University of Brighton

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Modelling and experimental studies of aerosols and sprays for medical and automotive applications
Kazan Federal University , University of Brighton

Artur Gilfanov
(Kazan Federal University)

Modelling of evaporation in quadrature method of moments.

Governing equations

$n(t, x, v, s)dvds$ - particle concentration with velocity [v; $v + dv$] and size [s; $s + ds$]

$$\frac{\partial n}{\partial t} + \frac{\partial (vn)}{\partial x} + \frac{\partial (An)}{\partial v} + \frac{\partial (Gn)}{\partial s} = 0$$

Williams equation

$$\frac{\partial n}{\partial t} + \frac{\partial (Gn)}{\partial s} = 0$$

$G = Bs^p$ - evaporation law

B – some coefficient p - power (0, 1/3 or 2/3, etc.)

d – particle diameter, v – particle volume

$$\frac{dv}{dt} = \frac{2\pi D d v_m}{kT}(p - p_s)$$

d^2-law, continuum regime

$$\frac{dv}{dt} = \frac{\pi d^2 v_m}{(2\pi m kT)^{1/2}}(p - p_s)$$

d-law, free-molecular regime

D – vapour diffusivity

v_m – monomer volume

p – actual vapour pressure

p_s – saturation pressure

T – temperature

k – Boltzmann constant

m – mass of one molecule

(Friedlander, 2000)

d – particle diameter

	d^2-law	d-law
s - particle volume	$G = \frac{ds}{dt} = Bs^{1/3}$	$G = \frac{ds}{dt} = Bs^{2/3}$
s - particle surface area	$G = \frac{ds}{dt} = B$	$G = \frac{ds}{dt} = Bs^{1/2}$
s - particle diameter	$G = \frac{ds}{dt} = Bs^{-1}$	$G = \frac{ds}{dt} = B$

In a pure evaporation problem the particle surface area or the particle diameter is a good choice for phase variable.

$$\frac{\partial n}{\partial t} + \frac{\partial (Gn)}{\partial s} = 0$$

Let us multiply by s^k and integrate over size range

$$\frac{\partial M_k}{\partial t} + \int_0^{+\infty} s^k \frac{\partial (Gn)}{\partial s} ds = 0$$

$$\int_0^{+\infty} s^k \frac{\partial (Gn)}{\partial s} ds = \int_0^{+\infty} s^k d(Gn) = Gns^k \Big|_0^{+\infty} - \int_0^{+\infty} Gnd(s^k) =$$

$$= Gns^k \Big|_0^{+\infty} - \int_0^{+\infty} ks^{k-1} Gnds$$

If $k = 0$ $$\left. Gns^k \right|_0^{+\infty} - \int_0^{+\infty} ks^{k-1} Gn ds = -Gn(s=0) = -\psi$$ disappearance of particles due to evaporation

If $k > 0$ $$\left. Gns^k \right|_0^{+\infty} - \int_0^{+\infty} ks^{k-1} Gn ds = -\int_0^{+\infty} ks^{k-1} Gn ds$$

$$G = Bs^p$$

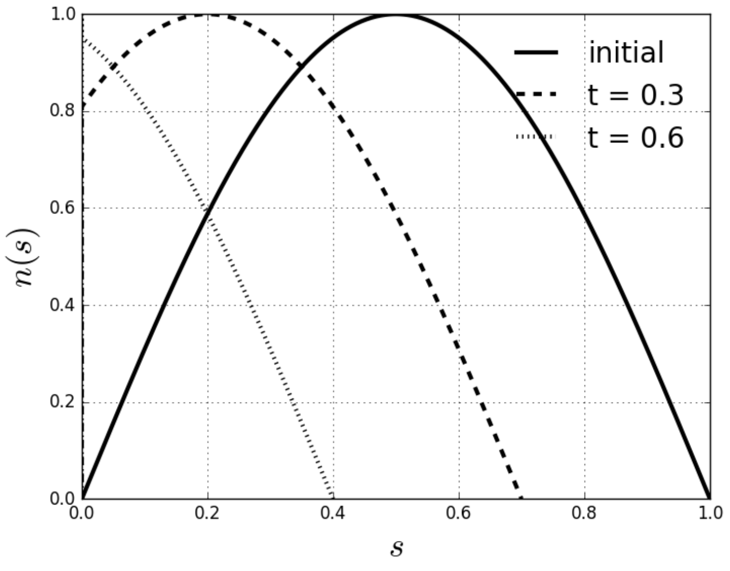
	If $p = 0$	If $p = 1/3$
$\frac{\partial M_0}{\partial t} = \psi$	$\frac{\partial M_0}{\partial t} = \psi$	$\frac{\partial M_0}{\partial t} = \psi$
$\frac{\partial M_1}{\partial t} = \int_0^{+\infty} Gnds$	$\frac{\partial M_1}{\partial t} = BM_0$	$\frac{\partial M_1}{\partial t} = BM_{1/3}$
$\frac{\partial M_2}{\partial t} = 2\int_0^{+\infty} Gnsds$	$\frac{\partial M_2}{\partial t} = 2BM_1$	$\frac{\partial M_2}{\partial t} = 2BM_{4/3}$
$\frac{\partial M_3}{\partial t} = 3\int_0^{+\infty} Gns^2ds$	$\frac{\partial M_3}{\partial t} = 3BM_2$	$\frac{\partial M_3}{\partial t} = 3BM_{7/3}$

$$n(s) = \sum_{i=1}^{2} w_i \delta(s - s_i)$$

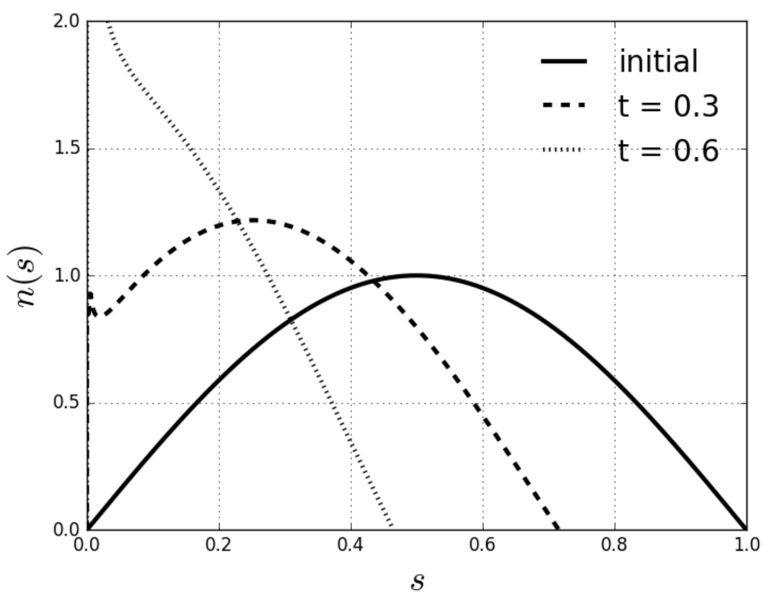
Right parts for M_1, M_2, M_3 can be calculated, but not for M_0

$$\frac{\partial n}{\partial t} + \frac{\partial (Gn)}{\partial s} = 0$$

$$G = \frac{ds}{dt} = \text{const}$$

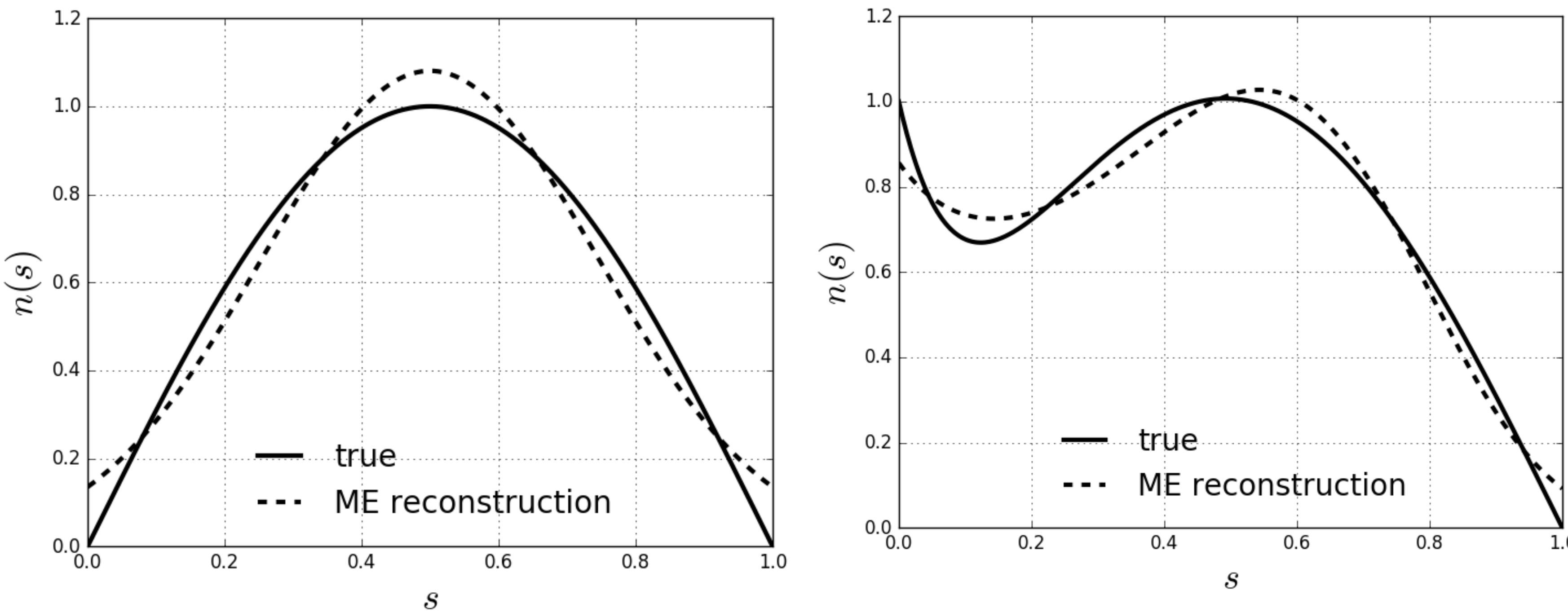


$$G = \frac{ds}{dt} = -s^{1/3}$$



Maximum entropy method

$$n_{ME}(s) = \exp(-\sum_{i=0}^{N} \xi_i s^i) \qquad L(n) = -\int n(s) \ln n(s) ds \to \max$$



Massot, M. A robust moment method for evaluation of the disappearance rate of evaporating sprays / M. Massot, F. Laurent, D. Kah, S. De Chaisemartin // SIAM Journal on Applied Mathematics. – 2010. – V.70, I.8. – P.3203-3234.

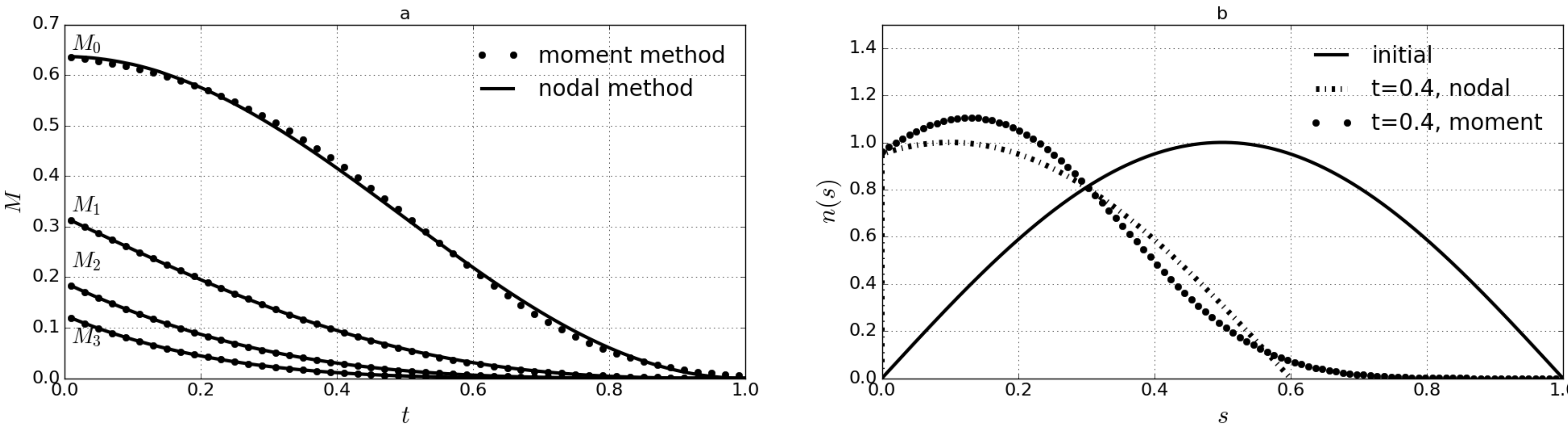
Calculation scheme

$$M_0^j, M_1^j, M_2^j, M_3^j$$

1) reconstruction of the particle size distribution by maximum entropy method
2) estimation of loss of the moments due to disappearance of particles
3) PD-reconstruction (determination of abscissas and weights) using residual values of the moments
4) transport of the abscissas in phase space (evaporation)

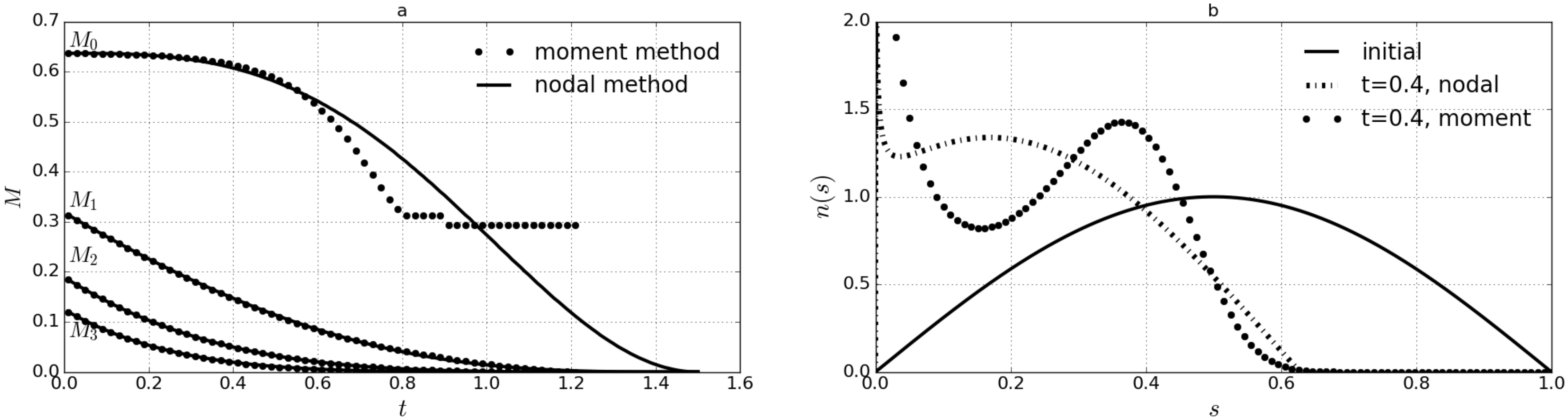
$$M_0^{j+1}, M_1^{j+1}, M_2^{j+1}, M_3^{j+1}$$

Constant evaporation law



$$G = \frac{ds}{dt} = \text{const}$$

Power evaporation law



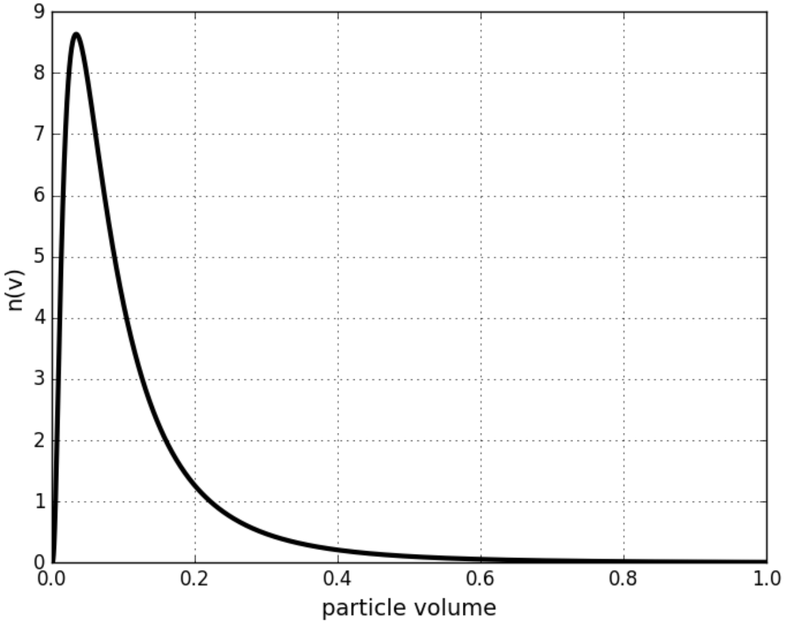
$$G = \frac{ds}{dt} = -s^{1/3}$$

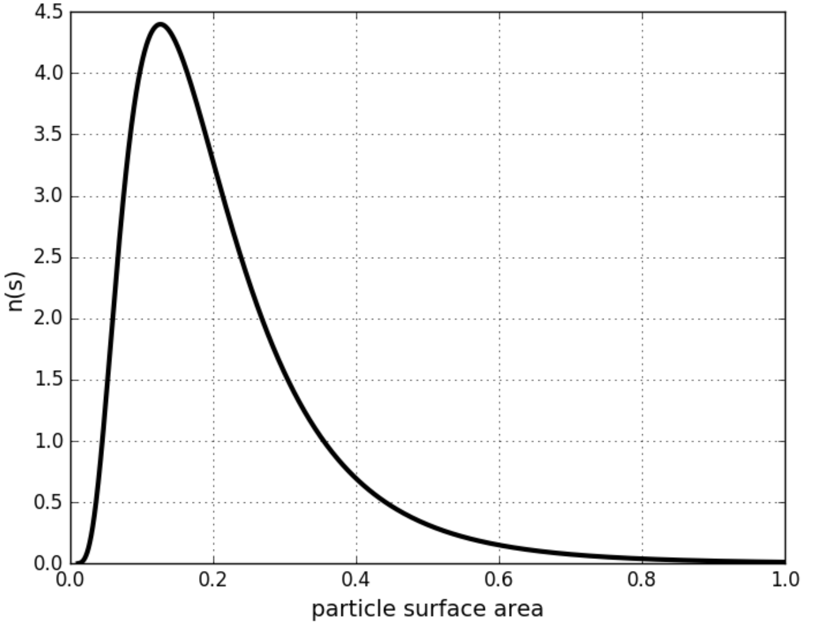
Evaporation for lognormal distribution

$d_g = 50 \cdot 10^{-6}$ m – geometric mean diameter

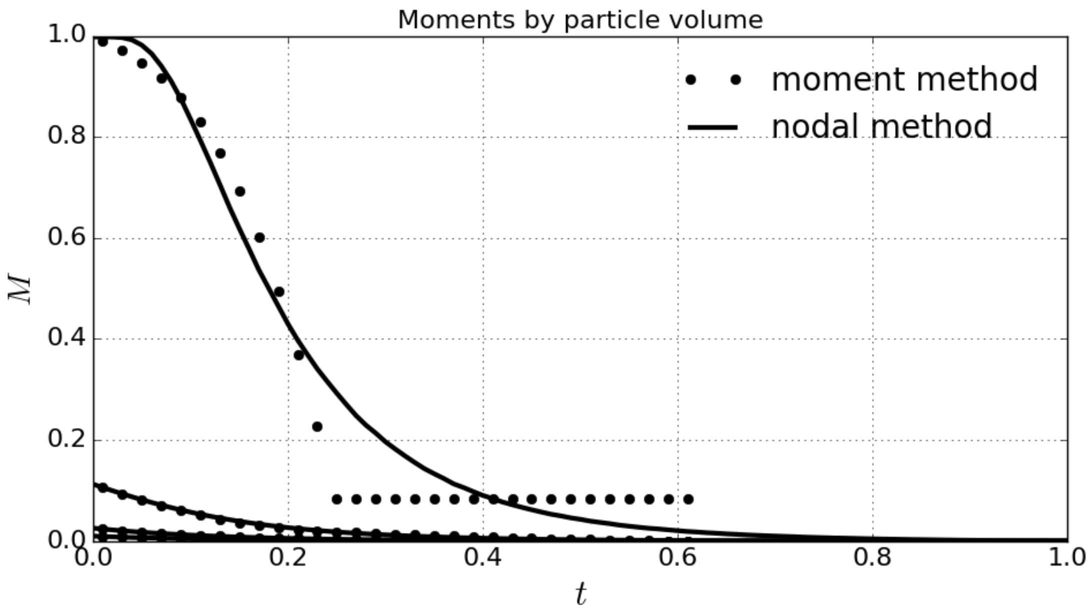
$\sigma = 1.35$ – standard geometric deviation

Normalized distributions



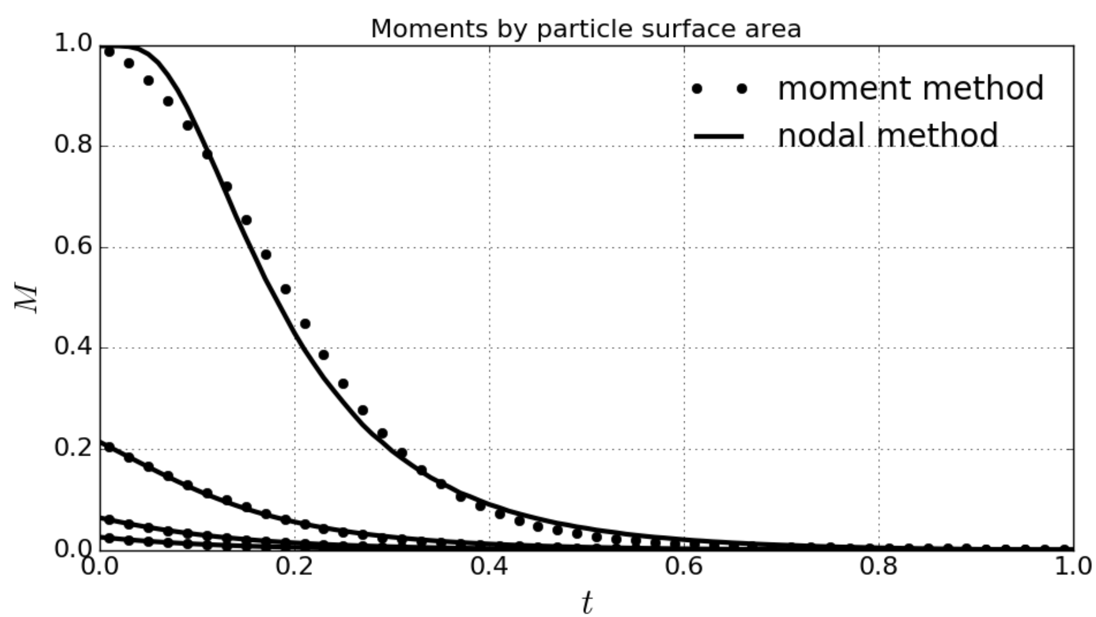


Evaporation for lognormal distribution



power law evaporation

constant evaporation law



Extended quadrature method of moments

$$n(s)=\sum_{i=1}^{N} w_i \delta(s-s_i) \quad \Rightarrow \quad n(s)=\sum_{i=1}^{N} w_i \delta_\sigma(s,s_i)$$

$\delta_\sigma(x,y)$ - kernel density function

σ – parameter (deviation)

An additional moment is needed to determine σ

seminfinite support

$$\delta_\sigma(x,y)=\frac{1}{\sigma\Gamma(y/\sigma)}\left(\frac{x}{\sigma}\right)^{y/\sigma-1} e^{-x/\sigma}$$

Gamma

infinite support

$$\delta_\sigma(x,y)=\frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(x-y)^2}{2\sigma^2}\right)$$

Gaussian

finite support

$$\delta_\sigma(x,y)=\frac{x^{y/\sigma-1}(1-x)^{(1-y)/\sigma-1}}{B(y/\sigma,(1-y)/\sigma)}$$

Beta

(Yuan, Fox, 2012)

Acknowledgments

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Thank you for your attention!