# Chamber model how-to

## Creating and initializing a chamber object

The chamber model is based on object-oriented programming. That is, every simulation is an object that has functions (methods) and variables. To run a simulation, one has to first create a chamber object by writing

simulation\_1 = chamber;

where “simulation\_1” is the name of the object, and “chamber” tells Matlab that this object is a chamber model object.

Now “simulation\_1” has all the functions needed to actually run the simulation. But before that, one must define the initial conditions. A simple case would be a log-normal particle distribution that develops by condensation, coagulation and dilution during the simulation.

All the initial parameters of a chamber object are found in structure chamber.initials, where “chamber” is the name of the chamber object, so in this case the initial values are seen by typing

simulation\_1.initials

in matlab, without the semicolon at the end. These values can be modified using function chamb.initialize(). All the parameter names and their descriptions are found in section “Initial parameters”.

Let us first set the initial log-normal distribution so that its mean diameter is 15 nm and geometric standard deviation is 1.6. The total number of particles is set to 1e5. This is done by writing

simulation\_1.initialize(‘mu’, 15e-9, ‘sigma’, 1.6, ‘N’, 1e5);

The name of variable is written first and after that its desired value. In addition, let us define the source and initial concentration of condensing vapor. If we want to have 1e7 molecules/cm^3 of vapor in the beginning, we shall write

simulation\_1.initialize(‘Cvap0’, 1e7);

To define a constant source of condensing vapor, say 1e5 molecules/cm^3, we write

simulation\_1.initialize(‘gas\_source’, 1e5);

The last setting we are going to do is the time vector. If we want to run the simulation 10 hours (=10\*3600 seconds) and we want the results for every 60 seconds, the time vector is set in the following way:

simulation\_1.initialize(‘tvect’, 0:60:10\*3600);

These settings are enough for this simple example, because coagulation and dilution are on as default and we don’t need to switch them on separately. The initialization parameter by parameter, but also all at once, by writing

simulation\_1.initialize(‘mu’, 15e-9,…  
 ‘sigma’, 1.6,…  
 ‘N’, 1e5,…  
 ‘Cvap0’, 1e7,…  
 ‘gas\_source’, 1e5,…

‘tvect’, 0:60:10\*3600);

To start the simulation, type

simulation\_1.run;

After this command, the time evolution of simulation is shown in Matlab command window. When the simulation is ready, some results can be studied by typing

simulation\_1.plot;

This command plots the particle size distribution, vapor concentration and the total volume and number concentration of particles as a function of time. All data is stored in *simulation\_1.output\_data*, whereas the initial values are still found in *simulation\_1.initials*.

## Advanced settings

The chamber model is based on sectional simulation, where the size distribution is divided in a number of sections into which the particles are distributed. Coagulation and condensation/evaporation affect the particle size distribution, and in this model there are two alternative methods how these mechanisms are implemented. It is crucial to understand the difference between these methods, so that one can decide which of the methods one should use in different simulations.

The first method is called “moving sectional model”, where condensation/evaporation moves the corresponding diameters of sections and coagulation re-distributes particles between the sections. This method is the fastest and often the best way of the two methods to simulate behavior of particle distribution. This method, however, has its limits: particle sources cannot be used in moving sectional model, so for example modeling experiments where nucleation occurs is impossible. For simulations with nucleation, one has to use “fixed sectional model” which is described below.

In the fixed sectional model, the size distribution is divided in sections just as in moving sectional model. However, the corresponding diameters of sections do not move by condensation or evaporation, but stay fixed throughout the simulation. This allows the implementation of nucleation, because the section into which particles are nucleated does not change its corresponding diameter. This is a simple description of the model. In reality, the corresponding diameters of sections do move, but they have certain limits. The diameter grows by condensation, but if it reaches its upper limit, the particles from that section are moved to the next one and the diameter is reset to its original value. So the sections are not totally fixed, but they are fixed between their limits, and that is enough for implementation of particle sources (or nucleation). In addition, this is much more accurate method than totally fixed sections. The fixed sectional model is not as fast as moving sectional model, and in addition, the size distribution plots created by the fixed sectional model do not look as smooth as the ones created by the moving sectional model.

The choice between the two different methods is done by a setting named *fixed\_sections*. If *fixed\_sections* is set to zero (by writing *simulation\_1.initialize(‘fixed\_sections’, 0);*), the moving sectional model is used. This is the default setting. If *fixed\_sections* is something else than zero, the fixed sectional model will be used.

## Vector parameters

Some of parameters in the chamber model can be defined as time-dependent. These parameters are dilution coefficient, vapor source and particle source. The time-dependent values are defined as matrices, where the first column is a time vector and the actual values are in the second column. Thus, the value in the second column corresponds to the time that is in the first column in the same row. The values between two time points are interpolated. An example of time-dependent vapor source vector is below. In that example, the vapor source is defined with different values till 240 seconds. Beginning from 300 seconds to the end (10\*3600 seconds), the vapor source will be zero. It is important that both the first value of time vector (0 seconds in this case) and the last value (10\*3600 seconds in this case) are defined in the vector so that it is possible to interpolate the values for all time points.

|  |  |
| --- | --- |
| 0 | 1e3 |
| 60 | 1e4 |
| 120 | 1.5e4 |
| 180 | 2e4 |
| 240 | 2.5e4 |
| 300 | 0 |
| 10\*3600 | 0 |

The particle source matrix is an exception among other matrices because it has to be defined as 3-column matrix instead of 2-column matrix like the other time-dependent variables. This is because in addition to nucleation rate, also the size of nucleating particles must be defined. The size is defined in the third column and first row of the matrix, so the time-dependent particle source is of the form:

|  |  |  |
| --- | --- | --- |
| 0 | 1.5 | 3e-9 |
| 60 | 1.5 | NaN |
| 120 | 1.5 | NaN |
| 180 | 1.5 | NaN |
| 240 | 1.5 | NaN |
| 300 | 0 | NaN |
| 10\*3600 | 0 | NaN |

Particle source above will create 3 nm particles with source rate of 1.5 particles/cm^3s in the beginning and no particles at all after first 300 seconds. If one wants to define nucleation rates for different particle sizes, the particle source matrix must be a 3d-matrix. For example, if there is one particle source for 3nm particles and another for 6 nm particles, the source should be defined in the following way:

source1=

|  |  |  |
| --- | --- | --- |
| 0 | 1.5 | 3e-9 |
| 60 | 1.5 | NaN |
| 120 | 1.5 | NaN |
| 180 | 1.5 | NaN |
| 240 | 1.5 | NaN |
| 300 | 0 | NaN |
| 10\*3600 | 0 | NaN |

source2=

|  |  |  |
| --- | --- | --- |
| 0 | 0 | 6e-9 |
| 60 | 0 | NaN |
| 120 | 0 | NaN |
| 180 | 0 | NaN |
| 240 | 0 | NaN |
| 300 | 0.3 | NaN |
| 10\*3600 | 0.3 | NaN |

*particle\_source(:,:,1) = source1;  
particle\_source(:,:,2) = source2;  
simulation\_1.initialize(‘part\_source’, particle\_source);*

The initial particle distribution can be also defined as a vector. This is necessary when the initial distribution consists of two or more log-normal distributions. For example, if the initial distribution is a sum of two distributions, so that the first distribution has mu=10e-9, sigma=1.3 and N=1000 and the second mu=100e-9, sigma=1.4 and N=10 000, it can be defined in the following way:

simulation\_1.initialize(‘mu’, [10e-9, 100e-9], ‘sigma’, [1.3, 1.4], ‘N’, [1000, 10000]);

## Automatizing simulations

One has often a need to run a number of simulations with different initial values. For that use, separate functions “*chamber\_runfile*” and *“chamber\_runfile2”* were implemented. Function *chamber\_runfile* reads a file that contains different initial settings and runs all the simulations in turn. In addition, this function saves the results of every simulation after it has been run, so that no data is lost even if one or more simulations were interrupted.

The settings file must be like the following

#

fixed\_sections = 1;

sedi\_on = 0;

coag\_on = 1;

Dp\_min = -9;

Dp\_max = -6;

tvect = 0:60:32400;

sigma = [1.25, 1.3];

N = [1e3 1e2];

mu=[50e-9, 140e-9];

dilu\_on = 0;

sections = 30;

output\_sections = 10\*sections;

Cvap\_const = 1;

Cvap0 = 2e7;

gas\_source = 0;

#

fixed\_sections = 1;

sedi\_on = 0;

coag\_on = 1;

Dp\_min = -9;

Dp\_max = -6;

tvect = 0:60:32400;

sigma = [1.25, 1.3];

N = [1e3 1e2];

mu=[50e-9, 140e-9];

dilu\_on = 1;

sections = 30;

output\_sections = 10\*sections;

Cvap\_const = 1;

Cvap0 = 2e7;

gas\_source = 0;

#

The script above defines the initial values for two simulations. The simulations are separated by “#” character, and the same character begins and ends the file. The only difference between these two simulations is that in the first one, dilution is switched off, whereas in the second one it is on.

The script is run by typing

[chamb, elapsed]=chamber\_runfile(filename);

This reads first the file and checks that all definitions are correct. After that, the program runs the simulations and saves the results of each simulation to file ‘temp\_timestamp.mat’, where timestamp is the current time (function *datestr(now,30)*). When all the simulations are successfully run, the program saves them all to file ‘run\_timestamp.mat’. After that, the temporary files are deleted. If the program is for some reason interrupted before that, the temp files are not deleted. The run\_timestamp.mat file contains all the results in an array named ‘chamb’. If there were two simulations defined in the definition script, the length of chamb is two: results of the first simulation is in *chamb(1).output\_data* and the second in *chamb(2).output\_data*. In addition, the *run\_timestamp.mat* file contains an array named *elapsed*; *elapsed(1)* tells the time (in seconds) elapsed running the first simulation run and *elapsed(2)* the same for the second simulation run.

Things to bear in mind when using chamber\_runfile:

* The settings file must start with “#” and end with “#”. In addition, there must be “#” between two simulation definitions.
* You can address to variables defined in the settings file. For example one can first define tvect, and then the gas source vector so that gas\_source=[tvect’, 10.\*tvect’], which means that the vapor source is directly proportional to time.
* You can define helper variables, that is, variables whose name does not correspond to any name in chamb.initials. However, the program will give a warning if this is done.
* You can use functions in the settings file. For example functions *ones()* and *zeros()* are useful when defining particle or vapour sources.

Another useful automatizing function is *chamber\_runfile2*. This function is especially handy when one wants to keep most of parameters constant and vary only some of them. In that case, the parameters that are varied are defined as vectors. An example of this is below

#

Dp\_min = -9;

Dp\_max = -6;

tvect = 0:60:32400;

sigma = [1.6];

mu=[50e-9];

sections = 25;

output\_sections = 10\*sections;

Cvap\_const = 1;

dilu\_on = 1;

Cvap0 = [1e6; 5e7];

N = [1e4; 1e5];

#

In the script above, the first ten definitions are constants, whereas the two last can have two values: *Cvap0* can be either 1e6 or 5e7, and *N* 1e4 or 1e5. The different values must be separated by semicolon. When this script is run by *chamber\_runfile2*, it automatically simulates all the possible combinations of *Cvap0* and *N* (number of combinations is 2\*2 = 4 in this case).

The distribution parameters can also have several different values, even when the distribution consists of two or more log-normal distributions. Consider a case where user wants to have a distribution that consists of two log-normal distributions, where mu\_1 = 10e-9, mu\_2 = 150e-9 and sigma\_1 = 1.3 and sigma\_2 = 1.6. User wants to test three different values for the total number concentration in the distribution. This would be done by writing a following script:

#

mu = [10e-9, 150e-9];

sigma = [1.3, 1.6];

N = [1000, 1000; 1000, 10000; 10000, 1000];

#

As in the first example, also here the different values for N are separated with semicolon.

For time-dependent variables, the definition of several values is different. As the time dependent variables are matrices, it is not possible to separate values by writing them in separate rows. Instead, the matrices must be defined as 3d-matrices. For example, defining two different vapor source matrices is done by writing:

#

tvect = 0:60:10800;

gas\_source(:,:,1) = [tvect’, 10.\*tvect’];

gas\_source(:,:,2) = [tvect’, 100.\*tvect’];

#

The program will now run two simulations: in the first one, the vapor source is 10\*t, and in the second one it is 100\*t. Particle source and dilution coefficient must be defined in the same way. Even when the dilution coefficient is constant throughout the simulation, it has to be defined

#

dilu\_coeff(:,:,1) = 1e-4;

dilu\_coeff(:,:,2) = 5e-4;

#

A known limit when using *chamber\_runfile2* is that it is not possible to define particle sources for different diameters.

## Initial parameters

|  |  |  |
| --- | --- | --- |
| Parameter | Description | Default value |
| SWITCHES |  |  |
| dilu\_on | Defines whether the dilution is on or not. If dilu\_on = 0, the aerosol will not dilute. If dilu\_on = 1, the aerosol will dilute with rate defined by parameter dilu\_coeff. | 1 |
| coag\_on | Defines whether the coagulation is on or not. If coag\_on = 0, the particles won't coagulate. If coag\_on = 1, the coagulation is set on. | 1 |
| sedi\_on | Defines whether the sedimentation is on or not. If sedi\_on = 0, sedimentation is turned off. If sedi\_on = 1, sedimentation will occur. Only usable for sedimentation in SAPPHIR chamber! | 0 |
| gas\_source\_is\_vect | Defines whether the parameter gas\_source is a vector or scalar. This cannot be set by user. Instead, the program checks if gas\_source is an array or not and sets the value to 1 or 0 respectively. |  |
| dilu\_vect\_on | Defines whether the parameter dilu\_coeff is an array or scalar. This cannot be set by user. Instead, the program checks if dilu\_coeff is an array or scalar and sets the value to 1 or 0 respectively. |  |
| part\_source\_is\_vect | Defines whether the parameter part\_source is a time-dependent vector or a constant. This cannot be set by user. Instead, the program checks if part\_source is an array or scalar and sets the value to 1 or 0 respectively. |  |
| coag\_mode | Defines whether the particles coagulate 'normally' or agglomerate. Value should be either 'coag' for normal coagulation or 'aggl' for agglomeration. Agglomeration works only for particles in the free-molecule region. Condensation and deposition might not work correctly for agglomerates. |  |
| coag\_num | Numerical representative of coag\_mode. If coag\_mode == 'coag' => coag\_num = 1. If coag\_mode == 'aggl' => coag\_num = 0. This cannot be set directly by user, but the program sets it based on the value of coag\_mode. |  |
| fixed\_sections | Defines whether the model will use fixed or moving sections. If fixed\_sections == 0, moving sections will be used. Otherwise the sections will be fixed.  When the model uses moving sections, the diameter defining the section grows or shrinks by condensation or evaporation.  When using fixed sections, the diameters defining sections are constant. If particles grow by condensation so that they reach the limit diameter, they will be moved to the next section. The limit diameter is logarithmically halfway between adjacent sections. |  |
| Cvap\_const | Defines whether the vapor concentration is constant or not.  If Cvap\_const == 1, the vapor concentration stays at value Cvap0 during the whole simulation time, so that the value gas\_source has no effect on vapor concentration.  If Cvap\_const ~= 1, the vapour concentration is not kept constant, but its value depends on Cvap0 and gas\_source. |  |
| vap\_wallsink\_on | Defines whether the vapor condenses on walls or not | 0 |
| Parameter | Description | Default value |
| BASIC VALUES |  |  |
| part\_source | Particle source rate (1/cm3/s).  If particle source is constant during the simulation, this parameter is a vector of following form:   |  |  | | --- | --- | | source rate (1/cm3/s) | particle size (m) |   where particle size is the diameter of particles created. For example part\_source=[1, 3e-9] will generate one 3-nanometer particle/cm3 every second during the simulation.  If user wants to create particle sources of different sized particles, this can be done by defining part\_source as a 3D-matrix. For example lines  part\_source(:,:,1) = [1, 3e-9];  part\_source(:,:,2) = [5, 5e-9];  will create one 3-nanometer particle/cm3 and five 5-nanometer particles/cm3 every second during the simulation.  Particle sources can also be defined as time-dependent vectors. In that case, the vector should be of following form:   |  |  |  | | --- | --- | --- | | t\_0 | source rate (1/cm3/s) | particle size (m) | | t\_1 | source rate (1/cm3/s) | NaN | | . . . | . . . | . . . | | t\_end | source rate (1/cm3/s) | NaN |   where the source rate in first line defines the source rate of particles at time t\_0, the next line defines it at time t\_1 etc. Particle size in first line defines the diameter of particles created; the values of column 3 in the rest of lines do not matter. |  |
| gas\_source | The condensing vapor source rate (1/cm3/s). Can be defined as a scalar or two-column array. When defined as scalar, the source rate will be constant during the simulation.  If gas\_source is an array, it must have two columns; the first column is a time vector and the second one tells the gas\_source value at respective time. The time vector doesn't need to have same length as parameter tvect. However, the first and last element of gas\_source's first column must have the same values as respective elements of tvect. If the length of the array is different than tvect's length, gas\_source will be interpolated to same length. |  |
|  |  |  |
| Parameter | Description | Default value |
| dilu\_coeff | Dilution coefficient (1/(cm3s)). Dilution affects particle concentration in following way: dN/dt = -dilu\_coeff\*N (N is particle concentration)  Parameter dilu\_coeff can be either a scalar or an array. When defined as a scalar, dilution coefficient will be constant during the simulation.  If dilu\_coeff is an array, it must have two columns; the first column is a time vector and the second one tells the dilu\_coeff value at respective time. The time vector doesn't need to have same length as parameter tvect. However, the first and last element of dilu\_coeff's first column must have the same values as respective elements of tvect. If the length of the array is different than tvect's length, dilu\_coeff will be interpolated to same length. |  |
| vap\_wallsink | The flux of vapor molecules that condense on walls (1/(cm3s)).  The change of vapor concentration by condensation on walls is then dCvap/dt = -vap\_wallsink\*Cvap. |  |
| satu\_conc | The condensing vapor saturation concentration (1/cm3). |  |
| lambda | The condensing vapor mean free path (m). |  |
| diff\_coeff | The condensing vapor diffusion coefficient (cm2/s). |  |
| vap\_molmass | Molecular mass of condensing vapor (g/mol). |  |
| particle\_dens | Density of particle matter. (g/cm3). |  |
| stick\_coeff | Sticking coefficient. The probability that vapor molecules will stick to aerosol particles. |  |
| Cvap0 | Initial condensing vapor concentration (1/cm3) |  |
| T | The temperature (K) |  |
| TIME VECTOR |  |  |
| tvect | The time vector (seconds). Define as row vector. The vector spacing does not remarkably affect calculation time, but defines only the spacing of the results. |  |
| DISTRIBUTION PARAMETERS |  |  |
| N0 | Initial total particle concentration (1/cm3).  If user wants to create a distribution that consists of several log-normal distributions, N0 can be defined as a vector. Then the total distribution will be a superposition of log-normal distributions. If N0 is defined as N0 = [1e3, 1e5], the first distribution has particle concentration N0(1) (= 1e3), standard deviation sigma(1) and mean diameter mu(1). The total particle concentration will then be N0(1) + N0(2).  Note that each distribution must have values for sigma and mu, so if N0 is a vector, mu and sigma must be vectors of same length. |  |
| mu | The mean of the lognormal size distribution.  If user wants to create a distribution that consists of several log-normal distributions, mu can be defined as a vector. Then the total distribution will be a superposition of n log-normal distributions, so that each distribution is defined by N0(i), mu(i) and sigma(i). Thus, if mu is a vector, N0 and sigma must be vectors of same length. |  |
|  |  |  |
| Parameter | Description | Default value |
| sigma | Sigma (standard deviation) of log-normal size distribution.  If user wants to create a distribution that consists of several log-normal distributions, sigma can be defined as a vector. Then the total distribution will be a superposition of n log-normal distributions, so that each distribution is defined by N0(i), mu(i) and sigma(i). Thus, if sigma is a vector, N0 and mu must be vectors of same length. |  |
| Dp\_min | The exponent of minimum diameter of the size grid.  The program will create a logarithmically spaced size grid between diameters and . The particle distribution will use this grid as x-axis and therefore Dp\_min and Dp\_max define limits inside which the distribution must stay. Thus, if particles for example grow during simulations, Dp\_max must be defined high enough so that the distribution stays inside the limits. |  |
| Dp\_max | The exponent of maximum diameter of the size grid.  The program will create a logarithmically spaced size grid between diameters and . The particle distribution will use this grid as x-axis and therefore Dp\_min and Dp\_max define limits inside which the distribution must stay. Thus, if particles for example grow during simulations, Dp\_max must be defined high enough so that the distribution stays inside the limits. |  |
| sections | The number of sections the model will use.  The size grid is created between and and the number of grid points is defined by parameter ‘sections’. The grid is logarithmically spaced. Particles are then placed in the sections according to their diameter.  The bigger the number of sections, the more accurate the model will be. However, increasing the number of sections slows down the model. |  |
| output\_sections | Defines the number of sections in output size grid.  After the simulation has run, the distribution at each time point is interpolated to the original size grid. The original size grid has however the same amount of sections as the calculated distributions, which causes error in interpolation. By defining output\_sections bigger than ‘sections’, the original size grid is made denser for the interpolation, minimizing the error. That is why output\_sections should always be bigger than ‘sections’, for example ten times bigger. |  |
|  |  |  |
| Parameter | Description | Default value |
| TOLERANCE PARAMETERS | Defines the tolerance settings for ode45. |  |
| Cvap\_tol | Vapor concentration tolerance. |  |
| N\_tol | Particle concentration tolerance. |  |
| Dp\_tol | Particle diameter tolerance. |  |

## Output data

The simulation results are found in *chamber.output\_data.* Descriptions of the contents of *output\_data* are in the table below.

## Known issues