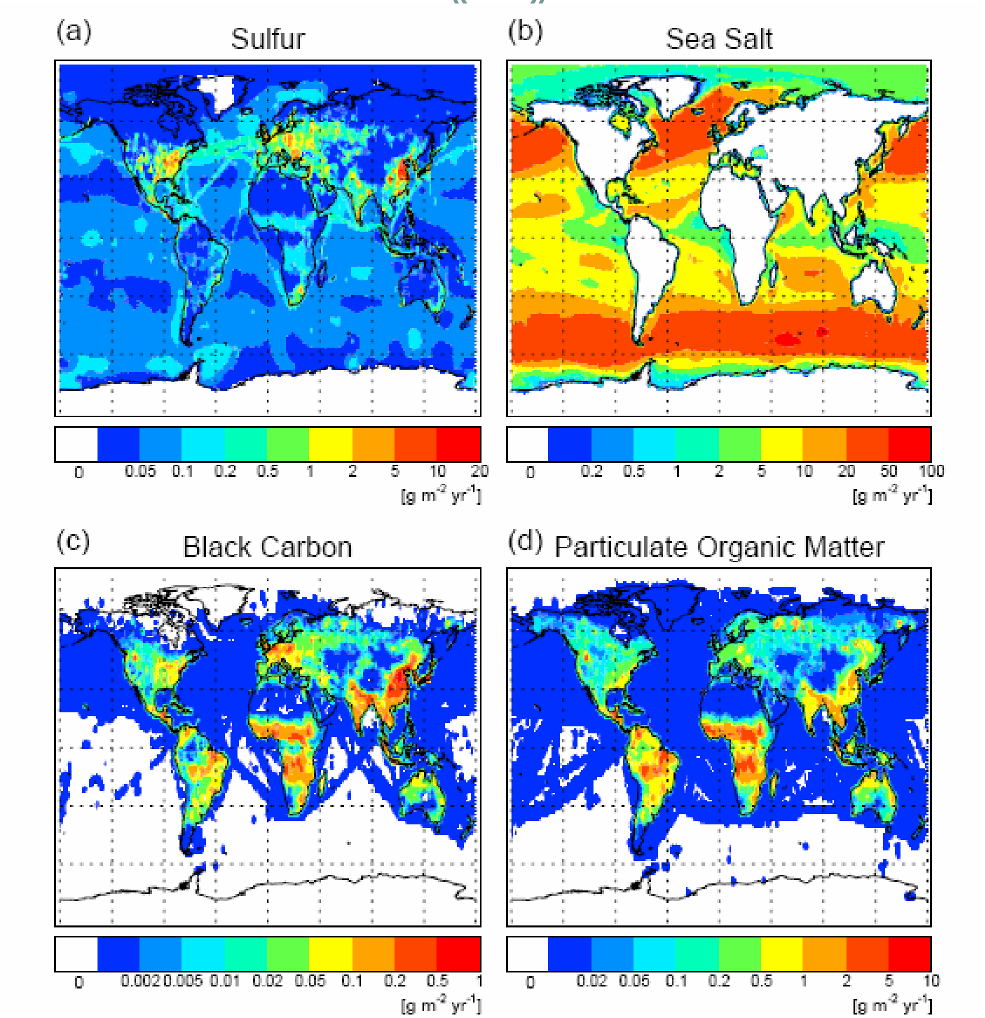


Total number flux vs. wind speed



Size dependent number flux

Annual global mass emissions



Aerosol removal

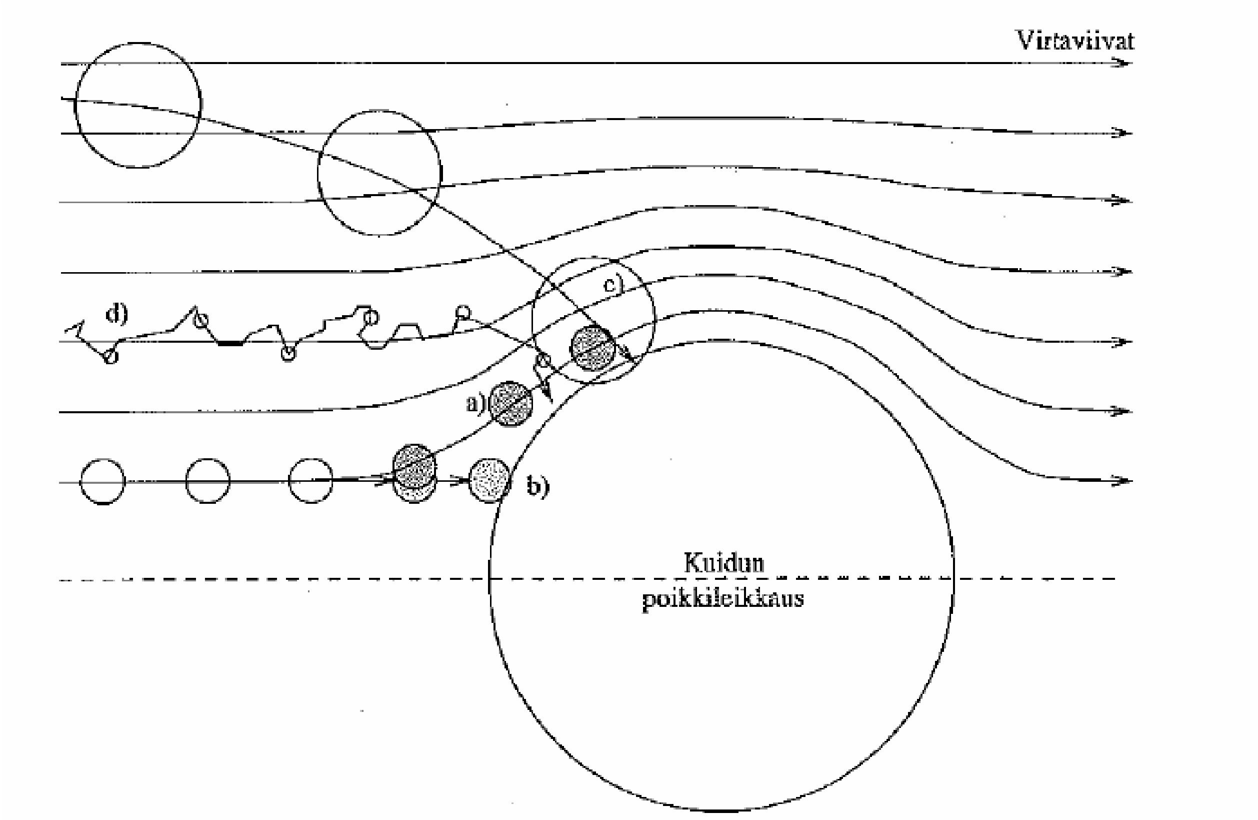
1) dry deposition

2) nucleation scavenging (~ in-cloud scavenging)

3) impaction scavenging (~ below-cloud scavenging)

} wet deposition

Dry deposition

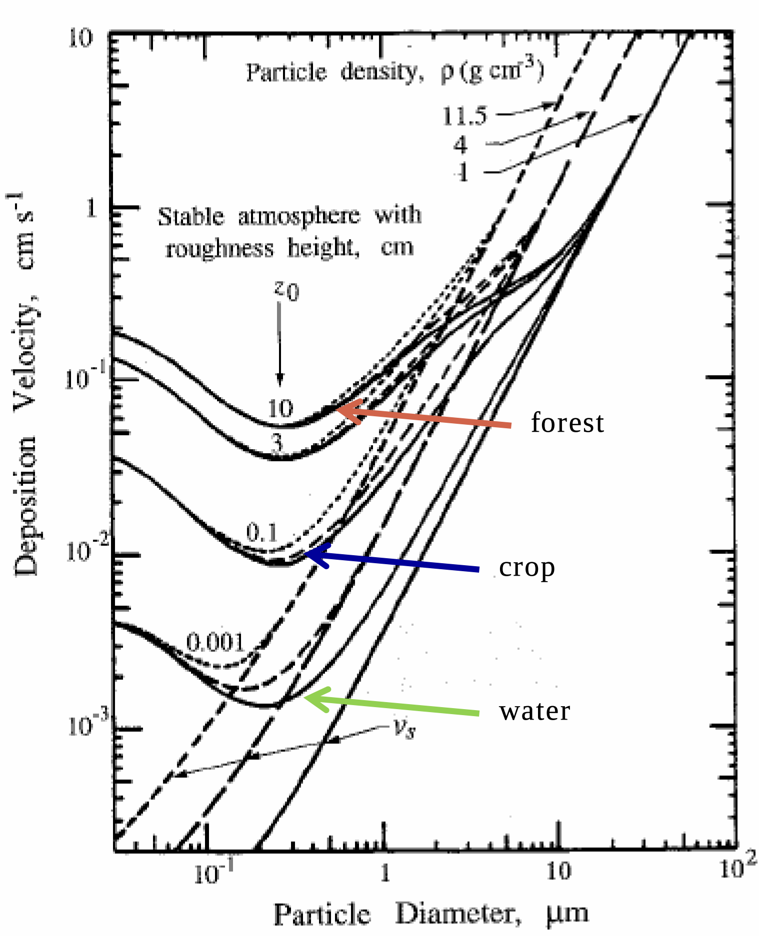


Dry deposition

Close to the surface deposition flux

$$F = -v_d C$$

Deposition velocity v_d is most strongly affected by particle size and the roughness of the surface



Dry deposition velocity

$$v_d = \frac{1}{r_a + r_b + r_c} + v_s$$

where r_a = aerodynamic resistance (determined by turbulence)

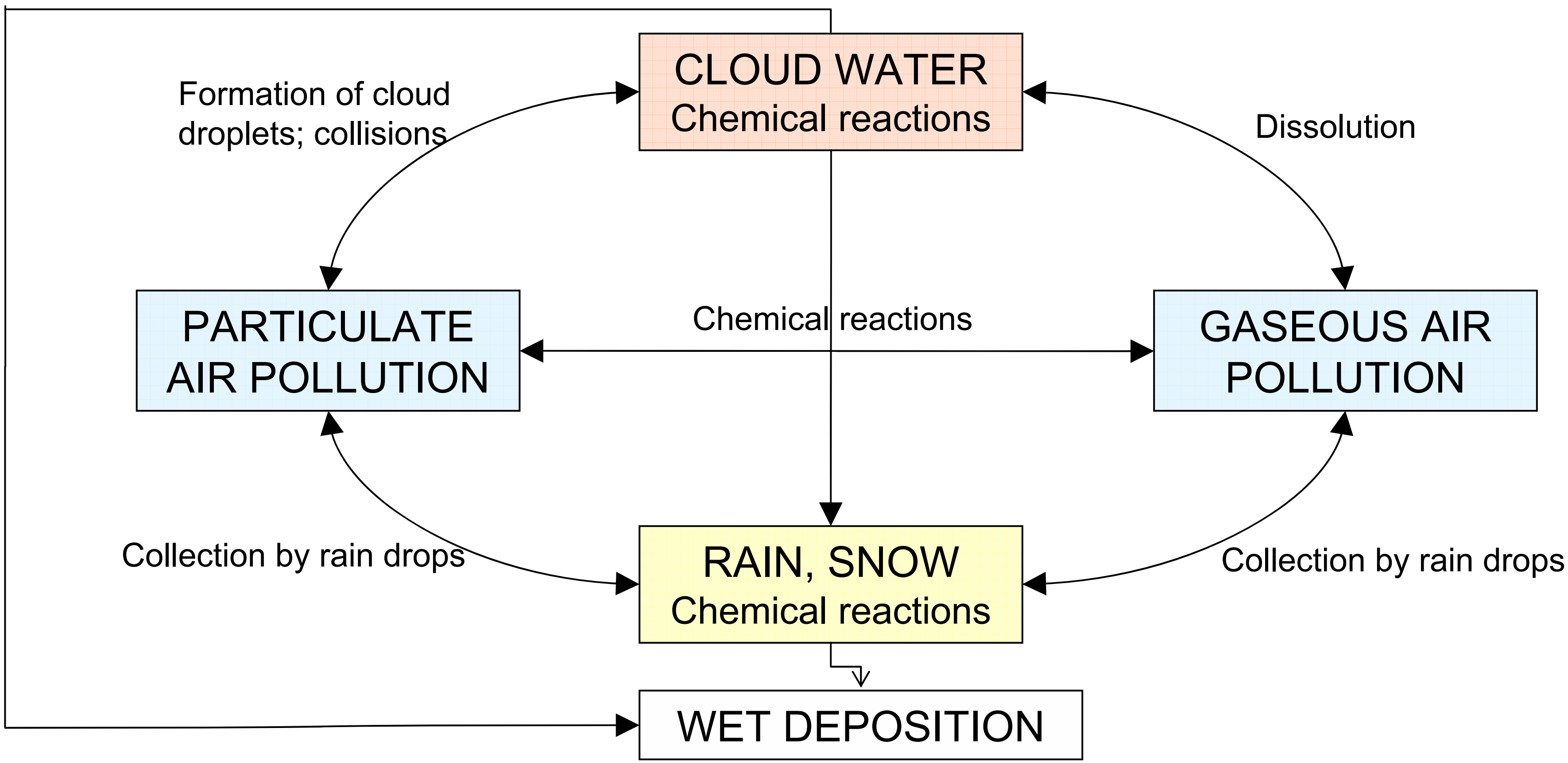
r_b = quasi-laminar layer resistance (determined by particle properties and surface characteristics)

r_c = canopy resistance (chemical reactions, perturbation of quasi-laminar layer)

v_s = particle settling velocity (determined by size)

Resistance equations complex, several "simplified" parameterisations for large scale models available

Wet deposition



In-cloud scavenging

Nucleation scavenging removes in practice all activated particles larger than a certain cut-off size.

Large scale models typically use a cut-off ~100-300 nm dry size in grid boxes where precipitation is formed.

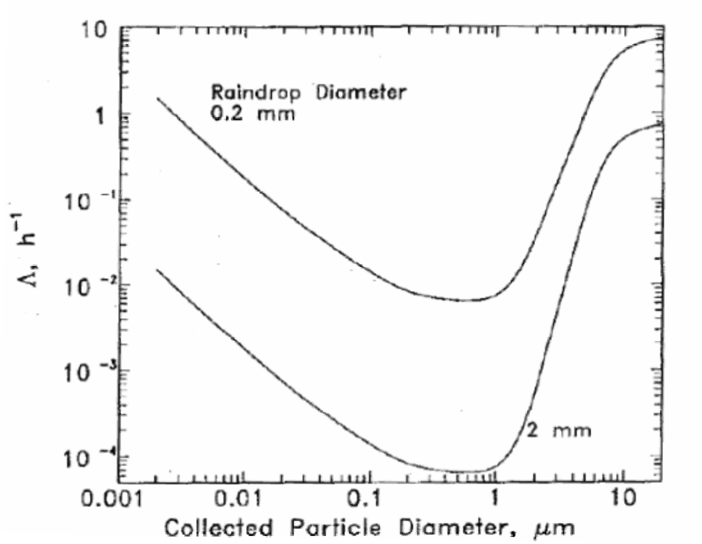
Autoconversion often (but not always) neglected.

Below-cloud scavenging

Scavenging minimum at accumulation mode

–smaller particles collected due to Brownian motion

– larger particles collected due to their inertia



Scavenging rate

$$\Lambda(d_p) = \frac{\pi}{4} D_{drop}^2 U_t(D_{drop}) E(D_{drop}, d_p) N_{drop}$$

where collision efficiency is

$$E = \frac{4}{\mathrm{Re}\, Sc}\left[1 + 0.4\sqrt{\mathrm{Re}}\sqrt[3]{Sc} + 0.16\sqrt{\mathrm{Re}}\sqrt{Sc}\right] + 4\phi\left[\frac{1}{\omega} + (1 + 2\sqrt{\mathrm{Re}})\phi\right] + \left[\frac{St - S^*}{St - S^* + 2/3}\right]^{3/2}$$

Summary

- Time evolution of atmospheric aerosol particles described with general dynamic equation (GDE)

- Although mathematical formulations possible to find for all processes, it is usually impossible to solve all processes simultaneously → time splitting

- Factors limiting accurate solution
  - incomplete information available (esp. emissions)
  - subgrid scale processes (clouds, emissions,...)
  - impossible to describe continuous size distribution in a model (see next lecture!)