Simulator of atmospheric aerosol nucleation bursts

User manual, version 20110324

H. Tammet

Introduction

The program *Burstsimulator.exe* is an implementation of the numerical model for atmospheric aerosol nucleation bursts described in the papers by Tammet and Kulmala (2005, 2007). The model is based on computationally efficient parameterization of submodels, which allow considering the ion-induced and homogeneous nucleation, depletion of nanoparticles and ions on the pre-existing aerosol, the nano-Köhler growth function, the molecule-particle interception geometry, quantum retardation of sticking, the electric charges of particles, the molecular dipole moments, the polarization interaction, and the dry deposition of ions and freshly nucleated particles onto the needles of trees in a coniferous forest. The evolution of the size distribution is computed using a sectional model with several thousands of sections. Computing time on an ordinary PC is counted in seconds in case of a typical task with several thousands of time steps and several thousands of size sections. The applications of the model are testing of effects of environmental conditions on the development of nucleation bursts and search for parameters that could provide diagrams, which are similar to the results of real measurements.

The present simulator is an updated version of the old program dated 20060912. Main changes are:

- function *Mobility* is corrected for multiply charged particles, however, without any effect in the functionality and the results of the present program,
- the output of mobility distributions, which was declared in the manual of the old version but not properly realized in the old program, is implemented in the new version,
- two new types of output tables is available: *diagram tables* support convenient drawing of distribution diagrams corresponding to the end of the evolution period and *plot tables* help to draw the contour plots using the MatLab function *Burstplot.m*, which is included into the package *Burstsimulator.zip*,
- the output files can be ordered in any combination using the modified control line 61,
- three additional control lines are included into the control file where the last four lines are:
  95) geometric standard deviation of the size distribution of positive small ions,
  96) geometric standard deviation of the size distribution of negative small ions,
  97) version of the plot table composition,
  98) the symbol of indeterminacy.

The nucleation process is calculated assuming the monodisperse small ions and the standard deviations above are considered only when compiling the plot tables, where the small ions are spread around the average mobility according to the lognormal law taking into account the control lines 95 and 96.

Standard distribution package **`burstsimulator.zip`** consists of ten files:

- **`burstsimulator.exe`** − the executable program,
- **`burstcontrol_demo.txt`** − an example of the control file,
- **`burstplot.m`** – the MatLab function for drawing of contour plots,
- **`burstsimulatormanual.pdf`** − the present document,
- **`burstdiagramtemplates.doc`** − the diagram templates.
- **`paper_2005.pdf`** − the manuscript of the first journal paper,
- **`paper_2006.pdf`** − a copy of the second journal paper,
- **`paper_2007.pdf`** − a copy of the third journal paper,
- **`burstsimulator.txt`** − the Pascal source code of the program,
- **`readme.txt`** − introductory explanations to the package.

Theory and methods

The theory and methods used in the simulator are described in three journal papers:

Tammet, H. & Kulmala, M. (2005) Simulation tool for atmospheric aerosol nucleation bursts. *J. Aerosol Sci.* **36**, 173–196, http://dx.doi.org/doi:10.1016/j.jaerosci.2004.08.004.

Tammet, H., Hõrrak, U., Laakso, L., & Kulmala, M. (2006) Factors of air ion balance in a coniferous forest according to measurements in Hyytiälä, Finland. *Atmos. Chem. Phys.*, **6**, 3377–3390, http://www.atmos-chem-phys.net/6/3377/2006/.

Tammet, H. & Kulmala, M. (2007) Simulating aerosol nucleation bursts in a coniferous forest, *Boreal Env. Res.*, **12**, 421–430, http://www.borenv.net/BER/pdfs/ber12/ber12-421.pdf.

The content of these papers is not repeated in the present document. The main concepts and principles of the simulator have been described in the first paper. This paper does not consider the dry deposition of ions and nanometer particles on the forest canopy and uses an oversimplified submodel of the sink of air ions on large aerosol particles. The second paper consists of improved theoretical models describing the sinks of air ions on background aerosol particles and on the needles of conifer trees. The third paper is a continuation of the first one and describes enhancements of the simulator. The papers are attached to the distribution package.

Program of the simulator

The program is written in Pascal language and compiled in the environment of Delphi 6. The computer must run under a 32-bit Windows. The minimum performance of the computer is 64 MB of RAM, a few megabytes of free disk space, and at least a 200 MHz processor. If Delphi is installed in the computer then the file *burstsimulator.txt* (available in the package *Burstsimulator.zip*) could be renamed to *burstsimulator.dpr*. After that a double click on the icon of this file will launch Delphi and load the source code of the simulator. The source code can be freely used and modified. Some universal subroutines can be useful in different projects. These subroutines do not use specific tools provided by Delphi and can be used inside of any Pascal-program. A set of subroutines is published in web, see http://ael.physic.ut.ee/tammet/a_tools/.

Additionally, the package includes the ready-compiled program file

`burstsimulator.exe`,

which can be used without Delphi. This file should be saved in any folder on the computer disk and it does not require installation. The control data should be prepared as a separate plain text file often named as

`burstcontrol.txt`.

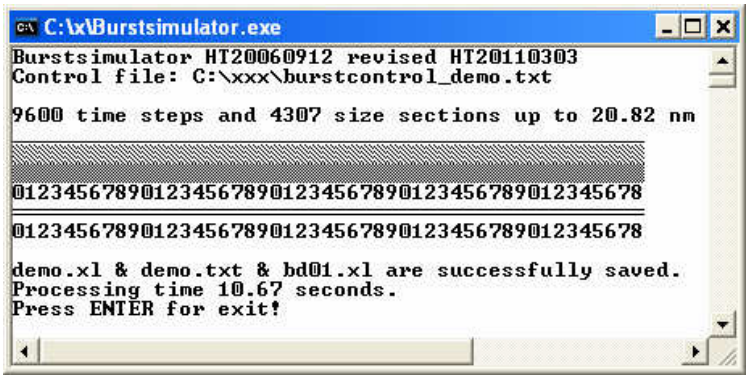
The content of the control file is explained below. It can be edited using *Notepad* or some other plain text editor.

The normal method to run the simulator is to drag the icon of the control file onto the icon of the exe-file of the program. In this occasion the control file may have an arbitrary name and may be located in an arbitrary folder. An alternative method is the double-clicking the icon of the exe-file. In this case the control file must have the name **`burstcontrol.txt`** and must be located in the same folder as the program. In both cases the output data will be saved in the folder where the control file is located. This folder is called the control folder. If an output file is used as the data for MS Office diagrams, then the most convenient control folder is *My Documents*.

The algorithm of the program includes five stages. At first, the control file is analyzed and the values of the time-dependent ruling parameters are calculated and tabulated in memory as functions of time for the full period under consideration. At the second stage the evolution of ions and particles in free air is integrated by the steps of about a second or few seconds. The third stage includes the preparative calculations for the optimization of the integration of air ion and aerosol dynamics in forest. The fourth stage is calculation of the evolution of air ions and aerosol particles inside of the forest canopy. In the fifth stage the export values are found using the data

collected during the previous stages. The third and fourth stages can be avoided setting the control parameter 51 (conifer needle length in a unit volume) equal to zero.

The program opens an information window and shows minimum technical information including three or five progress indicators as in the figure below:



The progress indicators show:

1) ▒▒▒▒▒▒▒▒▒▒▒▒▒▒▒▒ precalculation of sinks of ions and particles,
2) ▒▒▒▒▒▒▒▒▒▒▒▒▒▒▒▒ precalculation of the particle growth rates in the free air,
3) 01234567890123 evolution of ions and particles in the free air,
4) ═══════════════ precalculation of the particle growth rates and sink in a forest,
5) 01234567890123 evolution of ions and particles inside of the forest canopy.

The last two progress indicators appear only when the forest effect is included.

The accuracy of the results and the computing time are generally in the inverse relation. Main arguments of the computing time are:

- t_{per} – time period under consideration (control parameter 1),
- n_{min} – number of evolution steps in a minute (control parameter 2),
- t_{int} – duration of a time interval in the output table (control parameter 58).

The progress indicators on the computer screen count the time intervals. Number of intervals is t_{per} / t_{int}, typically few tens to few hundreds. The computing is arranged in such a way that the ruling parameters like ion sinks, nanoparticle sinks, growth rates etc are precalculated as mean values in the time intervals. This may consume considerable computing time. If the time intervals are long, e.g. more than 5 minutes, then the computing is quick but the results are not accurate due to the rough steps of estimating the ruling parameters. The time step of integrating the ion-aerosol evolution is dt = 1 minute / n_{min} and the total number of steps is $t_{per} \times n_{min}$. This number is responsible for the computing time used for integrating. The third main factor of the accuracy and the computing time is the number of size sections, which is chosen automatically and has usually a value of few thousands.

The control file allows to reduce the computing time using an acceleration coefficient. In the normal regime, the acceleration coefficient is 1. In an extreme situation (a very long period under consideration), the acceleration coefficient can be increased. The width of a particle size section is multiplied by the acceleration coefficient, reducing the number of the sections. It is not recommended to work with the number of size sections less than 1000. Otherwise, an effect called the numerical diffusion may appear as considerable.

Controls

The content of the control data is explained below using an expanded version of the control file **`burstcontrol_demo.txt`**. All lines printed without indent in bold **`Courier`** are the lines of the control file and the indented lines in *Italic Times* are additional comments that do not belong to the control file **`burstcontrol_demo.txt`**.

A line of the control file is a comment or a control line. Any line that begins with the equals sign is a comment line and contains only explanations. Other lines up to a special comment line

=== THE END ===

are the control lines. Possible leading and trailing spaces in a line are ignored.

A control line begins with a control value or two slash-separated control values. Follow a delimiting space and the explanation. The end of the line consists of the number of the control line and, usually, of a brief identifier of the control variable. The numbers are helpful for the diagnostics of possible errors made when editing the control file. The identifiers are used in the output files. Slash-separated values can be used in the control lines, which are marked with an asterisk. The first number of a slash-separated combination presents the value of the parameter in the free air and the second, in the forest. A single number in the place of a slash-separated combination is also legal. In this case, the value of the parameter is considered the same as in the free air as in the forest.

Only the control values can be changed during routine editing of the control file.

Attention: the space after a control value or two slash-separated values is important as a delimiter and must not be deleted!

The control file includes 98 control lines. The simulator program recognizes the control lines according to their positions. Thus, not a single control line should be deleted or added to the file. If a formal rule is ignored, then the processing will be interrupted immediately after reading the control data and a corresponding message appears in the information window.

In addition, an advanced user can edit the identifiers at the ends of the control lines. An identifier is a text from the last colon up to the end of the line. Identifiers will appear in the header of the output data table and in diagrams just as they are presented in the control file. An important limitation is that an identifier may contain no more than 9 symbols.

The model used in the simulator includes a large number of physical effects. This does not mean that all effects must be considered in a specific simulation. An effects can be easily neglected choosing the zero or unit parameters. However, all control lines should still be present in the file.

The control parameters are explained in an example of the control file on the following pages.

```
======= BURSTCONTROL_DEMO.TXT for BURSTSIMULATOR version HT20110306 =======
= The lines beginning with a symbol "=" in the first position and all lines
= after THE END are the comment lines. The lines beginning with a different
= symbol are the control lines. A control line consists of a control value
= followed by a space and a comment. A dual control value consists of the
= free-air value, slash, and the forest value. The number and the identifier
= of the control variable are shown at the end of a control line.
= The control values can be modified by the user of the simulator.
=== NB: Do not add or delete any control lines in this file! ===
=== Symbol # indicates that the value must be a whole number.
=== Symbol * allows to present slash-separated dual values e.g. 4.5/6.7
=== where the first is valid in the free air and the second in the forest.
= Full instruction is available as a separate document.
================================================================================
240 #min : Time period under consideration (<= 1440), 1
```

The sign # means here and below that the value must be a whole number.

```
40 #: Number of evolution steps in a minute (recommended 20...60), 2:nst
```

Time step is 60/nst seconds when calculating the evolution of ions and particles. The computing time is proportional to square of nst. The number of size sections will be determined by the program and it is proportional to the number of evolution steps. It is strongly recommended to notice the number of sections displayed on the screen and increase the number of time steps when the number of sections appears less than 1000.

```
1 : Acceleration coefficient dd/dd_min, normal value is 1, 3:acc
```

A multiplier to the section width, which decreases the computation time and accuracy. The value of the coefficient is recommended to be kept equal to 1. It can be increased only in extreme situations.

0 Celsius: Air temperature, 4:t

1013 millibar: Air pressure, 5:p

=== IONIZATION PARAMETERS ===

4/5 *cm-3 s-1: Initial ionization rate, 6:I0

Here a dual value is presented: the ionization rate is expected to be 4 in the free air and 5 in the forest.

4.5/5 *cm-3 s-1: Halftime ionization rate, 7:I1

5/5 *cm-3 s-1: Final ionization rate, 8:I2

Three values of the ionization rate allow to describe a parabolic trend. If an interpolated value turns up negative, then it is replaced with zero.There is a linear trend in the free air and no trend in the forest in the present example.

1.4 cm2 V-1 s-1: Electric mobility of positive cluster ions, 9:Z+

1.6 cm2 V-1 s-1: Electric mobility of negative cluster ions, 10:Z-

Mobilities must be given in respect to the actual temperature and air pressure.

1.5e-6 cm3 s-1: Cluster ion mutual recombination coefficient, 11:rec

2 g cm-3: Density of ions (standard value is 2.08), 12:idn

The density has a minor effect on the resuls via the small ion size-mobility conversion.

=== NUCLEATION PARAMETERS ===

1.5 nm: Birth size of particles, 13:d0

The nucleation is considered as a genesis of particles of a given size. If the birth size is defined as very small, then it may happen that the particles will not grow at due to the quantum rebound and/or nano-Köhler process. The parameters of the growth are presented when describing the condensing substances.

0 *cm-3 s-1: Maximum nucleation rate for positive ion nucleation, 14:J+

A single number in an asterisk-line means that the value is the same both in the free air and in the forest. Example: a presentation 3.2 has the same meaning as 3.2/3.2.

0.1 *cm-3 s-1: Maximum nucleation rate for negative ion nucleation, 15:J-

1/2 *cm-3 s-1: Maximum nucleation rate for neutral nucleation, 16:J0

The actual nucleation rate is calculated as the product of the maximum rate and the nuclation variation function that is common for positive, negative, and neutral nuclation. The variation function begins and ends with zero and is described using the following five parameters.

10 min: Rise time of the nucleation activity, 17:rt

3 #: Shape code of rise: 1=linear, 2=sinus, 3=square_of_sinus, 18:shr

The argument of the sine is zero at the beginning of the rise phase and pi/2 at the end of the rise phase.

60 min: Time of steady nucleation activity, 19:st

30 min: Time of dropping nucleation activity, 20:dt

Nucleation rate decreases from the maximum value until zero.

3 #: Shape of dropping: 1=linear, 2=sinus, 3=square_of_sinus, 21:shd

The argument of sine is pi/2 at the beginning of decrease and 0 at the end. The total nucleation time is rt + st + dt.

=== PARAMETERS OF THE FIRST CONDENSING SUBSTANCE ===

The first condensing substance (e.g. sulphuric acid) is responsible for initial particle growth. The first substance is expected to be non-evaporating. The condensation may be retarded at extra low sizes by the quantum rebound of growth units.

2 g cm-3: Density of growth units, 22:u1r

This value has a minor effect on the results via the diffusion coefficient of growth units.

0.115 nm: Extra distance of the Van der Waals capture, 23:h

0.55 nm: Diameter of a growth unit, 24:u1d
149 Å^3 : Polarizability, 25:pol1

Polarizability of a conducting sphere is $(d/2)^3$. The polarization effect can be ignored when writing here 0. In case of the permanently polarized growth units, the polarizability may be presented by the effective polarizability as done in this example.

1 : Nadykto-Yu dipole enhanchement factor for d = 1 nm, 26:Yu1

Nadykto and Yu presented a model of permanent dipole effecting condensation. If the method of effective polarization is used, then the Nadykto-Yu factor must be bypassed assigning the value 1 to the factor as at d = 1 nm as well at d = 2 nm.

1 : Nadykto-Yu dipole enhanchement coefficient for d = 2 nm, 27:Yu2

If Yu1 > 1 then Yu2 must be less than Yu1.

1 *nm/h: Initial plain Knudsen growth rate of neutral particles, 28:G10

The plain Knudsen growth rate neglects the interception size of growth units, Van der Waals capture, polarization effect and quantum rebound of growth units.

2/3 *nm/h: Halftime plain Knudsen growth rate of neutral particles, 29:G11
1 *nm/h: Final plain Knudsen growth rate of neutral particles, 30:G12

Three values allow to describe a parabolic trend. If the interpolated value appears to be negative, then it is replaced with zero.

2.5 nm: Critical size of quantum rebound, 31:dq0
600 K: Extra temperature of quantum rebound, 32:Tq0
=== PARAMETERS OF THE SECOND CONDENSING SUBSTANCE ===

The second condensing substance (e.g. some organic compound) is responsible for the ongoing accelerated particle growth. The condensation is expected to follow the approximated nano-Köhler law.

0.8 nm: Diameter of a growth unit, 33:u2d
32 Å^3: Polarizability, 34:pol2

The Nadykto-Yu factor cannot be applied for the second condensing substance and the effect of permanent dipole can be included using the method of effective polarizability.

2 *nm/h: Initial plain Knudsen growth rate of neutral particles, 35:G20

The plain Knudsen growth rate neglects the interception size of growth units, Van der Waals capture, polarization effect and quantum rebound of growth units.

3/7 *nm/h: Halftime plain Knudsen growth rate of neutral particles, 36:G21
3 *nm/h: Final plain Knudsen growth rate of neutral particles, 37:G22

Three values allow to describe a parabolic trend. If the interpolated value appears to be negative, then it is replaced with zero.

3 nm: Critical diameter when the condensation starts, 38:nKd
2 : Power of nano-Koehler approximation, 39:nKp
=== PARAMETERS OF THE PRE-EXISTING BACKGROUND AEROSOL ===
50 nm: Initial average diameter of background aerosol particles, 40:bd0
60 nm: Halftime average diameter of background aerosol particles, 39:bd1
60 nm: Final average diameter of background aerosol particles, 42:bd2

If an interpolated value turns up less than 20 nm, then it is replaced with 20 nm.

1500 cm-3: Initial concentration of background aerosol particles, 43:bn0
2000 cm-3: Halftime concentration of background aerosol particles, 44:bn1
3000 cm-3: Final concentration of background aerosol particles, 45:bn2

If an interpolated value turns up negative, then it is replaced with zero.

=== PARAMETERS OF THE CONIFER FOREST ===
180 m: Air residence distance (time * wind) in forest, 46:rd
1 m s-1: Initial wind in the forest, 47:w0
1 m s-1: Halftime wind in the forest, 48:w1
1 m s-1: Final wind in the forest, 49:w2

If an interpolated value turns up less than 0.1, then it is replaced with 0.1.

0.9 mm: Conifer needle diameter, 50:dn

150 m-2: Conifer needle length in a unit volume m/m3, 51:L

Wind speed and the needle parameters are important only in the calculation of dry deposition in the forest. If the measurement site is not in the forest, then the needle length should be written 0 and other forest parameters may have arbitrary values.

=== PRESENTATION CONTROL ===

1 #: Particle distribution argument is 1) diameter or 2) mobility, 52:d/Z

1.333 nm or cm2 V-1 s-1: Low end of the particle presentation range, 53:dmn

7.5 nm or cm2 V-1 s-1: High end of the particle presentation range, 54:dmx

These two size boundaries do not influence the processing of the particle evolution. They are used as the limits when computing the size distribution subtable, limited-range concentrations and average diameters (see the list of possible output variables in the section of ranks below)

6 #: Number of size fractions in distribution tables (<= 99), 55:nfr

Has no effect on computing time. A large number may convert a table hard to survey.

2 #: Scale of size or mobility 1) linear 2) logarithmic, 56:scl

Fraction intervals in the size distribution subtables are uniform in the selected scale.

3 #: Distr. 1) fraction concentrations 2) dN/dd 3) dN/d(log(d)), 57:dst

Decimal logarithm is used according to the tradition.

5 #min: Duration of a time interval in the output table, 58

Has a minor effect on the results due to the interpolation of environmental trends with a step in one interval. Does not influence the computing time for the free air but has some effect on the computing time for the forest. The number of intervals in the data table will be (time period) / (time interval). This number should not exceed 360. It is reasonable to keep the number of intervals in the range of 20-90. A number below of 10 is not good because most of the trends of environmental parameters are interpolated with a step of one interval. The number of intervals in the example is 48.

1 #min: Unit of time in the output table, 59:unit

The unit affects only the numbers in the time column of the output tables. The time column is always the first. Write here 60 for the hour scale or 1440 for the day scale.

0 #: Delimiter in the signature file 0) gap 1) tab 2) comma, 60

TL : Output: T = st-table, L = par-list, D = distr, P = plot-table 61

Order of the output files up to 4 symbols from the set of T, L, D, and P. The files are delivered according to the included symbols. T marks the standard table, L the parameter list, D the diagram table for the last time interval, and P the plot table, which allows to draw the contour plot by means of the MatLab function Burstplot.m.

=== RANKS OF VARIABLES AND SUBTABLES (RANK 0 = SKIP VARIABLE) ===

All variables which can be included into the output data table are listed below in the section of ranks. At first, the columns of the first rank variables are included into the data table, then of the second rank etc. Inside of the variables of the equal rank, the order of the list is followed. The variables of zero rank and of rank > 99 are skipped in the output.

0 #: Free air positive nucleation rate, 62:J+a

J+ will be skipped in the output table due to the zero rank.

0 #: Free air negative nucleation rate, 63:J-a

0 #: Free air neutral nucleation rate, 64:Joa

0 #: Forest positive nucleation rate, 65:J+f

1 #: Forest negative nucleation rate, 66:J-f

This parameter will occupy the first column in the output table after the time.

1 #: Forest neutral nucleation rate, 67:Jof

1 #: Concentration of positive ions, 68:n+

1 #: Concentration of negative ions, 69:n-

Follow seven averages calculated over the full size range:

0 #: Average diameter of positive particles, 70:d+

2 #: Concentration of positive particles, 71:N+
0 #: Average diameter of negative particles, 72:d-
2 #: Concentration of negative particles, 73:N-
1 #: Average diameter of neutral particles, 74:do
1 #: Concentration of neutral particles, 75:No
0 #: Polarity balance index of charged particles, 76:balance5

*The balance index = 10 * N^+ / (N^+ + N^-), where N^+ and N^- are the concentrations of positive and negative freshly nucleated particles. The values of the balance index may vary between 0 and 10.*

The next seven variables are similar to the above, but they are calculated not for the full size range but for the limited range betveen dmn and dmx.

0 #: Average diameter of positive particles between dmn&dmx, 77:d<+
0 #: Concentration of positive particles between dmn&dmx, 78:N<+
0 #: Average diameter of negative particles between dmn&dmx, 79:d<-
0 #: Concentration of negative particles between dmn&dmx, 80:N<-
0 #: Average diameter of neutral particles between dmn&dmx, 81:d<o
0 #: Concentration of neutral particles between dmn&dmx, 82:N<o
0 #: Polarity balance index between dmn&dmx, 83:balance<
2 #: Charge of background aerosol particles multiplied by 100, 84:100q

Average charge considers all background aerosol particles. If the numbers of positive and negative particles are equal, then the average charge is zero. The value of the average charge expressed in elementary charges is multiplied by 100 with the aim of making convenient the drawing of diagrams using common axes for different parameters.

0 #: Charge concentration of background aerosol, 85:Nq

The charge concentration equals to the product of the average charge and the particle concentration.

0 #: Effective diameter concentration of background aerosol, 86:Nd

Effective diameter concentration controls the sink of ions. It is calculated as the product of (diameter – 1.5 nm) and the particle concentration (see paper_2007.pdf) and is expressed in m / m^3 = m^{-2}.

Every line above with a nonzero rank includes one column into the data table but the following three lines can include each of nfr columns.

0 #: Distribution subtable of positive particles, 87:p
0 #: Distribution subtable of negative particles, 88:n
0 #: Distribution subtable of neutral particles, 89:z
=== SCALE DENOMINATORS FOR DIAGRAMS ===

The diagrams can be drawn in common axes when the variables are individually scaled. Thus the values of variables in the output data table are divided with the nominators below. The nominators will be automatically shown in the heading ot the table and they can be automatically transferred into the legend of the MS Word diagram. The denominators are not applied to the columns of the distribution subtables, which are always presented in the original units cm^{-3} and nm.

100 #: Concentration of ions cm-3, 90
50 #: Concentration of charged nanoparticles cm-3, 91
500 #: Concentration of neutral nanoparticles cm-3, 92
-10 #: Concentration of background aerosol charge m-3, 93

The background aerosol is usually negative. In the example, the polarity is inverted using a negative denominator. This is helpful when drawing the diagrams in common axes for different variables.

100 #: Effective diameter concentration of background aerosol m-2, 94
=== INFORMATION ABOUT PLOT TABLE ===
1.18 : geometric std of the distribution of positive ions, 95:gs+
1.22 : geometric std of the distribution of negative ions, 96:gs-

```
1 #: table composition: 1 = + & -, 2 = + & neutral, 3 = - & neutral, 97
=== REPLACEMENT FOR INDETERMINED VALUES ===
? : Symbol(s) of indeterminacy (- = gap, # = presumable limit), 98
```

Some values are indetermined, e.g. an average diameter before the nucleation burst when the concentration is zero. Symbols ? or - are recommended when the data are used for diagrams. Any numerical value, e.g. -999, may be used when the data are appointed for numerical processing. In case of # the program makes an attempt to estimate a limit value.

```
=== THE END ===
COMMENTS:
1. The columns of the output standard table are delivered in the order
   of ranks and when of equal rank, then in the order of control lines.
   The columns of zero rank are skipped in the table.
2. Scale denominators are applied to the integral concentrations only,
   the distributions are delivered in cm-3 or cm-3 nm-1 independent
   of denominator values.
```

Use of tabulated growthrate

In some extra situations the growth rate can be prescribed via a table. The tabulated growth rate is considered as independent of time and the particle charge. Thus the applications are limited. The table should be saved into the control folder and have the name *burstgrowthtable.txt*. The table includes two space-separated columns and *n* lines, where *n* is the number of control diameters:

$$d_1 \quad Gr_1$$
$$d_2 \quad Gr_2$$
$$\ldots\ldots\ldots$$
$$d_n \quad Gr_n$$

Gr_i is the growth rate (nm/h) at the diameter d_i (nm). All diameters must be positive. The number of diameters *n* should be at least 2 and no more than 99. If the file *burstgrowthtable.txt* is found in the control folder then the growth parameters presented in the control file have no effect and the growth rate is calculated as the linear interpolation according to the table. If the diameter of a particle is out of the range $d_1 ... d_n$ then the growth rate is expected to be Gr_1 or Gr_n.

Output files

Simulator delivers up to four output files according to the order presented in the control line no. 61. The names of the output files are compiled using the number, which is asked to be entered in the beginning of calculations. The number should be in range of 1…999 and it is indicated with ### in the conventional filenames below. If a file already exists in the control folder, then the computer asks to choose overwrite or escape from the program. However, if the preexisting file is read-only or locked for editing (e.g. open in MS Excel), then a corresponding message appears and a forced interruption of the program occurs.

Technical hints: an immediate *ENTER* is an equivalent of the answer "y" and the running program can be broken up intentionally by pressing the key combination Ctrl+C.

A parameter list has a filename L###.txt and consists of a single long line that can be wrapped when copying it into a document. In this line the values of the control parameters are listed. The identifiers of the parameters are taken from the ends of the control lines and they are explained in the control file. An example of the list, which corresponds to the sample control file:

```
nst=40 acc=1 t=0 p=1013 I0=4/5 I1=4.5/5 I2=5 Z+=1.4 Z-=1.6 rec=1.5e-6 idn=2
d0=1.5 J+=0 J-=0.1 J0=1/2 rt=10 shr=3 st=60 dt=30 shd=3 u1r=2 h=0.115 u1d=0.55
pol1=149 Yu1=1 Yu2=1 G10=1 G11=2/3 G12=1 dq0=2.5 Tq0=600 u2d=0.8 pol2=32 G20=2
G21=3/7 G22=3 nKd=3 nKp=2 bd0=50 bd1=60 bd2=60 bn0=1500 bn1=2000 bn2=3000
rd=180 w0=1 w1=1 w2=1 dn=0.9 L=150 d/Z=1 dmn=1.333 dmx=7.5 nfr=6 scl=2 dst=3
sct=4307 max=20.82 ?=? unit=1
```

Two identifiers close to the end of the list are not explained in the control file. The value of **sct** is the number of size sections actually used in the calculations and **max** is the maximum diameter up to which the particles could grow. This diameter is a technical limit and it is intentionally somewhat overestimated.

If the growthrates are defined by the file *burstgrowthtable.txt* then a remark *tabulated growth* is appended to the parameter list.

A standard table has a filename T###.xl and it can be opened in MS Excel with a double-click on the file icon. However, the standard table is not a complete Excel worksheet but a simple tab-separated text that can be read using any plain text editor.

The first line of the standard table is the heading where the identifiers of columns are shown. The following lines contain the data. Standard units are cm^{-3} and nm. If a denominator is used, it is shown in the heading and the values in a corresponding column are divided with the nominator. The nominators are used to keep the values in a range that is convenient in diagram presentation.

The first column of a table is the time column. The following columns are assembled according to the ranks defined in the control file. The contents of the columns are explained in the corresponding control lines of the control file.

The symbols ? in the tables mark the unknown values. This symbol is chosen in the last control line of the control file and may be changed. The sample control file generates the table, which beginning and end are presented below:

time	J-f	Jof	n+ /100	n- /100	do	No /500	N+/50	N-/50	100q
0	0	0	9.71	9.01	?	0	0	0	-3.81
5	0.05	1	9.67	8.94	1.55	0.19	0	0.09	-3.78
10	0.1	2	9.63	8.8	1.61	0.79	0.01	0.41	-3.56
15	0.1	2	9.59	8.7	1.7	1.28	0.02	0.69	-3.20
20	0.1	2	9.54	8.62	1.81	1.76	0.05	0.89	-2.87

.....

220	0	0	6.61	5.93	15.28	5.63	5.62	5.97	-2.04
225	0	0	6.55	5.88	15.63	5.58	5.75	6.1	-2.00
230	0	0	6.49	5.82	15.96	5.54	5.87	6.22	-1.96
235	0	0	6.44	5.77	16.29	5.49	5.98	6.34	-1.92
240	0	0	6.38	5.72	16.61	5.45	6.09	6.45	-1.88

A diagram table has a filename D###.xl and it is could be ordered only in a special situation when the distribution of the nucleating particles at the end of the evolution process is to be visualised using the MS Word graph routine. The argument of the table is diameter of mobility according to the control line no. 52. A diagram table includes the same data as the distribution subtables in the last row of the standard table. The difference is that the data are tabulated just as convenient for building the diagrams in MS Word. An application of the diagram tables is the study of nearly stationary distributions when the the nucleation period (control line 19) lasts until the end of a long enough full time period (control line 1). Firste column of the table is the central mobility or the size of the particle fraction depending on the control line 52. Three following columns present distribution of the fraction concentrations for the positive, negative and neutral nanoparticles. If the argument is the mobility then two more columns follow: the diameter of particle and the free air growth rate at the central mobility of the fraction.

NB: The data in the distribution subtables are always presented in the original units cm^{-3} and nm. Thus the values may differ from the values presented in a standard table, where the denominators defined in the lines 91 and 92 of the control file are applied.

A plot table has a filename P###.xl and it can be used for drawing the contour plots by means of the MatLab function *Burstplot.m*, which is available in the package and below in the present document.

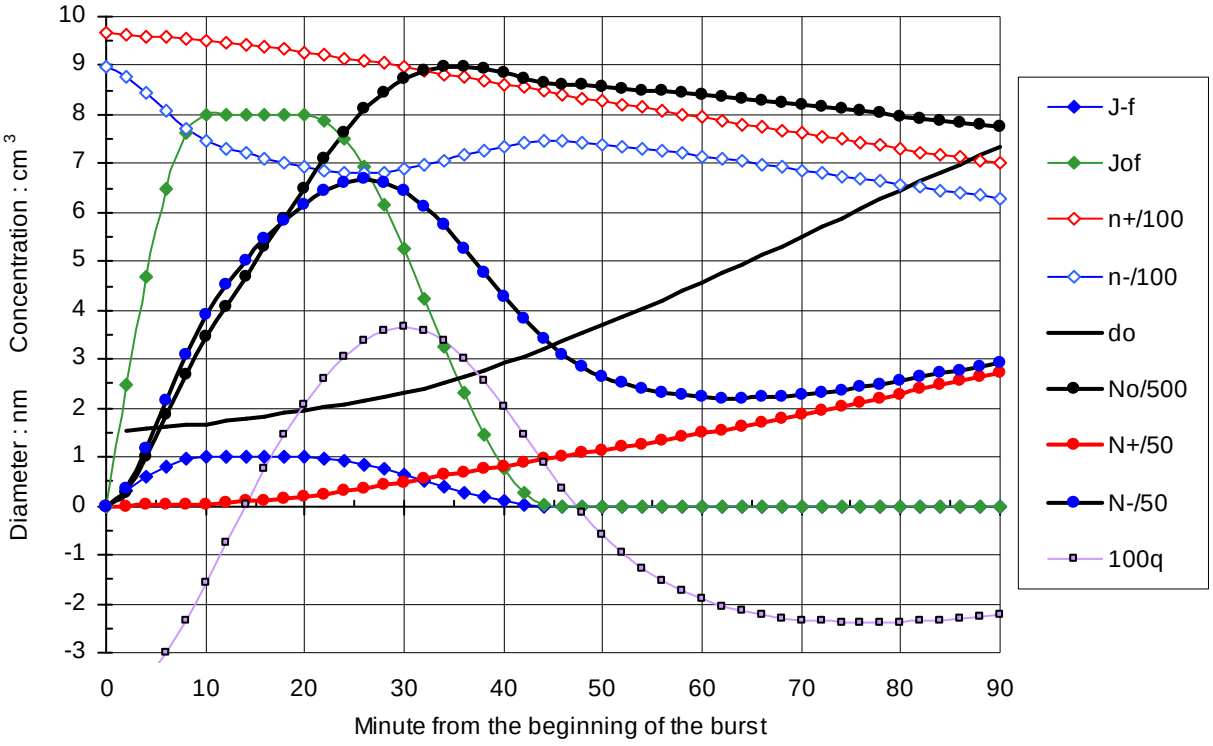
Drawing of diagrams in MS Word

Compiling a diagram without a prepared template is a troublesome job. Thus some diagrams could be stored in a special document and used as diagram templates. A special file *burstdiagramtemplates.doc* is included into the distribution package of the simulator.

The document, where a diagram should be included, may be located in an arbitrary folder. Locating of the data table in *My Documents* makes the processing easy. At first a diagram template has to be copied into the document. Then the diagram should be double-clicked to open it for editing. The full datasheet of the diagram should be selected (click in the upper left corner of the datasheet) and its content deleted (press *Delete* key). As a result the diagram appears empty. Next the cursor must be placed in the cell A0, which includes the prompt "X Values". Now the operation *Edit / Import file* should be performed and the new diagram appears ready. It may be additionally edited according to the intentions of the user.

Compiling a new data table (*xl*-file) with the same name will not change the diagram because the diagram data are copied and saved in the *MS Word* document. To change the diagram, it should be edited again after every new simulation of the nucleation burst.

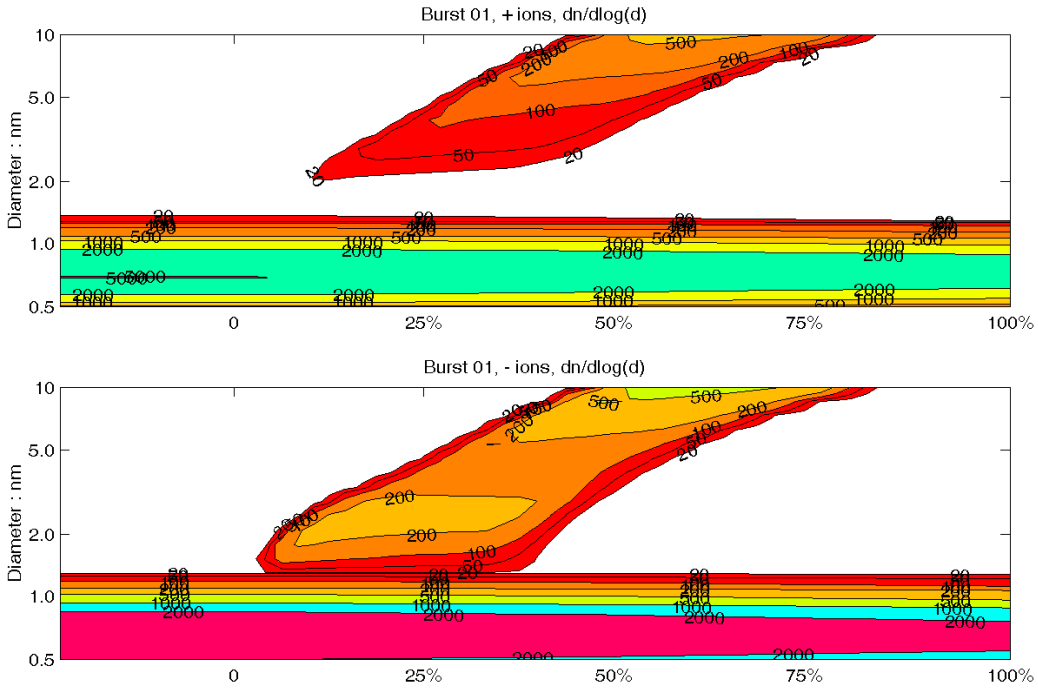
A sample diagram is presented below:



Drawing of contour plots

A plot table issued by Burstsimulator contains one header line and following data lines. The first element of the header line is the index of the table composition copied from the 97th control line. The index shows what two tables are presented: 1 = + & –, 2 = + & neutral, 3 = – & neutral. The table includes a prenucleation period and nucleation period. The length of the nucleation period is as specified in the first control line (240 minutes in the burstcontrol_demo.txt). The added prenucleation period is 25% of the nucleation period (60 minutes in the demo example). First column of the table is the number of the time interval, where the beginning of nucleation is marked with number 0 and the intervals of the prenucleation period have negative numbers. Following columns contain the values of the distribution function dn /dlogd while the first row shows the fraction center diameter expressed in nanometers. The span of diameter 0.5 to 10 nm is distributed into 20 fractions and the center diameters are: 0.539, 0.626, 0.727, 0.845, 0.981, 1.14, 1.324, 1.538, 1.786, 2.075, 2.41, 2.799, 3.252, 3.777, 4.387, 5.096, 5.92, 6.877, 7.988, 9.278 nm.

Before the drawing of the plots the plot files are recommended to be moved into are dedicated working folder. Next the MatLab should be launched and the function Burstplot.m should be loaded. The filepath indicated in the line 14 of Burstplot.m should coincide with the path of the working folder. If necessary the function should be edited. Now the operation Debug==>Run or key F5 will launch the processing. All plot table files located in the working folder will be automatically processed and the resulting png-files will be saved in the same folder. As the example the plot corresponding to the burstcontrol_demo.txt is presented below:



The text of the function Burstplot.m can be copied from the listing below:

```
% Burstplot - creates contour plots using Burstsimulator files - HT20110306
%=========================================================================
% Permanent sample of control lines, please keep unmodified:
% prefix = 'Burst'; % for output file name
% filepath = 'C:\Sci\nucleation\simulator\'; % where the files are located
% levels = [20 50 100 200 500 1000 2000 5000 10000 20000 50000 100000]; % for dn/dlogd
% pos_axes = [50 320 700 200]; % left, bottom, width, height
% neg_axes = [50 60 700 200]; % width (standard is 700) may be sometimes modified
% y_ticknumbers = [1 2.18 3.43 4.85 6.65 8.3 10];
% y_ticklabels = {'0.5';'0.7';'1.0';'1.5';'2.5';'4.0';'6.5'};
%=========================================================================
```

```
% The control lines to be modified by the user (the permanent sample is preserved
above):
   prefix = 'Burst'; % for output file name
   filepath = 'C:\_A\Sci\Nucleation\simulator\arendus\'; % where the files are located
   levels = [20 50 100 200 500 1000 2000 5000 10000 20000 50000 100000]; % for dn/dlogd
% The controls, which could be modified only in special situations:
   pos_axes = [50 320 700 200]; % left, bottom, width, height
   neg_axes = [50 60 700 200];  % left, bottom, width, height
   x_tickpositions = [1 12 24 36 48 61]; % horizontal positions
   x_ticklabels = {'';'0';'25%';'50%';'75%';'100%'}; % of the processing time
   y_tickpositions = [1 5.4 9.7 15.6 20]; % vertical positions
   y_ticklabels = {'0.5';'1.0';'2.0';'5.0';'10'}; % nanometers
%=========================================================================
% Modification of the text below of this line is not recommended
   for nr = 1:999;
      dd = num2str (nr);
      if nr < 100
         dd = ['0' dd];
      end;
      dd = num2str (nr);
      if nr < 10
         dd = ['0' dd];
      end;
      if exist ([filepath 'p' dd '.xl'], 'file')
         xx = load([filepath 'p' dd '.xl']);
         composition = xx (1, 1); % 1 = +&-, 2 = +&0, 3 = -&0
         [rows, columns] = size (xx);
         x = xx (2 : rows, 2:21); % first sector of ions + or -
         if sum (sum (x)) > 9999 % empty plot is skipped
            colormap(hsv);
            axes ('units', 'pixels', 'position', pos_axes);
            [c,h] = contourf (x', levels);
            brighten (0.6);
            clabel (c, h);
            set (gca, 'xtick', x_tickpositions);
            set (gca, 'xticklabel', x_ticklabels);
            set (gca, 'ytick', y_tickpositions);
            set (gca, 'yticklabel', y_ticklabels);
            ylabel('Diameter : nm');
            if composition < 3
                title(['Burst ' dd ', + ions, dn/dlog(d)']);
            else
                title(['Burst ' dd ', - ions, dn/dlog(d)']);
            end;
            print ('-dpng', [filepath prefix dd '.png']);
         end; % if sum > 9999
         x = xx (2 : rows, 22:41); % second sector of -ions or neutrals
         if sum (sum (x)) > 9999 % empty plot is skipped
            colormap(hsv);
            axes ('units', 'pixels', 'position', neg_axes);
            [c,h] = contourf (x', levels);
            brighten (0.6);
            clabel (c, h);
            set (gca, 'xtick', x_tickpositions);
            set (gca, 'xticklabel', x_ticklabels);
            set (gca, 'ytick', y_tickpositions);
            set (gca, 'yticklabel', y_ticklabels);
            ylabel('Diameter : nm');
            if composition < 2
                title(['Burst ' dd ', - ions, dn/dlog(d)']);
            else
                title(['Burst ' dd ', neutral particles, dn/dlog(d)']);
            end;
            print ('-dpng', [filepath prefix dd '.png']);
         end; % if sum > 9999
         close all;
      end; % of if exist
   end; % of nr
```