TAMPERE UNIVERSITY OF TECHNOLOGY

Lagrangian Tampere University of Technology Aerosol Model (L-TUTAM) Manual

Miska Olin

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CONTENTS

LIST OF SYMBOLS AND ABBREVIATIONS

Latin symbols

$\bar{c}$	mean thermal velocity of a particle
D_1	the lowest particle diameter in a power law distribution
D_2	the highest particle diameter in a power law distribution
D_{coag}	cut diameter for coagulational transfer
D_{p}	particle diameter
$\mathcal{D}_{\mathrm{p}}$	particle diffusion coefficient
$f(\mathrm{Kn}_{\mathrm{coag}})$	transition regime function
g	condensational growth rate
i	index for the distribution, PL or LN
j	index for a size section
J	new particle formation rate
k	order of the moment
k_{dep}	deposition coefficient
$\mathrm{Kn}_{\mathrm{coag}}$	Knudsen number for coagulation
l_{bg}	exponent for the coagulational losses
m	index for a vapor
$M_{i,0}$	0^{th} moment, i.e. the number concentration, in distribution i
$M_{i,2}$	2^{th} moment in distribution i
$M_{i,3}$	3^{th} moment in distribution i
$M_{i,k}$	k^{th} moment in distribution i
N	particle number concentration
N_{bg}	number concentration of the background distribution
n_i	mode i density function
N_j	number concentration in the size section j
n_{LN}	the density function of the LN distribution
N_{LN}	the number concentration of the LN distribution
n_{PL}	the density function of the PL distribution
N_{PL}	the number concentration of the PL distribution
t	time
T	temperature
X	index for a moment

Greek symbols

α	slope parameter of the power law distribution
β	coagulation coefficient

γ	condensational transfer factor
ΔD_j	diameter width of the size section j
ρ_p	particle density
σ	geometric standard deviation of the LN distribution

Abbreviations

CMD	count median diameter
FS	fixed-sectional representation of the distribution
GMD	geometric mean diameter
GSD	geometric standard deviation
LN	log-normal distribution
NPF	new particle formation
PL	power law distribution
PL+LN	combined power law and log-normal distribution

1. CAPABILITIES AND LIMITATIONS

L-TUTAM is an aerosol dynamics model used in Lagrangian simulations with Matlab. New particle formation, condensation (not evaporation), coagulation, coagulational losses, and depositional losses can be simulated with the model. The model contain two submodels: 1) simple model using new particle formation rate and growth rate as inputs, 2) gas-particle-coupled model where those rates are calculated using nucleation and condensation theories. Particle size distribution can be represented modally or sectionally in the simple model, and only modally in the coupled model. The modal representation is computationally efficient but the distribution must have a pre-defined shape. Table 1.1 shows the main limitations of the model.

Table 1.1: *Limitations of L-TUTAM.*

Size distribution represented modally	PL (power law), LN (log-normal), PL+LN
Size distribution represented sectionally	no limitations (only in simple model)
Number of distributions	1
Immiscible phases in a particle	1
Miscible species in a particle	1 (simple), no limitations (coupled)
Particle diameter D_p	no limitations (works best when $D_\mathrm{p} < 100$ nm)
Particle morphology	spherical
Temperature T	no limitations
Pressure p	no limitations

2. THEORY

2.1 Particle size distributions

The particle size distribution is represented, by default, as a log-normal (LN) distribution, which provides the fastest simulation. In the case of simultaneous new particle formation and growth, the combined power law (PL) and log-normal distribution (PL+LN) can also be used. Additionally, it can be represented as a power law (PL) distribution only. If the size distribution cannot be fixed to a pre-defined shape, a fixed-sectional (FS) representation can be used. Figure 2.1 represents a sample of a LN distribution. LN distribution has the following density function

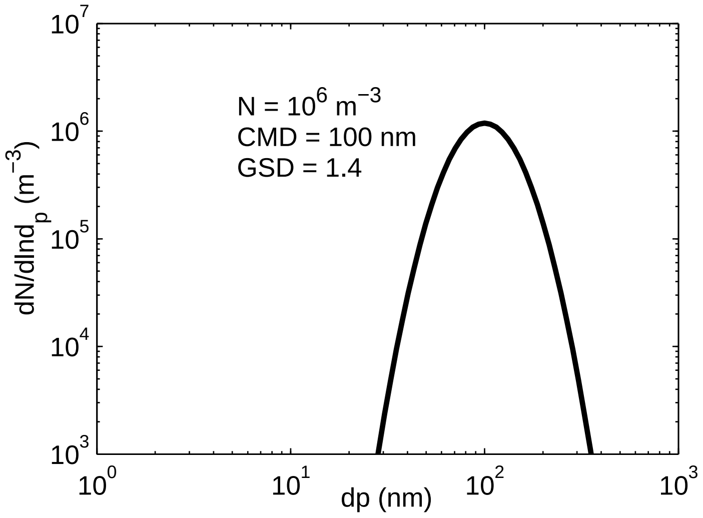

Figure 2.1: *A log-normal aerosol distribution.*

$$n_{\mathrm{LN}} = \left.\frac{\mathrm{d}N}{\mathrm{d}\ln D_{\mathrm{p}}}\right|_{\mathrm{LN}} = \frac{N_{\mathrm{LN}}}{\sqrt{2\pi}\ln\sigma}\exp\left[-\frac{\ln^2\left(\frac{D_{\mathrm{p}}}{CMD}\right)}{\ln^2\sigma}\right], \tag{2.1}$$

where N_{LN} is the total particle number concentration, $\mathrm{d}N$ is the particle number concentration within a logarithmic size range $\mathrm{d}\ln D_{\mathrm{p}}$, CMD is the count median diameter, σ is the geometric standard deviation, and D_{p} is the particle diameter (Hinds, 1999).

Figure 2.2 represents samples of PL distributions and of a combined PL+LN distribution. PL distribution has the following density function

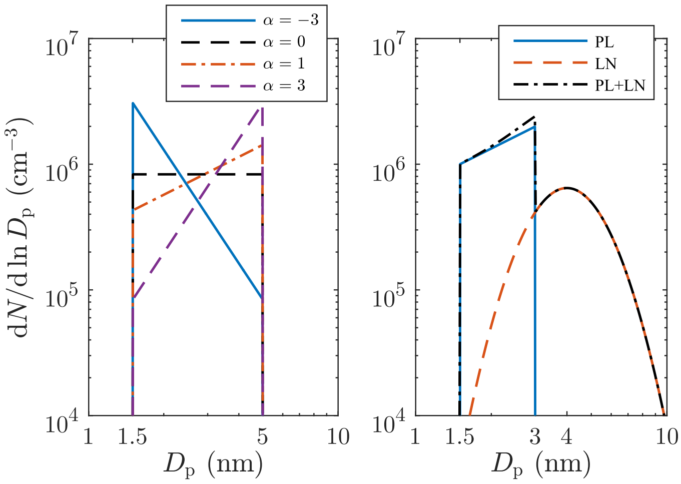

Figure 2.2: *Left pane represents examples of the power law distribution with different values of α. Right plane represents the combination of power law and log-normal distributions. (Olin et al., 2016)*

$$n_\mathrm{PL} = \left.\frac{\mathrm{d}N}{\mathrm{d}\ln D_\mathrm{p}}\right|_\mathrm{PL} = \begin{cases} \frac{N_\mathrm{PL}\alpha}{D_2^\alpha - D_1^\alpha} D_\mathrm{p}^\alpha, & D_1 \leq D_\mathrm{p} \leq D_2,\ \alpha \neq 0 \\ \frac{N_\mathrm{PL}}{\ln(D_2/D_1)}, & D_1 \leq D_\mathrm{p} \leq D_2,\ \alpha = 0 \\ 0, & \text{otherwise} \end{cases} \tag{2.2}$$

where α is the slope parameter, D_1 is the smallest diameter, and D_2 is the largest diameter of the PL distribution (Olin et al., 2016). In the PL+LN model, the total distribution is expressed with

$$n_\mathrm{PL+LN} = n_\mathrm{PL} + n_\mathrm{LN}. \tag{2.3}$$

More information on the PL+LN model can be found in Olin et al. (2016).

Figure 2.3 represents a sample of an FS40 (fixed-sectional distribution having 40 size sections between 1.6 and 100 nm) distribution.

2.2 Moments of a distribution

A log-normal distribution function (Eq. 2.1) requires 3 parameters (N, CMD, σ) to represent the particle concentration dN for a size D_p. Therefore, modelling of a log-normal distribution requires 3 variables and 3 equations to be modelled. A power law distribution requires 4 parameters (N, α, D_1, D_2) of which D_1 has a constant value. Therefore, 3 variables are required for the PL distribution also. These variables are the k^th moments of a distribution that are defined as

$$M_{i,k} = \int_{-\infty}^{\infty} D_\mathrm{p}^k\, n_i \,\mathrm{d}\ln D_\mathrm{p}, \tag{2.4}$$

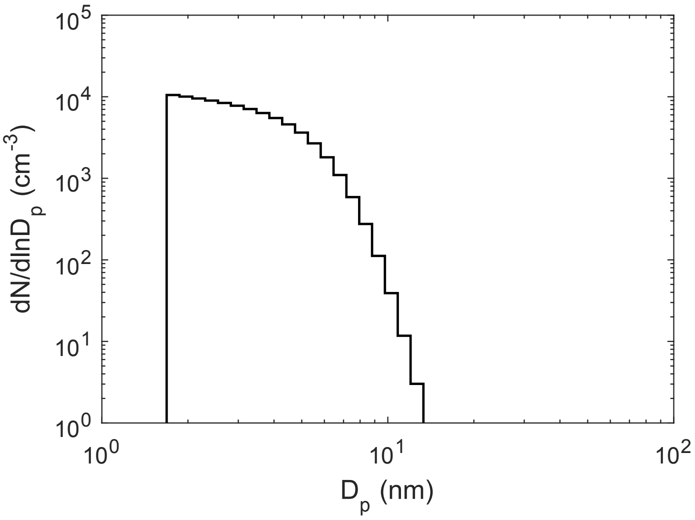

Figure 2.3: *Particle size distribution represented by the FS40 model.*

where i denotes the distribution, PL or LN. The 3 moments [and their units] used in L-TUTAM are

$$\begin{aligned} &M_{i,0} \quad [1/\mathrm{cm}^3] \\ &M_{i,2} \quad [\mathrm{m}^2/\mathrm{cm}^3] \\ &M_{i,3} \quad [\mathrm{m}^2/\mathrm{cm}^3] \end{aligned} \tag{2.5}$$

which correspond to number concentration, surface area concentration (times π^{-1}), and mass concentration (times $6\pi^{-1}\rho_\mathrm{p}^{-1}$), respectively. In the coupled model, mass concentration is also divided into the number of different vapor species

$$M_{i,3} = \sum_m M_{i,3,m}, \tag{2.6}$$

where the index m denotes a vapor.

When 3 moments are known, the 3 parameters of a log-normal distribution can be calculated by (Whitby and McMurry, 1997)

$$\begin{aligned} N_\mathrm{LN} =& M_\mathrm{LN,0} \\ \sigma =& \exp\left(\sqrt{\ln\frac{M_\mathrm{LN,3}^{\frac{2}{3}} M_\mathrm{LN,0}^{\frac{1}{3}}}{M_\mathrm{LN,2}}}\right) \\ CMD =& \left(\frac{M_\mathrm{LN,3}}{M_\mathrm{LN,0}}\right)^{\frac{1}{3}} e^{-1.5\ln^2\sigma}, \end{aligned} \tag{2.7}$$

Reconstruction of the parameters of PL distribution from 3 moments is done either using an interpolation table as described in Olin et al. (2016) or using the Levenberg-Marquardt iteration algorithm. In the PL+LN model, totally 6 moments are modelled.

2.3 General dynamic equation for the moments in modal method

Aerosol dynamics is modelled with the following equation

$$\frac{\mathrm{d}X}{\mathrm{d}t} = \mathrm{npf}_X + \mathrm{cond}_X + \mathrm{coag}_X + \mathrm{loss}_X^{\mathrm{coag}} + \mathrm{loss}_X^{\mathrm{dep}} + \mathrm{transfer}_X^{\mathrm{coag}} + \mathrm{transfer}_X^{\mathrm{cond}}, \tag{2.8}$$

where X denotes a particular moment.

2.3.1 New particle formation

The new particle formation (NPF) term in Eq. 2.8 is

$$\begin{aligned} \mathrm{npf}_{M_{i,0}} =& J(t) \\ \mathrm{npf}_{M_{i,2}} =& J(t) D_1^2 \\ \mathrm{npf}_{M_{i,3}} =& J(t) D_1^3, \end{aligned} \tag{2.9}$$

where $J(t)$ is the new particle formation rate [1/cm^{3}s] as a function of time, D_1 is the diameter of a newly formed particle. In the PL+LN model, new particles are formed only in the PL distribution.

2.3.2 Condensation

The condensation term in Eq. 2.8 is

$$\mathrm{cond}_X = \begin{cases} 0, & X = M_{i,0} \\ 2\, g(t) \int_{-\infty}^{\infty} D_\mathrm{p}\, \mathrm{d}N_i, & X = M_{i,2} \\ 3\, g(t) \int_{-\infty}^{\infty} D_\mathrm{p}^2\, \mathrm{d}N_i, & X = M_{i,3} \end{cases} \tag{2.10}$$

where $g(t)$ is the condensational growth rate [m/s] as a function of time and $\mathrm{d}N_i$ is an abbreviation of $n_i \, \mathrm{d} \ln D_\mathrm{p}$. An analytical solution for the term is included in the model code.

2.3.3 Coagulation

Coagulation is modelled as intramodal coagulation within the PL distribution and within the LN distribution, and, in the PL+LN model, as intermodal coagulation from the PL distribution to the LN distribution. The coagulation terms derived from the equations of

Whitby and McMurry (1997) are

$$\begin{aligned}\mathrm{coag}_{M_{\mathrm{PL},0}} =& -\frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\beta(D_{\mathrm{p}},D'_{\mathrm{p}})\,\mathrm{d}N_{\mathrm{PL}}\,\mathrm{d}N'_{\mathrm{PL}}\\ &-\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\beta(D_{\mathrm{p}},D'_{\mathrm{p}})\,\mathrm{d}N_{\mathrm{PL}}\,\mathrm{d}N'_{\mathrm{LN}}\end{aligned}\tag{2.11}$$

$$\begin{aligned}\mathrm{coag}_{M_{\mathrm{PL},2}} =& -\frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left[2D_{\mathrm{p}}^{2}-\left(D_{\mathrm{p}}^{3}+D_{\mathrm{p}}^{\prime 3}\right)^{\frac{2}{3}}\right]\beta(D_{\mathrm{p}},D'_{\mathrm{p}})\,\mathrm{d}N_{\mathrm{PL}}\,\mathrm{d}N'_{\mathrm{PL}}\\ &-\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}D_{\mathrm{p}}^{2}\,\beta(D_{\mathrm{p}},D'_{\mathrm{p}})\,\mathrm{d}N_{\mathrm{PL}}\,\mathrm{d}N'_{\mathrm{LN}}\end{aligned}\tag{2.12}$$

$$\mathrm{coag}_{M_{\mathrm{PL},3}} = -\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}D_{\mathrm{p}}^{3}\,\beta(D_{\mathrm{p}},D'_{\mathrm{p}})\,\mathrm{d}N_{\mathrm{PL}}\,\mathrm{d}N'_{\mathrm{LN}}\tag{2.13}$$

$$\mathrm{coag}_{M_{\mathrm{LN},0}} = -\frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\beta(D_{\mathrm{p}},D'_{\mathrm{p}})\,\mathrm{d}N_{\mathrm{LN}}\,\mathrm{d}N'_{\mathrm{LN}}\tag{2.14}$$

$$\begin{aligned}\mathrm{coag}_{M_{\mathrm{LN},2}} =& -\frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left[2D_{\mathrm{p}}^{2}-\left(D_{\mathrm{p}}^{3}+D_{\mathrm{p}}^{\prime 3}\right)^{\frac{2}{3}}\right]\beta(D_{\mathrm{p}},D'_{\mathrm{p}})\,\mathrm{d}N_{\mathrm{LN}}\,\mathrm{d}N'_{\mathrm{LN}}\\ &+\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left[\left(D_{\mathrm{p}}^{3}+D_{\mathrm{p}}^{\prime 3}\right)^{\frac{2}{3}}-D_{\mathrm{p}}^{\prime 2}\right]\beta(D_{\mathrm{p}},D'_{\mathrm{p}})\,\mathrm{d}N_{\mathrm{PL}}\,\mathrm{d}N'_{\mathrm{LN}}\end{aligned}\tag{2.15}$$

$$\mathrm{coag}_{M_{\mathrm{LN},3}} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}D_{\mathrm{p}}^{3},\beta(D_{\mathrm{p}},D'_{\mathrm{p}})\,\mathrm{d}N_{\mathrm{PL}}\,\mathrm{d}N'_{\mathrm{LN}},\tag{2.16}$$

where $\beta(D_{\mathrm{p}},D'_{\mathrm{p}})$ is the coagulation coefficient of particles with the diameters of D_{p} and D'_{p} calculated with the equation

$$\beta(D_{\mathrm{p}},D'_{\mathrm{p}}) = 2\pi(D_{\mathrm{p}}+D'_{\mathrm{p}})(\mathcal{D}_{\mathrm{p}}+\mathcal{D}'_{\mathrm{p}})f(\mathrm{Kn}_{\mathrm{coag}}),\tag{2.17}$$

where $f(\mathrm{Kn}_{\mathrm{coag}})$ is the transition regime function of Dahneke (1983)

$$f(\mathrm{Kn}_{\mathrm{coag}}) = \frac{1+\mathrm{Kn}_{\mathrm{coag}}}{1+2\mathrm{Kn}_{\mathrm{coag}}+2\mathrm{Kn}_{\mathrm{coag}}^{2}},\tag{2.18}$$

where $\mathrm{Kn}_{\mathrm{coag}}$ is the Knudsen number for coagulation

$$\mathrm{Kn}_{\mathrm{coag}} = \frac{4(\mathcal{D}_{\mathrm{p}}+\mathcal{D}'_{\mathrm{p}})}{(D_{\mathrm{p}}+D'_{\mathrm{p}})\sqrt{\bar{c}^{2}+\bar{c}^{\prime 2}}},\tag{2.19}$$

where $\bar{c}$ and $\bar{c}'$ are the mean thermal velocities of particles with the diameters of D_{p} and D'_{p}. Diffusion coefficients $\mathcal{D}_{\mathrm{p}}$ and $\mathcal{D}'_{\mathrm{p}}$ are calculated according to Hinds (1999) with the slip correction coefficient.

The integrals in Eqs. (2.11) – (2.16) cannot be solved analytically in the transition regime because Eq. (2.18) cannot be presented in a polynomial form. Therefore, the integrals are calculated numerically or by using quadrature techniques. By default, in the case of the PL distribution, the integrals are solved numerically using 20 size sections, when $D_2/D_1 > 3$, and using the Gauss-Olin quadrature described in Olin et al. (2016), otherwise. In the case of the LN distribution, the Gauss-Hermite quadrature is used in calculation of the integrals.

2.3.4 Coagulational losses

Particles in the background distribution excluded from the modelled distribution are assumed to be significantly larger than the other particles. Therefore, the particle diameters of the background distribution can be approximated with a single diameter value, e.g., $\mathrm{CMD_{bg}}$ (count median diameter). According to Kerminen and Kulmala (2002), the coagulation coefficient will then become

$$\beta(D_\mathrm{p}, \mathrm{CMD_{bg}}) \approx \beta(D_1, \mathrm{CMD_{bg}}) \left(\frac{D_\mathrm{p}}{D_1}\right)^{l_\mathrm{bg}}, \tag{2.20}$$

where l_bg is the exponent depending on $\mathrm{CMD_{bg}}$. The value of l_bg ranges between -2 and -1 (Lehtinen et al., 2007), the default value being -1.6. The coagulational loss term for zeroth moment is

$$\mathrm{loss}^\mathrm{coag}_{N_i} = -N_\mathrm{bg}\, \beta(D_1, \mathrm{CMD_{bg}}) D_1^{-l_\mathrm{bg}} \int_{-\infty}^{\infty} D_\mathrm{p}^{l_\mathrm{bg}}\, \mathrm{d}N_i, \tag{2.21}$$

where N_bg is the number concentration of the background distribution (Olin et al., 2016). An analytical solution is included in the model code.

2.3.5 Depositional losses

The depositional losses are modelled with

$$\mathrm{loss}^\mathrm{dep}_{N_i} = -k_\mathrm{dep} \int_{-\infty}^{\infty} D_\mathrm{p}^{-1} \mathrm{d}N_i \tag{2.22}$$

where k_dep is the deposition coefficient [m/s] (Olin et al., 2016). An analytical solution is included in the model code.

2.3.6 Coagulational transfer

Particles in the PL mode can be transferred to a LN mode using

$$\mathrm{transfer}_{M_{\mathrm{PL},0}} = -\,\mathrm{transfer}_{M_{\mathrm{LN},0}} = -\frac{1}{2}\int_{-\infty}^{\infty}\int_{\ln D_\mathrm{coag}}^{\infty} \beta(D_\mathrm{p}, D'_\mathrm{p})\, \mathrm{d}N_\mathrm{PL}\, \mathrm{d}N'_\mathrm{PL} \tag{2.23}$$

$$\mathrm{transfer}_{M_{\mathrm{PL},2}} = -\,\mathrm{transfer}_{M_{\mathrm{LN},2}} = -\frac{1}{2}\int_{-\infty}^{\infty}\int_{\ln D_\mathrm{coag}}^{\infty} \left(D_\mathrm{p}^3 + D'^3_\mathrm{p}\right)^{\frac{2}{3}} \beta(D_\mathrm{p}, D'_\mathrm{p})\, \mathrm{d}N_\mathrm{PL}\, \mathrm{d}N'_\mathrm{PL} \tag{2.24}$$

$$\mathrm{transfer}_{M_{\mathrm{PL},3}} = -\,\mathrm{transfer}_{M_{\mathrm{LN},3}} = -\frac{1}{2}\int_{-\infty}^{\infty}\int_{\ln D_\mathrm{coag}}^{\infty} \left(D_\mathrm{p}^3 + D'^3_\mathrm{p}\right) \beta(D_\mathrm{p}, D'_\mathrm{p})\, \mathrm{d}N_\mathrm{PL}\, \mathrm{d}N'_\mathrm{PL}, \tag{2.25}$$

where D_{coag} is the cut diameter

$$D_{\mathrm{coag}} = \left(D_2^3 - D_{\mathrm{p}}'^3\right)^{1/3} \tag{2.26}$$

which is the smallest particle that forms a particle larger than D_2 after coagulating with a particle having a diameter of D_{p}', assuming full coalescence (Olin et al., 2016).

2.3.7 Condensational transfer

Some of the particles are transferred from the PL mode to the LN mode using the condensational transfer. It is modelled with

$$\mathrm{transfer}_X^{\mathrm{cond}} = \gamma \frac{g(t)}{D_2} n_{\mathrm{PL}}(D_{\mathrm{p}} = D_2) \cdot \begin{cases} -1, & X = M_{\mathrm{PL},0} \\ -D_2^2, & X = M_{\mathrm{PL},2} \\ -D_2^3, & X = M_{\mathrm{PL},3} \\ +1, & X = M_{\mathrm{LN},0} \\ +D_2^2, & X = M_{\mathrm{LN},2} \\ +D_2^3, & X = M_{\mathrm{LN},3} \end{cases}, \tag{2.27}$$

where γ is the condensational transfer factor having the value of 0.5 by default (Olin et al., 2016).

2.4 General dynamic equation in sectional method

Aerosol dynamics is modelled with the following equation

$$\frac{\mathrm{d}N_j}{\mathrm{d}t} = \mathrm{npf}_j + \mathrm{cond}_j + \mathrm{coag}_j + \mathrm{loss}_j^{\mathrm{coag}} + \mathrm{loss}_j^{\mathrm{dep}}, \tag{2.28}$$

where j denotes a size section.

2.4.1 New particle formation

The new particle formation (NPF) term in Eq. 2.28 is

$$\mathrm{npf}_j = \begin{cases} J(t), & j = 1 \\ 0, & j > 1 \end{cases}. \tag{2.29}$$

2.4.2 Condensation

The condensation term in Eq. 2.28 is

$$\mathrm{cond}_j = \begin{cases} -N_j \frac{g(t)}{\Delta D_j}, & j = 1 \\ -N_j \frac{g(t)}{\Delta D_j} + N_{j-1} \frac{g(t)}{\Delta D_{j-1}}, & j > 1 \end{cases} \tag{2.30}$$

where ΔD_j is the diameter width of the section j.

2.4.3 Coagulation

The coagulation term is

$$\mathrm{coag}_j = -N_j \sum_{j'=1}^{\infty} \beta(D_j, D_{j'}) N_{j'} + \frac{1}{2} \sum_{j'=1}^{j-1} \beta(D_{j'}, D_{j-j'}) N_{j'} N_{j-j'}. \tag{2.31}$$

2.4.4 Coagulational losses

The coagulational loss term is

$$\mathrm{loss}_j^{\mathrm{coag}} = -N_{\mathrm{bg}} \beta(D_1, \mathrm{CMD}_{\mathrm{bg}}) D_1^{-l_{\mathrm{bg}}} D_j^{l_{\mathrm{bg}}} N_j. \tag{2.32}$$

2.4.5 Depositional losses

The depositional loss term is

$$\mathrm{loss}_j^{\mathrm{dep}} = -\frac{k_{\mathrm{dep}}}{D_j} N_j. \tag{2.33}$$

3. USING THE SIMPLE L-TUTAM

The L-TUTAM model is used with Matlab. The model is developed to operate in Matlab R2015b, but may also work with older releases.

3.1 Launching the model

The model uses two structs, `p` and `out`, which denote input parameter setup and the output of the simulation, respectively. If `p` does not exist in the workspace, it needs to be created by typing the command `initialize`, which loads the default parameter setup, asks your own setup file, and creates `p` struct into the workspace. At this point, the code also asks whether you want to use the simple or the coupled model.

You can make your own setup file in `.m` format that contains at least the input variables that do not have the default values. You can use `defaultSetupFile.m` file as a model in making your own setup file. The parameters and their default values are described next.

p.coupled Is simple (0) or coupled (1) model used? The value should not be changed here. If you want to change the submodel, run `initialize` again.

p.model How the distribution is modelled: power law (`'PL'`), log-normal (`'LN'`, default), combination (`'PLLN'`), fixed-sectional with n size sections (`'FSn'`). The LN model is the fastest model and it can be used in the most cases. The PL+LN model provides more accuracy especially in the cases of simultaneous new particle formation and growth. The most accurate model is the FS model, but the computational cost is significantly higher.

p.PLEquations How the system of equations in the PL model is solved: interpolation table (1), Levenberg-Marquardt iteration algorithm (2, default).

p.JMatrix New particle formation rate, $J(t)$ [1/cm^3 s], in a matrix form. The top row denotes the times [s] and the bottom row the rates at those times. The default matrix

$$\begin{bmatrix} 0 & 3600 \\ 0 & 1 \end{bmatrix} \tag{3.1}$$

denotes the following function

$$J(t) = \begin{cases} 0\,\mathrm{cm^{-3}\,s^{-1}}, & t \le 0\,\mathrm{s} \\ 1\,\mathrm{cm^{-3}\,s^{-1}}, & t \le 3600\,\mathrm{s} \end{cases} . \tag{3.2}$$

Make sure that the highest time in the matrix is not less than the highest simulation time. The number of columns in the matrix is not limited, and it can also be one. E.g., the matrix

$$\begin{bmatrix} \mathrm{inf} \\ 1 \end{bmatrix} \tag{3.3}$$

denotes that J has a constant value of $1\,\mathrm{cm^{-3}\,s^{-1}}$.

p.dCluster The diameter of a newly formed particle [m]. It also describes the smallest diameter that is modelled in the FS model. The default value is 1 nm.

p.highestDiameter The highest diameter in the FS model. The default value is 100 nm.

p.GRMatrix Condensational growth rate, $g(t)$ [m/s], in a matrix form. The default matrix

$$\begin{bmatrix} 0 & 3600 \\ 0 & \text{3e-12} \end{bmatrix} \tag{3.4}$$

denotes the following function

$$g(t) = \begin{cases} 0\,\mathrm{m\,s^{-1}}, & t \le 0\,\mathrm{s} \\ 3 \cdot 10^{-12}\,\mathrm{m\,s^{-1}}, & t \le 3600\,\mathrm{s} \end{cases} . \tag{3.5}$$

p.condensationalTransfer Is the condensational transfer on with the PL+LN model? Is Eq. 2.27 calculated? 1 (on, default) or 0 (off). In the most cases, it should be on.

p.condensationalTransferFactor The condensational transfer factor, γ, in Eq. 2.27 with the PL+LN model. The range is 0 ... 1 and the default value is 0.5. You can add log-normal features to the output distribution by increasing the value towards unity. More guidelines to choose the value can be found in Olin et al. (2016).

p.coag Is coagulation on? 1 (on, default) or 0 (off).

p.coagulationalTransfer Is the coagulational transfer on with the PL+LN model? Are Eq. 2.23 – Eq. 2.25 calculated? 1 (on, default) or 0 (off). Either the condensational transfer or the coagulational transfer must be on for the LN distribution to form with the PL+LN model. If γ is high, the coagulational transfer can be neglected to save some computing time.

p.binsInCoagulation Size bins in the numeric integration of coagulation terms with the modal method. The default values is 20. Integrals in calculating coagulation terms are double integral; thus, increasing the number of size bins increases the associated computing time squarely.

p.numericCoagulation Are integrals in the coagulation terms always calculated numerically with the modal method? 1 (on) or 0 (off, default). If you experience numerical problems, you can try to set this on.

p.T Temperature [K] of the carrier gas. The default value is 300 K. It can also be a time dependent function, as in the case of `p.JMatrix`. However, coagulation equations use only the mean temperature.

p.visc Dynamic viscosity [Pa s] of the carrier gas. The default value is $1.85 \cdot 10^{-5}$ Pa s which is calculated through `viscosity` function. The size is the same as the size of p.T.

p.rho Particle bulk density [kg/m^3]. The default value is 1000 kg/m^3.

p.sizeDependentGR Is a size-dependent function, $g(t, D_\mathrm{p})$, used for the condensational growth? It is not yet supported in this version; thus, the value must be 0.

p.coagSink Are the coagulational losses to the background distribution included? Is Eq. 2.21 or Eq. 2.32 calculated? 1 (on, default) or 0 (off).

p.coagSinkCMD CMD [m] of the background distribution causing the coagulational losses. The default value is 100 nm.

p.coagSinkExponent The exponent for the coagulational losses, l_bg. The range is -2 ... -1 and the default value is -1.6 that corresponds to the CMD of 100 nm. Refer, e.g., Lehtinen et al. (2007) to choose the appropriate value.

p.coagSinkN The number concentration [cm^{-3}] of the background distribution causing the coagulational losses. The default value is 1000 cm^{-3}.

p.losses Are the depositional losses included? Is Eq. 2.21 or Eq. 2.33 calculated? 1 (on, default) or 0 (off).

p.lossesCoeff The deposition coefficient, k_dep [m/s]. The default value is $5 \cdot 10^{-13}$ m/s, which corresponds to the deposition rate of small particles ($D_\mathrm{p} < 100$ nm) in a chamber with the dimensions of 3 m × 2 m × 2 m.

p.lossesExponent The exponent for the depositional losses. The default value is -1 that works well with particles smaller than 100 nm.

p.timeVec Time [s] vector to be simulated with the model. The default value is 0:3600 which denotes that the time domain to be simulated is from the time of 0 s to the time of 3600 s and that the simulation result is output with 1-second time resolution.

p.initialMomentVec The vector of the moments or the concentrations of the size sections, initially. The vector must be in the size of $1 \times n$ where n is 6 with the modal method, and the number of size sections with the sectional method. The meanings of the cells in the vector are, with the modal method, $[M_{\mathrm{PL},0}, M_{\mathrm{PL},2}, M_{\mathrm{PL},3}, M_{\mathrm{LN},0}, M_{\mathrm{LN},2}, M_{\mathrm{LN},3}]$. The default value is `zeros(1,6)` that denotes there are initially no particles. You can also set it to a scalar value of 0, which means there are no particles initially.

p.solverName The name of the ODE-solver. The default value is `'ode45'`. Refer Matlab documentation to choose the solver.

p.relativeTolerance The relative tolerance for the ODE solver. The default value is 10^{-3}.

p.plotDistrDuringSim Are distributions plotted during the simulation? 1 (on, default) or 0 (off). Plotting slows down the simulation.

p.plotWaitbarDuringSim Is waitbar shown during the simulation? 1 (on, default) or 0 (off). Showing the waitbar slows down the simulation.

p.plotOutputAfterSim Is the model output plotted after the simulation? 1 (on, default) or 0 (off).

3.2 Running a simulation

The simulation can be run by typing the command `simulate`. After the simulation is complete, `out` struct is created to the workspace. It contains the time series of the output variables, depending on the time vector, `p.timeVec`. The contents of `out` struct are described next.

out.t Time [s] vector. Same as `p.timeVec` but transposed.

out.Y Time series of the moments (modal method) or the number concentrations of the size sections (sectional method). The meanings of the cells are the same as with `p.initialMomentVec`.

out.p The input parameter set used in the simulation. Some additional variables for the internal usage of the model are also included in that.

out.N_LN The number concentrations [cm^{-3}] of the log-normal distribution with the modal method.

out.CMD Count median diameters [m] of the log-normal distribution with the modal method.

out.sigma Geometric standard deviations σ [m] of the log-normal distribution with the modal method.

out.N_PL The number concentrations [cm^{-3}] of the power law distribution with the modal method.

out.alpha The slope parameters α of the power law distribution with the modal method.

out.D2 The largest particle diameters D_2 [m] of the power law distribution with the modal method.

out.N The total number concentrations N [cm^{-3}].

out.M_2 The total 2$^{\mathrm{nd}}$ moments M_2 [m^2 cm^{-3}].

out.M_3 The total 3$^{\mathrm{rd}}$ moments M_3 [m^3 cm^{-3}].

out.GMD Geometric mean diameters [m] of the total distribution.

out.GSD Geometric standard deviations of the total distribution.

3.3 Running another simulation

Once `p` struct exist, a simulation can be run with different parameter set (1) by changing the variables directly in the Matlab's workspace, (2) by changing the variables through the Matlab's command line, or (3) by loading another setup file by typing the command `initialize`. After that, type the command `simulate`.

If you want to run the model in a batch process, make a script that alters the parameter set struct `p`, runs a simulation with the command `simulate`, and stores the output from `out` struct to another variable.

3.4 Plotting results

If `p.plotDistrDuringSim` is set to 1, the distribution at the end of the simulation is seen when the simulation is finished. If `p.plotOutputAfterSim` is set to 1, the time series of the outputs are plotted when the simulation is finished. You can plot the time series after the simulation by typing the command `plotOutput(out)`. The output plotted contains the time series of number concentration and 2$^{\mathrm{nd}}$ and 3$^{\mathrm{rd}}$ moments. In the case of the modal method, the parameters of the distributions are also plotted.

4. USING THE COUPLED L-TUTAM

The L-TUTAM model is used with Matlab. The model is developed to operate in Matlab R2015b, but may also work with older releases.

4.1 Launching the model

The model uses two structs, `p` and `out`, which denote input parameter setup and the output of the simulation, respectively. If `p` does not exist in the workspace, it needs to be created by typing the command `initialize`, which loads the default parameter setup, asks your own setup file, and creates `p` struct into the workspace. At this point, the code also asks whether you want to use the simple or the coupled model.

You can make your own setup file in `.m` format that contains at least the input variables that do not have the default values. You can use `defaultSetupFileCoupled.m` file as a model in making your own setup file. The parameters and their default values are described next.

p.coupled Is simple (0) or coupled (1) model used? The value should not be changed here. If you want to change the submodel, run `initialize` again.

p.model How the distribution is modelled: power law (`'PL'`), log-normal (`'LN'`, default), combination (`'PLLN'`). The LN model is the fastest model and it can be used in the most cases. The PL+LN model provides more accuracy especially in the cases of simultaneous new particle formation and growth.

p.PLEquations How the system of equations in the PL model is solved: interpolation table (1), Levenberg-Marquardt iteration algorithm (2, default).

p.dCluster The smallest diameter of the PL distribution [m]. The default value is 1 nm.

p.condensationalTransfer Is the condensational transfer on with the PL+LN model? Is Eq. 2.27 calculated? 1 (on, default) or 0 (off). In the most cases, it should be on.

p.condensationalTransferFactor The condensational transfer factor, γ, in Eq. 2.27 with the PL+LN model. The range is 0 ... 1 and the default value is 0.5. You can add log-normal features to the output distribution by increasing the value towards unity. More guidelines to choose the value can be found in Olin et al. (2016).

p.coag Is coagulation on? 1 (on, default) or 0 (off).

p.coagulationalTransfer Is the coagulational transfer on with the PL+LN model? Are Eq. 2.23 – Eq. 2.25 calculated? 1 (on, default) or 0 (off). Either the condensational transfer or the coagulational transfer must be on for the LN distribution to form with the PL+LN model. If γ is high, the coagulational transfer can be neglected to save some computing time.

p.binsInCoagulation Size bins in the numeric integration of coagulation terms with the modal method. The default values is 20. Integrals in calculating coagulation terms are double integral; thus, increasing the number of size bins increases the associated computing time squarely.

p.numericCoagulation Are integrals in the coagulation terms always calculated numerically with the modal method? 1 (on) or 0 (off, default). If you experience numerical problems, you can try to set this on.

p.p Absolute pressure [Pa]. The default value is 101325 Pa. It can also be a time dependent function as in the case of `p.JMatrix`.

p.T Temperature [K] of the carrier gas. The default value is 300 K. It can also be a time dependent function as in the case of `p.JMatrix`. However, coagulation equations use only the mean temperature.

p.rhoFunc Function to calculate particle density [kg/m^3]. You can make your own function using the default function `rhoSulfuricAcidWater.m` as a template.

p.visc Dynamic viscosity [Pa s] of the carrier gas. The default value is $1.85 \cdot 10^{-5}$ Pa s which is calculated through `viscosity` function. The size is the same as the size of p.T.

p.timeVec Time [s] vector to be simulated with the model. The default value is 0:3600 which denotes that the time domain to be simulated is from the time of 0 s to the time of 3600 s and that the simulation result is output with 1-second time resolution.

p.nVapor Number of vapors. The default value is 2.

p.initialMomentVec The vector of the moments, initially. The vector must be in the size of $1 \times (2 \cdot \texttt{p.nVapor} + 4)$. The meanings of the cells in the vector are $[M_{\mathrm{PL},0}, M_{\mathrm{PL},2}, M_{\mathrm{PL},3,m}, M_{\mathrm{LN},0}, M_{\mathrm{LN},2}, M_{\mathrm{LN},3,m}]$ where the index m runs over all the vapors. The default value is `zeros(1,8)` that denotes there are initially no particles. You can also set it to a scalar value of 0, which means there are no particles initially.

p.initialVaporVec The vector of the vapor concentrations [kg/cm^3], initially. The vector must be in the size of $1 \times \texttt{p.nVapor}$. You can also set it to a scalar value of 0, which means there is no vapor initially.

p.solverName The name of the ODE-solver. The default value is `'ode45'`. Refer Matlab documentation to choose the solver.

p.relativeTolerance The relative tolerance for the ODE solver. The default value is 10^{-3}.

p.plotDistrDuringSim Are distributions plotted during the simulation? 1 (on, default) or 0 (off). Plotting slows down the simulation.

p.plotWaitbarDuringSim Is waitbar shown during the simulation? 1 (on, default) or 0 (off). Showing the waitbar slows down the simulation.

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The simulation can be run by typing the command `simulate`. After the simulation is complete, `out` struct is created to the workspace. It contains the time series of the output variables, depending on the time vector, `p.timeVec`. The contents of `out` struct are described next.

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out.N_PL The number concentrations [cm^{-3}] of the power law distribution with the modal method.

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out.D2 The largest particle diameters D_2 [m] of the power law distribution with the modal method.

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