Identification of Distributed Parameters in Size-Structured Aerosol Populations using Bayesian State Estimation

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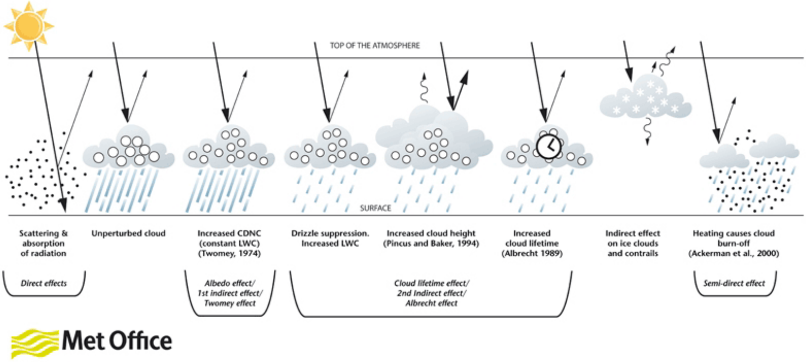
Aerosol, why is it worth understanding them?

1) Implication in the climate change



IPCC reports website [PAB$^+$14, PAP$^+$13] and earlier work [CSH$^+$92].

Aerosol, why is it worth understanding them?

2) Public health impact: in Europe ~ 403000 deaths per year due to $PM_{2.5}$ (cardiovascular diseases ~ 1830000)

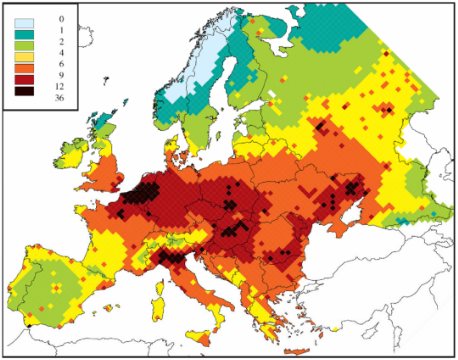
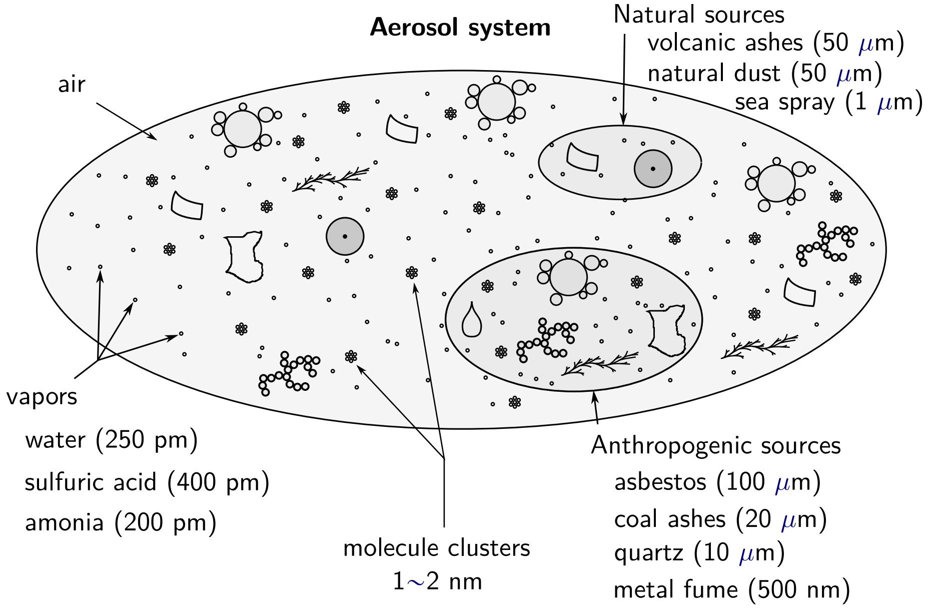
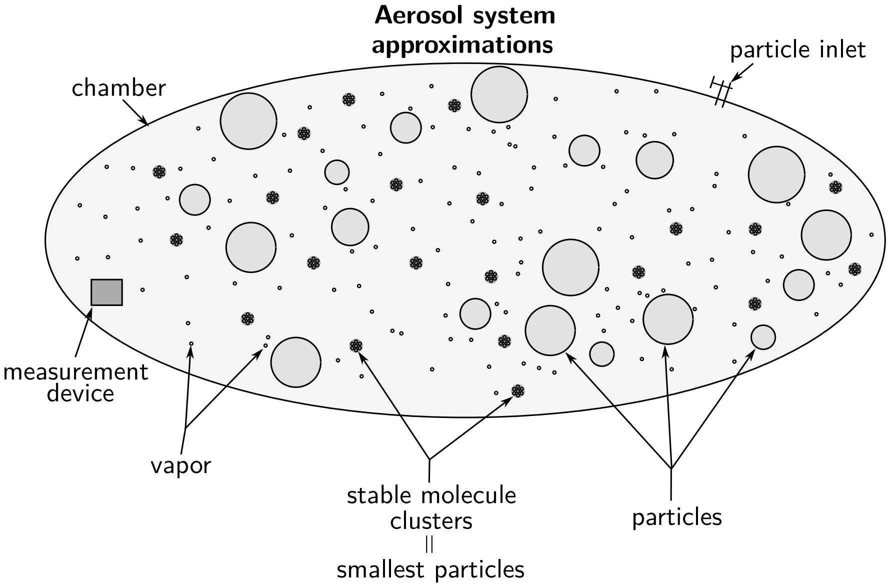


Figure: Loss in life expectancy attributable to exposure to fine particulate matter - 2000 (European Environment Agency)

Aerosol system

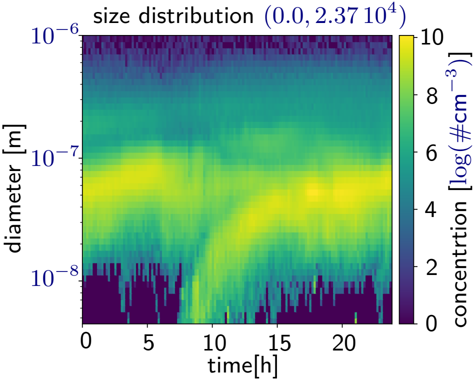


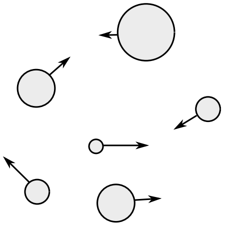

Aerosol system
approximations
particle inlet
chamber
measurement
device
vapor
stable molecule
clusters
||
smallest particles
particles

Representation of an aerosol system:

- box model: uniform in space
- size perfectly describes a particle

Therefor, the system can be represented by a size density.



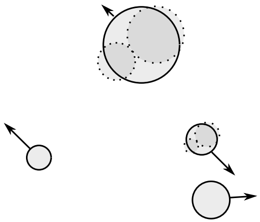


Coagulation

Brownian motion

$+$

sticking collision

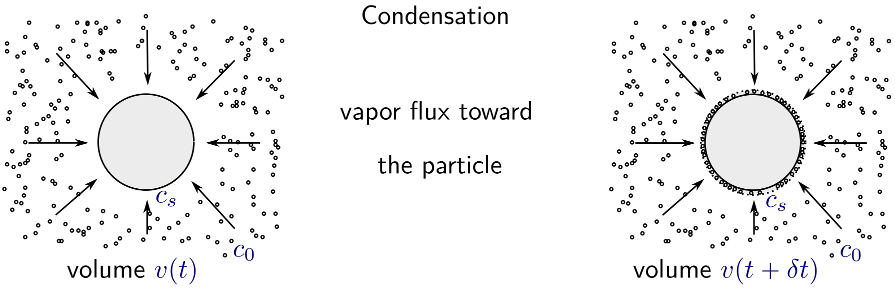


state $u(t)$ state $u(t+\delta t)$

For the Brownian coagulation, the collision frequency factor is given by [FW66]:

$$\beta(v_1, v_2) = \frac{2k_bT}{3\mu}\left(v_1^{\frac{1}{3}} + v_2^{\frac{1}{3}}\right)\left(\frac{1}{v_1^{\frac{1}{3}}} + \frac{1}{v_2^{\frac{1}{3}}}\right)$$

where T is the temperature, μ is the fluid viscosity and v_1 and v_2 the volumes of the coagulating particles

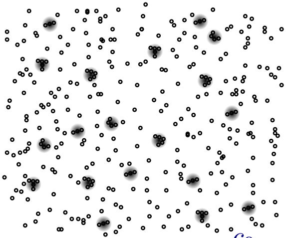


The growth rate of a particle of diameter $d(t)$ and denoted g depends on many parameters:

$$g(t) = f(d_{\text{par}}, d_{\text{vap}}, \frac{\lambda}{\ell}, \eta_{\text{par}}, \eta_{\text{vap}}, [X] \dots)$$

where λ is the mean free path of the particle and ℓ the characteristic size of the problem — $d_{\text{par}}, d_{\text{vap}}$ — the particle and vapor diffusivity η_{par} and η_{vap}, the vapor concentration $[X]$, *etc.* For more details cf. [SP98, Hin12].

Nucleation

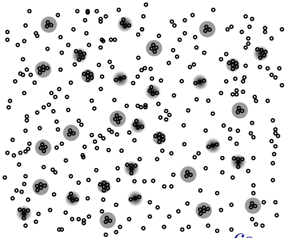


c_0
unstable clusters (t)

some unstable clusters

undergo some events

the energy barrier may be overcome

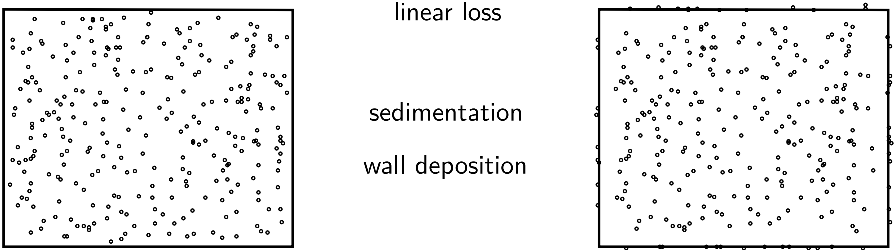


c_0
stable cluters ($t + \delta t$)

The nucleation rate also depends on many parameters — especially if more than one kind of vapor is involved — but two mechanisms — kinetic and activation — can be described a polynomial function of the vapor concentration:

$$J(t) = a[X]^2 + b[X]$$

whose coefficient a and b are not well defined [RSK$^+$07, SP98]



state $u(t)$ state $u(t + \delta t)$

The losses due to sedimentation or deposition on the wall of a chamber can be characterized by a single coefficient

$$\lambda = f(v, \ldots)$$

where v is the particle size. It may depend on the shape of the chamber and on other parameters.

How to describe the evolution of a population of aerosols whose characteristics depend on size? Size-structured Population Balance Equation (PBE).

$$\frac{\partial u}{\partial t} + \frac{\partial g u}{\partial s} = F_{\mathsf{n}}(t, s, u; \theta)$$

This PBE is a scalar conservation law where u is the particle size density, g the growth rate and F_{n} is the term that describes the mechanisms that make the density evolve — it depends on some parameter θ. We refer to this equation as the General Dynamic Equation for aerosols, or simply GDE.

Note: without going into details, each aerosol particle cannot be described only by a size. By nature, particles are complex objects of different shape, size and chemical composition, but we model them as spherical objects of equivalent volume without considering chemistry. Therefore, it cannot be a perfectly precise model (source of uncertainty, potentially modelled by SPDE).

Putting all terms together, the GDE becomes:

$$\underbrace{\frac{\partial u}{\partial t}(t,v) + \frac{\partial gu}{\partial v}(t,v)}_{\text{scalar conservation law}} = \underbrace{\int_{v_\star}^{v-v_\star} \beta_v(s, v-s)u(t,s)u(t,v-s)\mathrm{d}s}_{\text{coagulation source}}$$
$$- \underbrace{u(t,v)\int_{v_\star}^{\infty} \beta_v(v,s)u(t,s)\mathrm{d}s}_{\text{coagulation sink}}$$
$$- \underbrace{\lambda(t,v)u(t,v)}_{\text{linear losses}} + \underbrace{S(t,v)}_{\text{sources}}$$

with the conditions

$$\begin{aligned} u(0,v) &= u_0(v) && \text{initial condition} \\ g(t,v_\star)u(t,v_\star) &= J(t) && \text{lower boundary: nucleation} \\ g(t,v_\infty)u(t,v_\infty) &= L(t) && \text{upper boundary: loss } (L=0 \text{ if } v_\infty \text{ large enough}) \end{aligned}$$

The goal is to estimate some parameters not easily measured, such as:

- growth rates,
- nucleation rate,
- loss rates

based on "easily" measured quantities such as time series of number concentrations. The estimation is an inverse problem of the form:

$$(\hat{u}, \hat{\theta}) \in \arg\max_{u,\theta} \mathbf{P}(u, \theta | \mathcal{Y}, F, H)$$

where $\mathcal{Y}$ is a dataset, F the evolution model and H the measurement model.

Discretization

Dimensionality reduction: high resolution finite difference for PBE depending on the environment Shen et al [SSZ07], FEM for Fokker-Planck equation Harrison [Har88], FEM for GDE Fu et al [FLWC15] Tsang and Rao [TR90].

Age-structured

History "principle of population" by T. R. Malthus [Mal98] when demography begun to be a political concern, P.F. Verhulst in 1838 who formulated the "law of population growth", a.k.a the Verhulst-Pearl equation. Only in 1911, McKendrick and Kesava Pai rediscovered this equation and intended to estimate the rate of multiplication [MP11].

DPI inverse problems: birth rate estimation in Rundell [Run89], death rate estimation in Rundel [Run93] or both in Cho [CK97].

Fokker-Planck

discretization and DPI by minimization of some criteria such as least square Banks et al [BTW93] and Dimitriu [Dim02], or regularized least square Kravaris and Seinfeld [KS85].

Sinko-Streifer

age-and-size-structured equation [SS67]: 1) a growth rate, 2) a linear loss term, and 3) a Fredholm integral boundary condition. The DPI problem for modified versions of the equation:

- Ackleh [Ack97, Ack99]: growth, birth, fragmentation and loss rates
- Banks and Fitzpatrick [BF91]: growth rate via constrained least square
- Ackleh and Miller [AM18]: birth and growth rates, and sticking probability via least square
- Banks and Davis [BD07]: growth rate distribution and uncertainty estimation

GDE

The GDE for aerosol is a generalization of the Smoluchowski equation [Smo16] and is similar to Sinko-Streifer equation, except for the Dirichlet boundary condition and the coagulation integral terms. Only few studies for the DPI:

- Ramachandran [RB10]: experimental investigation of the feasibility
- Bortz et al. [BBM15, BB]: theoretical framework for the estimation of the post-fragmentation probability density of particles

The continuous form of the GDE is not really suitable for our purpose (parameter estimation from time series of number concentration), hence we define:

$$\forall k \in [\![0,T]\!], i \in [\![1,N]\!], \quad N_i^k = \frac{1}{t_{k+1}-t_k}\int_{t_k}^{t_{k+1}}\int_{\Omega_i} u(s,t)\mathrm{d}s\mathrm{d}t$$

the number of particles in the size range $\Omega_i = (v_0 r_v^{i-\frac{3}{2}}, v_0 r_v^{i-\frac{1}{2}}]$ per unit of volume (or at the lower boundary $\Omega_1 = [v_0 r_v^{-\frac{1}{2}}, v_0 r_v^{\frac{1}{2}}]$). Considering a logarithmic scale and assuming a piecewise constant approximation, the evolution equation becomes:

$$N_1^{k+1} = N_1^k + \Delta_t^k\left(J^k - \left(\frac{g_1^k}{\Delta_1} + \lambda_1\right)N_1^k - C_1^{\mathsf{sink}}(N^k)N_i^k\right) + \varepsilon_1^k \tag{1}$$

$$\begin{aligned} N_i^{k+1} = N_i^k + \Delta_t^k\Bigg(&\frac{g_{i-1}^k}{\Delta_{i-1}}N_{i-1}^k - \left(\frac{g_i^k}{\Delta_i} + \lambda_i\right)N_i^k \\ &+ C_i^{\mathsf{source}}(N^k) - C_i^{\mathsf{sink}}(N^k)N_i^k\Bigg) + \varepsilon_i^k \end{aligned} \tag{2}$$

Note that both discretization steps — time and size — add errors. The overall errors/uncertainties are encompassed in the terms ε_i^k.
Note everything is coded in Julia

The problem we were trying to solve is continuous (state space infinite dimension):

$$(\hat{u}, \hat{\theta}) \in \arg\max_{u,\theta} \mathbf{P}(u, \theta | \mathcal{Y}, F, H)$$

but the one we are solving is discrete (discretization by projection onto a subspace):

$$((\hat{N}_i^k)_{i,k}, (\hat{\theta}_i^k)_{i,k}) \in \arg\max_{(N_i^k)_{i,k}, (\theta_i^k)_{i,k}} \mathbf{P}((N_i^k)_{i,k}, (\theta_i^k)_{i,k} | \mathcal{Y}, F, H).$$

We use the Fixed Interval Kalman Smoother.
Note: the question of the convergence of the discrete solution to the continuous one will not be considered, but I assume that it does converge.

Kalman Filter (KF) [Kal60]

Estimation of the expected state and its uncertainty

$$X^{k|k} = \mathbb{E}[X^k|\mathcal{Y}_k] \quad \text{and} \quad \Gamma^{k|k} = \mathrm{Cov}[X^k|\mathcal{Y}_k],$$

Initialization

Set $X^{0|0} \in \mathbb{R}^N$ and $\Gamma^{0|0} \in \mathbb{R}^{N\times N}$ (Prior knowledge)

Recursion

While $k \leqslant K$, do

Prediction

$X^{k|k-1} = F^{k-1}\left(X^{k-1|k-1}\right)$ *(state expectation)*

$\Gamma^{k|k-1} = \partial F^{k-1}\Gamma^{k-1|k-1}(\partial F^{k-1})^T + \Gamma_w^{k-1}$ *(state covariance)*

Calculation of Kalman's gain

$K^k = \Gamma^{k|k-1}(H^k)^T(H^k\Gamma^{k|k-1}(H^k)^T + \Gamma_v^k)^{-1}$

Updating

$\Gamma^{k|k} = (I - K^kH^k)\Gamma^{k|k-1}$

$X^{k|k} = X^{k|k-1} + K^k(y^k - H^kX^{k|k-1})$

Update iterator

$k \Leftarrow k+1$

end(while)

Fixed Interval Kalman Smoother (FIKS) [KS06]

$$X^{k|K} = \mathbb{E}[X^k|\mathcal{Y}_K] \quad \text{and} \quad \Gamma^{k|K} = \mathrm{Cov}[X^k|\mathcal{Y}_K],$$

Initialization
Run KF and store all variables
Set $X^K_{smo} = X^{K|K}$ *and* $\Gamma^K_{smo} = \Gamma^{K|K}$
$k \leftarrow K - 1$
Recursion
While $k \geqslant 1$, do
Compute smoothing gain
$K^k_{smo} = \Gamma^{k|k}(\partial F^{k+1})^T(\Gamma^{k+1|k})^{-1}$
Smoothing
$X^k_{smo} = X^{k|k} + K^k_{smo}\left(X^{k+1}_{smo} - X^{k+1|k}\right)$
$\Gamma^k_{smo} = \Gamma^{k|k} + K^k_{smo}\left(\Gamma^{k+1}_{smo} - \Gamma^{k+1|k}\right)(K^k_{smo})^T$
Update iterator
$k \Leftarrow k - 1$
end(while)

To run the FIKS algorithm, we need the following elements:

- Evolution model (with its error covariance matrix)
- Measurement model (with its error covariance matrix)
- Data: simulation or measurement (with its error covariance matrix)
- Initial guesses: state and covariance

So far, we have

- the evolution model of the number concentrations

and we still need:

- the evolution models of the parameters
- the measurement model
- the data

Surrogate evolution models

Time invariant Some parameter are time invariant, so their time evolution model is a random walk:

$$k \geqslant 1, \quad p^{k+1} = p^k + \eta^k, \quad \text{with} \quad \eta^k \sim \mathcal{N}(0, \Gamma_\eta)$$

where Γ_η is the covariance of the model uncertainty.

Second order If a parameter is known to evolve smoothly with time, it can be modelled as a second order stochastic process such as:

$$G^k = \begin{bmatrix} p^k \\ p^{k-1} \end{bmatrix} = \begin{bmatrix} 2r_p & -r_p^2 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} p^{k-1} \\ p^{k-2} \end{bmatrix} + \begin{bmatrix} \eta_k \\ 0 \end{bmatrix} = B(r_p)G^{k-1} + \begin{bmatrix} \eta^k \\ 0 \end{bmatrix}$$

where r_p is the smoothness lever and $\eta^k \sim \mathcal{N}(0, \sigma_\eta^2)$ with σ_η controlling the amplitude of the process. The latter is given by its covariance matrix defined by:

$$\Gamma_G^k = \mathrm{cov}(G^k) = B(r_p)\Gamma_G^{k-1}B(r_p)^T + \begin{bmatrix} \sigma_\eta^2 & 0 \\ 0 & 0 \end{bmatrix}.$$

We are interested in the asymptotic behavior, i. e. $\Gamma_G^k = \Gamma_G^{k-1} = \Gamma_G^\infty = \begin{bmatrix} \sigma_p^2 & c \\ c & \sigma_p^2 \end{bmatrix}$, and how the variance of η controls the variance of p, σ_p^2. By expanding the previous relation, we find that:

$$\sigma_\eta^2 = \sigma_p^2 \left(1 - r_p^2 \left(4 + r_p^2 \left(1 - \frac{8}{1 + r_p^2}\right)\right)\right), \quad c = \frac{2r_p}{1 + r_p^2}\sigma_p^2.$$

Size correlation Some parameters are distributed, yet, the size dependence may be unknown or only approximately known. For most parameter, it is safe to assume that size dependence is continuous, and even rather smooth.

Let $p^k \in \mathbb{R}^N$ follow a random walk, the covariance Γ_η contains the size dependence information, and it can be constructed as:

$$\Gamma_\eta = \tilde{D}^{\frac{1}{2}} \bar{D}^{-\frac{1}{2}} \bar{\Gamma} \bar{D}^{-\frac{1}{2}} \tilde{D}^{\frac{1}{2}}$$

where $\bar{\Gamma}$ is the Toeplitz matrix build with the sequence $(\bar{\sigma}_i)_{i \in [\![1,N]\!]}$ which determines how the size dependence evolves with the size difference. We choose the sequence

$$\forall i \in [\![1, N]\!], \quad \bar{\sigma}_i = \bar{\sigma}_0 e^{\frac{1-i}{\delta}}$$

with δ so that only the first δ neighboring sizes significantly contribute to the evolution of one variable. The diagonal matrix $\bar{D} = \bar{\sigma}_1^2 I_N$ normalize the covariance $\bar{\Gamma}$ and the diagonal matrix $\tilde{D} = \text{diag}([\sigma_{\eta,1}^2 \, \sigma_{\eta,2}^2 \ldots \sigma_{\eta,N}^2])$ scales the variance of each size.

Size correlation

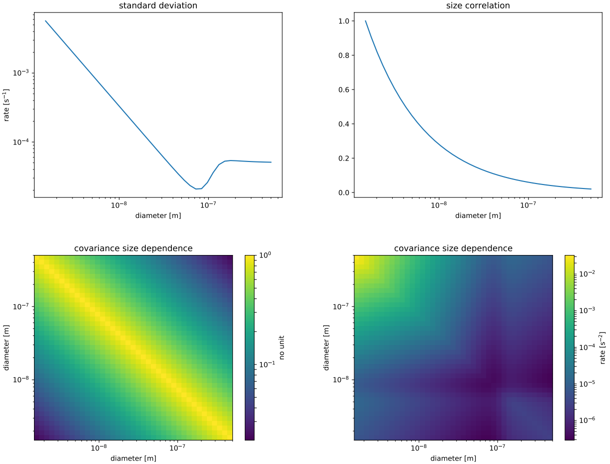


Figure: Creation of the covariance matrix of a model. a) size-dependence of the variances, b) correlation, c) Toeplitz matrix of the correlation, and d) covariance matrix of the model.

What if we know the possible range of a parameter?

Lower bound a

$$\zeta \in \mathbb{R},\ \alpha > 0, \quad p = a + \frac{1}{\alpha} \log\left(1 + e^{\alpha\zeta}\right),$$

Range $[a, b]$

$$\zeta \in \mathbb{R},\ \alpha > 0, \quad p = a + \frac{b - a}{1 + \frac{1}{\alpha} e^{-\alpha\zeta}}$$

Monotone: increasing

$$p_1 \in \mathbb{R},\ i > 1,\ \zeta_i \in \mathbb{R},\ \alpha_i > 0, \quad p_i = p_{i-1} + \frac{1}{\alpha_i} \log\left(1 + e^{\alpha_i \zeta_i}\right)$$

DMA

This device acts as a selector of near monodisperse size distribution around a given size d_i; its size discrimination power determines the sets $\{d_i\}_{i\in[\![1,N]\!]}$ and $\{\Delta_i\}_{i\in[\![1,N]\!]}$. For each channel, we denote the time invariant kernel ψ_i, which models the efficiency of the device. The number concentration at the outlet of the DMA is approximated by:

$$z_i^k = \frac{1}{\Delta_t}\int_{t_0+(k-1)\Delta_t}^{t_0+k\Delta_t}\int_{\omega_i}\psi_i(s)u(s,t)\mathrm{d}s\mathrm{d}t + \iota_i^k = \varphi_i^k + \iota_i^k$$

where ω_i is the support of ψ_i — where it is not null — and ι_i^k accounts for the model uncertainties. The number of particle is then obtained by multiplying by the volume.

CPC

Let the number concentration of particles at the inlet of a CPC is z_i^k (coming from the i^{th} channel of the DMA), the output y_i^k is modeled by:

$$y_i^k = \frac{\tilde{y}_i^k}{V}, \quad \text{with} \quad \tilde{y}_i^k \sim \mathcal{P}\text{oisson}(V z_i^k)$$

where V is the volume of sample used in the CPC for counting. In most cases, the number of particle in the CPC is large enough ($V z_i^k > 20$), thus the Poisson distribution can satisfactorily be approximated by:

$$y_i^k \sim \mathcal{N}(z_i^k, \frac{z_i^k}{V}).$$

Note that from this model it is clear that the quality of the measurement is directly link to the volume of the sample.

We use simulated data in order to evaluate the performance of the method

- dense discretization of the size space
- non-approximated measurement model (Gaussian kernel and Poisson noise)

The dense discretization of the size space may lead to spurious oscillation (or diverge) if the following condition on the time step is not met:

$$0 < \Delta_t^k < \frac{1}{\max_i \{ \frac{g_i^k}{\Delta_i} + \lambda_i + C_i^{\mathsf{sink}}(N^k) \}}.$$

For a acceptable approximation of the size density the size discretization must be small enough: it implies a very small time step.

Nucleation event

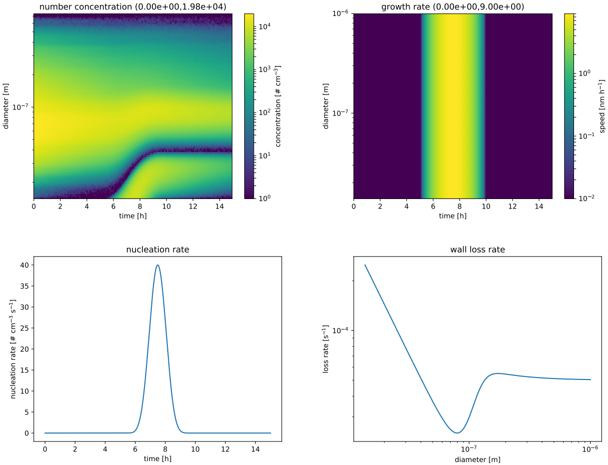


Figure: Simulation of a nucleation event. a) Number concentration contour plot, b) growth rate, c) nucleation rate at 14.1nm, and d) wall loss rate.

CLOUD simulation

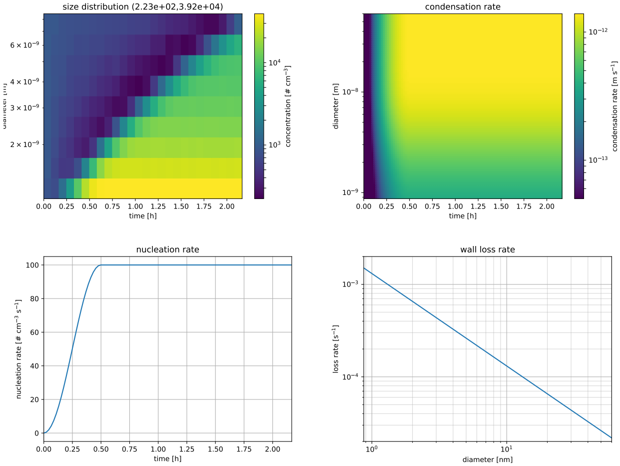


Figure: Simulation of a steady state. 1) Number concentration contour plot, 2) growth rate, 3) nucleation rate, and 4) wall loss rate.

Nucleation event

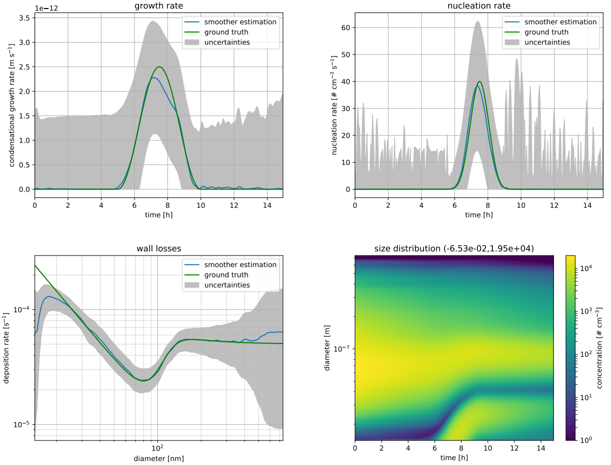


Figure: Estimation of the parameter of the GDE for aerosols from a simulated nucleation event data: 1) growth rate, 2) nucleation rate, 3) loss rate, and 4) number concentration.

CLOUD simulation

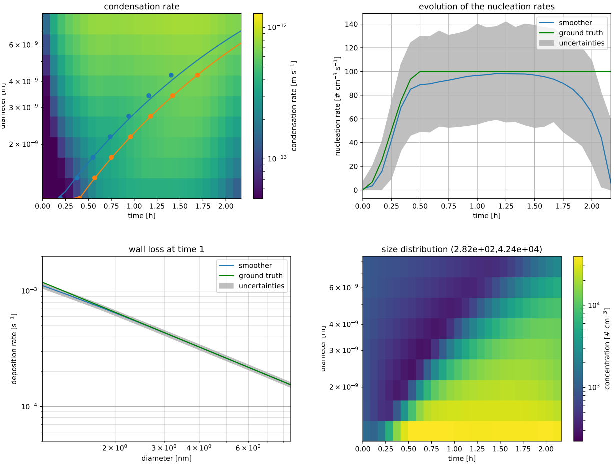


Figure: Estimation of the parameter of the GDE for aerosols from a simulated transition to steady state data: 1) growth rate, 2) nucleation rate, 3) loss rate, and 4) number concentration.

Take home messages:

- The requirements for applying the method are "weak": 1) the model must be well approximated by their Jacobian, and 2) the errors can be approximated as Gaussian
- The Fixed Interval Kalman Smoother is a suitable tool for the estimation of the GDE parameters along with uncertainties
- Need surrogate evolution models for the parameters of interest

Future work?

- Estimate coagulation coefficient
- CVG of the discrete to the continuous problem
- address the case of purely steady state (MAP estimate, but no uncertainty)
- more realistic model of the measurement device

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Thank you for your attention!