DMT-CCN instrument droplet growth simulations manual

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1. Introduction

- Obtaining the latest version of the code, sample files and this manual
  - http://nenes.eas.gatech.edu/CFSTGC
- The purpose of the code
  - Simulate droplet growth while accounting for water vapor depletion effects (Lathem and Nenes, *Aerosol Sci. Technol.*, 45:604–615, 2011), changes in instrument operation parameters (e.g. pressure, temperature and supersaturation), and changes in dry aerosol properties (hygroscopicity and size distributions)
  - If observed and simulated droplet sizes are different, there may be additional kinetic limitations

2. Generating model input files

- Can use IGOR Pro function (Appendix A) or just save from Excel
- Data files (*.ion)
  - The first row is a header line (free format)
  - Following rows contain the input data

    1: Scan index [instead of date and time]

    2: Total flow rate (L/min)

    3: Pressure (mbar)

    4: Supersaturation (%) [or column bottom temperature]

    5: Sheath-to-aerosol flow ratio

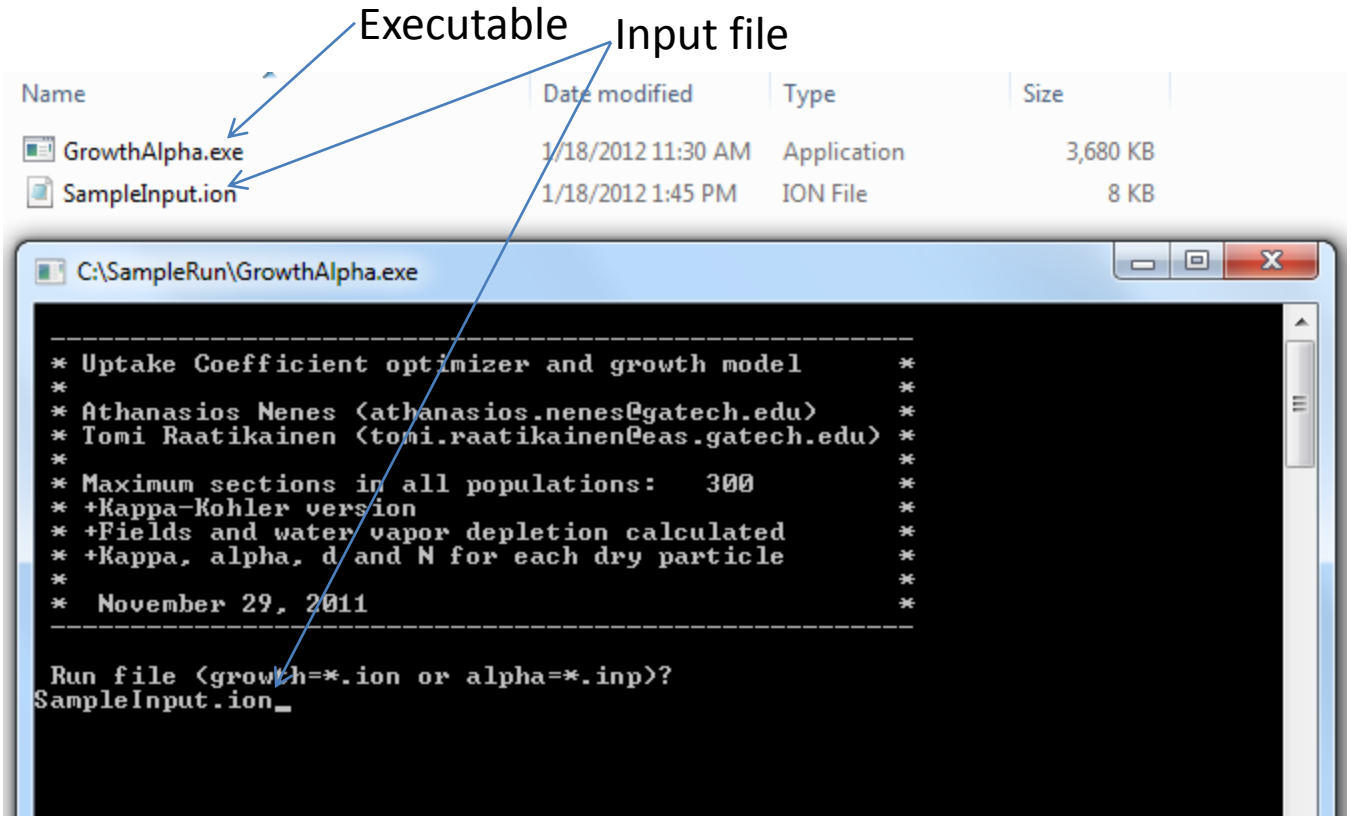
    6-7: Inlet and column top temperature (K) [usually the same values]

    8-11: Numbers of κ and α_c values, and dry particle number and size bins

    12->: κ and α_c values, number concentrations (cm^{-3} at instrument pressure and temperature) and dry sizes (nm)

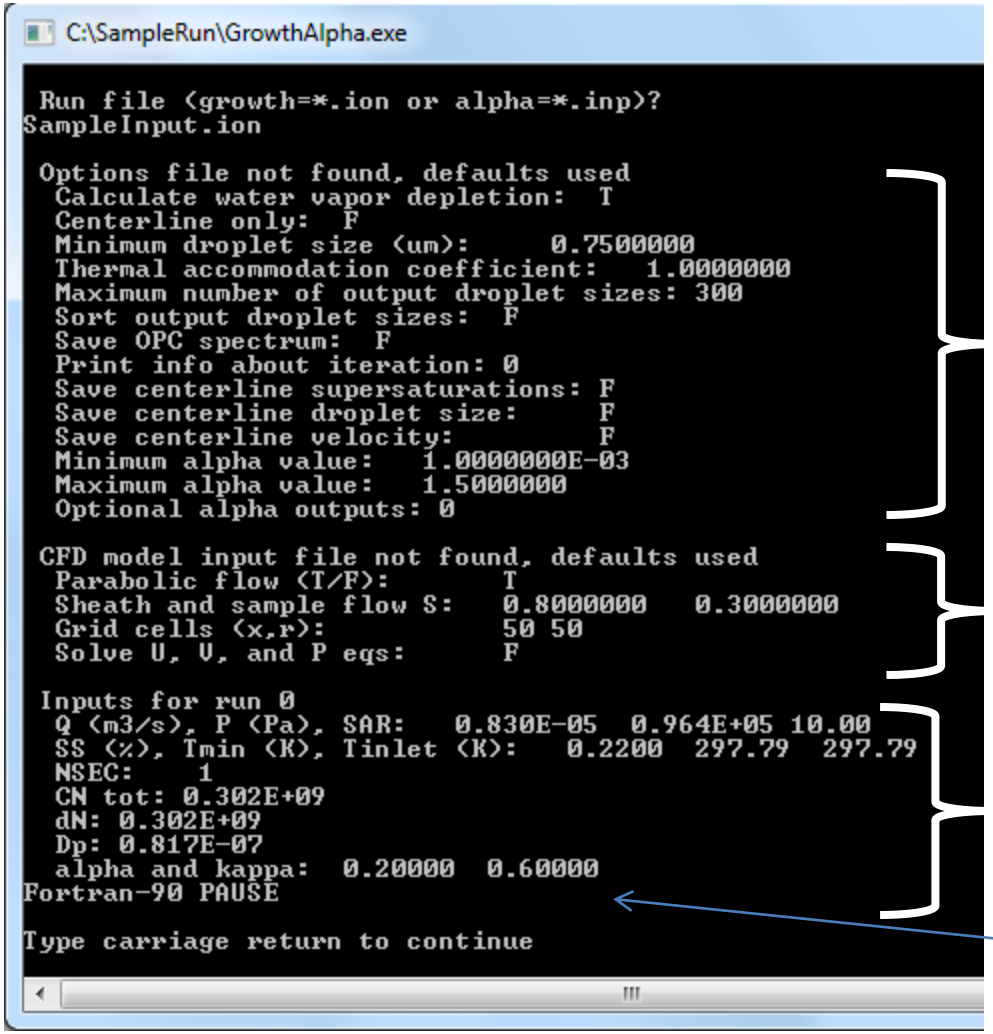
3. Running the growth code

1) Copy input data file and the executable (and option-files) to same folder
2) Start the executable by double-clicking it (opens command prompt)
3) Give the name of the input file name when asked and press return



… Running the growth code

4) Notice the initial information



General options for calculations
=> Default options used in this case

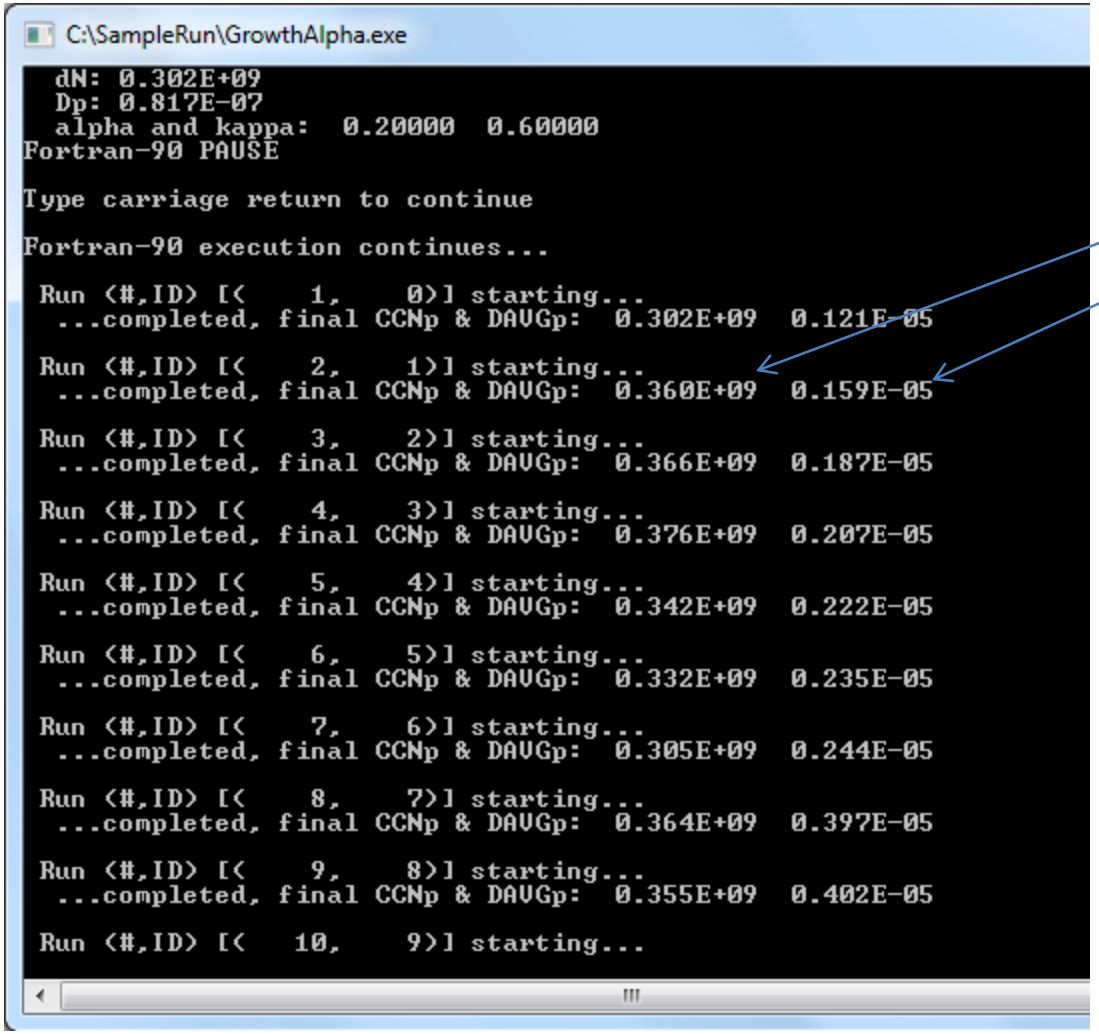
CFD (the gas-phase model) options
=> Defaults used

Inputs for the first run: OK

Possible warnings or error messages (no warning here)

… Running the growth code

5) Start simulations



Simulated CCN concentration (m^{-3})

Simulated average droplet size (m)

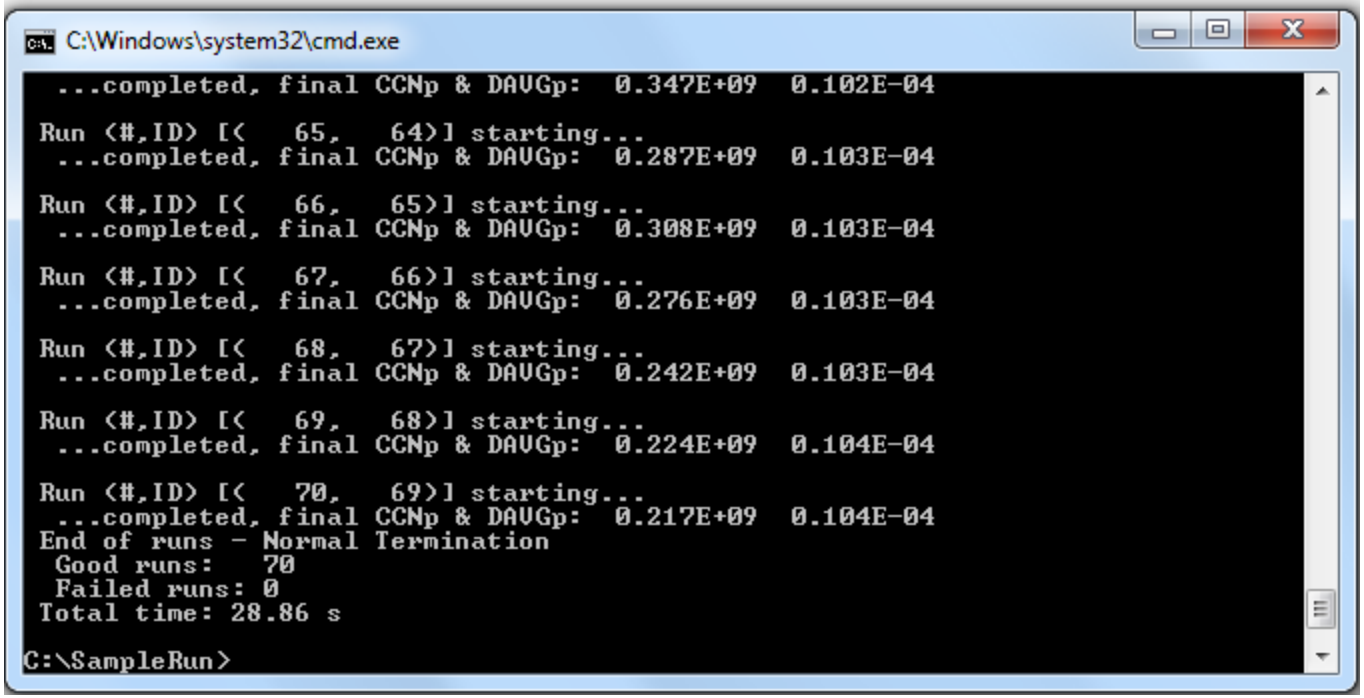
… Running the growth code

6) Finished!

A log file (list of failed runs)

The output file

Name	Date modified	Type	Size
GrowthAlpha.exe	1/18/2012 11:30 AM	Application	3,680 KB
SampleInput.ion	1/18/2012 1:45 PM	ION File	8 KB
SampleInput.log	1/18/2012 1:56 PM	Text Document	1 KB
SampleInput.res	1/18/2012 1:56 PM	RES File	29 KB



4. Model outputs (*.res)

- Can be opened by an IGOR Pro function (Appendix B) or Excel
- Data files
  - The first row is a header line
  - Following rows contain the output data

    1: Scan index
    2: Input supersaturation (%) [or column bottom temperature (K)]
    3: Particle free maximum supersaturation
    4: Supersaturation after the water vapor depletion effects
    5: Column bottom temperature
    6: Column top temperature (input)
    7: Inlet temperature (input)
    8: Pressure (input)
    9: Flow rate (input)
    10: SAR (input)
    11: CCN concentration (cm^{-3})
    12: Average droplet size (μm)
    13: Droplet size standard deviation (μm)
    14: Number of output droplet size bins (n)
    15-(15+2*n): Number of particles and droplet sizes
    16+2*n: Number of averaged output size distribution bins
    17+2*n-: Simulated CCN spectrum (cm^{-3})

5. Additional model options

- Two text files for model options
  - GrowthModelInputs.txt – General settings
  - setting.inp – Setting for the gas-phase model
- Default values used if an option file is not in the same folder as the executable

GrowthModelInputs.txt – General settings

```
* ============================================================================
* +++     Options for the droplet growth model                           +++
* +++                                                                    +++
* +++      Version: November 29, 2011                                    +++
* +++                                                                    +++
* +++      Tomi Raatikainen                                              +++
* +++                                                                    +++
* ============================================================================

...

*
*
* Common options
* +++++++++++++++
* Water vapor depletion effects, i.e. supersaturation is decreased due to
* condensation of water vapor, can be calculated or ignored.
* Default=TRUE (LOGICAL)
*CALCDPL=FALSE
*
* Use only centerline or all available aerosol trajectories. All fields
* should be used when water vapor depletion effects are accounted for.
* Default=FALSE (LOGICAL)
*USECENT=TRUE
*
* Thermal accommodation coefficient: negative value means that it is set
* equal to the mass accommodation coefficient. Otherwise, constant value
* is used.
* Default=1.0 (REAL)
*ALPHATK=-1.0
*
* Minimum droplet size in meters. Smaller droplets are not activated.
* Needed when calculating average droplet sizes. Do not set to zero!
* Default=0.75e-6 (REAL)
*OPCDCUT=1.0e-6
*
```

Comment line

A brief explanation

Variable (uncomment to set active)

Disable/enable water vapor depletion calculations

Should not be modified [faster calculations if only centerline aerosol growth is modeled]

Should not be modified [thermal accommodation coefficient set to unity]

Droplets smaller than this are ignored when calculating average droplet size

```
* Output options
* +++++++++++++++
* Maximum number of output droplet sizes (INTEGER). If possible, full size
* distribution with (NJAER-1)*NSEC points is saved. An empty array is a
* possible output.
* Default=300
*MAXDOUT=500
*
* Sort output droplet size distributions (TRUE/FALSE) so that droplet
* size is increasing. Otherwise, adjacent points are for aerosol
* sections with different trajectories.
* Default=FALSE
*SORTDAQ=TRUE
*
* Save averaged OPC or any other specified spectrum (TRUE/FALSE). Should
* use this is there are >> 1000 aerosol sections.
* Default=FALSE
*SAVEOPC=TRUE
*
* Read OPC bins from a text file. If no file name is given, default OPC
* bins (0.5-0.75, 0.75-1.0, 1.0-1.5, ... 9.5-10.0 um) are used.
* Default=
*OPCFILE=OPCbins.txt
*
* Print additional screen information about iteration
*     0    No printing
*     1    Print input values for each iteration
*     2    Print inputs and calculated numbers from each iteration
* Default=0 (INTEGER)
*OPTPRNT=2
*
```

Maximum number of output droplet size data. The total number is (number of different dry particles) x (number of aerosol grid cells); nothing saved if MAXDOUT is smaller than this.

Sort that droplet size data (not recommended)

Save averaged droplet size spectrum (should select this if not saving the full resolution droplet size distribution data)

Size bins for the averaged spectrum

Mainly for debugging purposes

```
* Save centerline supersaturation values to a text file
* Default=FALSE (LOGICAL)
*SAVESSC=TRUE
*
* Save centerline droplet size to a text file
* Default=FALSE (LOGICAL)
*SAVEDPC=TRUE
*
* Save centerline velocity to a text file
* Default=FALSE (LOGICAL)
*SAVEUVC=TRUE
*
*
* Alpha calculations only
* ++++++++++++++++++++++++
* Range of possible alpha values
* Default=0.001-1.5 (REAL)
*ALPHAMN=0.01
*ALPHAMX=1.5
*
* Save details from alpha iteration to an external text file
*     0   No saving
*     1   Save
* Default=0 (INTEGER)
*OPTDATA=1
*
* ========================================================================
```

Can save centerline supersaturations, droplet sizes (single dry particle κ, α_c and size) or axial flow velocities to text files. Axial distance from the aerosol inlet is the first line in each output file. The first row contains scan indexes.

Not used in the droplet growth calculations

Not used in the droplet growth calculations

setting.inp – Settings for the gas-phase model

Default values

```
*
* ==[ PARAMETERS FOR DMT CCN COUNTER SIMULATOR - UNITS IN SI ]==
*
===[ INLET PARAMETRES ]=============================================
Parabolic inlet velocity profile  [UPARAB]
.TRUE.
Sheath, Aerosol inlet RH (0-1 scale) [RHINS, RHINA]
0.8, 0.3
===[ GRID PARAMETERS ]==============================================
Number of cells in X-direction, Y-direction  [NI, NJ]
50, 50
===[ DEPENDENT VARIABLES ]==========================================
Solve for U, V, P equations ?
.false.
Solve for T, C equations ?
.true., .true.
===[ TERMINATION CRITERIA FOR ITERATIONS ]==========================
Maximum number of iterations per time step  [MAXIT]
5000
Maximum acceptable value of residuals  [SORMAX]
1e-7
===[ UNDER-RELAXATION ]=============================================
Under-relaxation factor for U, P equation  [URFU, URFP]
0.7, 0.1
Under-relaxation factor for T, C equation  [URFT, URFC]
1.0, 1.0
===[ EQUATION SOLVER SELECTION ]====================================
Solver selection for U, V, P equation  [ISLVU, ISLVP]
1, 1
Solver selection for T, C equation  [ISLVT, ISLVC]
2, 2
===[ INPUT-OUTPUT PARAMETERS ]======================================
Exit S is average over last (%) of chamber (0=exit point only) [SOAVGP]
0
```

Shouldn't be changed for constant velocity calculations

Best-guess relative humidity values; usually these values are good enough

Can be e.g. 100 x 100, but then calculations are slower

Shouldn't be changed for constant velocity calculations

Appendix A: Generating input files (*.ion) using the IGOR Pro function

1) Load data waves to an IGOR Pro experiment
   - Instrument settings (pressure, supersaturation, flows, temperature,…)
   - Dry particle properties (dry size and hygroscopicity)
2) Generate missing waves and perform unit conversions when needed
   - Eg. wave *Scan_ID=p*
3) Open procedure file “DropletGrowthKinetics.ipf”
4) Edit function output_model_data(opt,run_list,flag_name)
   - When needed, redefine the declared waves (Q_wave, P_wave, SS_wave, , SAR_wave, …)
   - Or give values for numerical variables (Q_val, P_val,…)
5) Execute
   output_model_data(0,””,””)
6) Save model input data

```
//
if (opt==0)
    // Sample calibarion experiment
    //
    // 1) Scan ID wave
    wave Scan_ID
    // 2) Instrument settings as P, Q , SS, SAR, Tcool and dTinlet waves
    wave Q_wave       // This wave exists, so this commad is not really needed (L/min)
    wave P_wave       // -||- (mbar)
    wave SS_wave=SS_cal     // The example supersaturation wave is called SS_cal (%)
    wave SAR_wave=SAR       // ... also the SAR wave is just called SAR
    wave Tinlet_wave=T_TEC1 // Inlet and column top temperatures should be equal (K)
    wave Tcool_wave=T_TEC1 // (K)
    // 3) Kappa and alpha: possible to use default values
    kappa_val=0.6     // Constant kappa for the calibration experiments
    alpha_val=0.2     // -||- alpha -||-
    // 4) Dry size distribution
    wave dN_wave=CCN_conc       // Here CCN concentration is used as is, but this could a
    wave dp_wave=DMA_Diameter // Scanning mobility, so dry size is varying
else
    print "Wrong option?"
    return 0
endif
//
```

Appendix B: Loading model inputs by the IGOR Pro function

1) Load the output text file (*.res) by executing ***load_res_file(0,0)***

Table0:tmp_data

R0C0 | 0

Row	tmp_data[][0]	tmp_data[][1]	tmp_data[][2]	tmp_data[][3]	tmp_data[][4]	tmp_data[][5]	tmp_data
	0	1	2	3	4	5	6
0	0	0.22	0.219982	0.219915	300.944	297.79	2
1	1	0.22	0.219983	0.219804	300.995	297.86	2
2	2	0.22	0.219983	0.21967	301.041	297.9	2
3	3	0.22	0.219982	0.219508	301.043	297.89	2
4	4	0.22	0.219982	0.219398	301.046	297.9	2
5	5	0.22	0.219982	0.219264	301.04	297.89	2
6	6	0.22	0.219984	0.219194	301.051	297.93	2
7	7	0.32	0.320041	0.316922	304.536	299.86	2
8	8	0.32	0.319987	0.316728	304.504	299.83	2
9	9	0.32	0.319989	0.316314	304.479	299.79	2

2) Convert the matrix wave to vector and matrix waves by executing ***res2wave_growth(1,"","",0)***

Table2:Scan_ID,sim_daq_avg,sim_ccn_nt...

R0C0 | 0

Row	Scan_ID	sim_daq_avg	sim_ccn_ntot	sim_daq_std	sim_io_mat[][0]	sim_io_mat[][1]	sim_io_mat[][2]	sim_io_mat[][3]
					0	1	2	3
0	0	1.21289	302.24	0.187431	0.22	0.219982	0.219915	300.944
1	1	1.58937	360.42	0.137761	0.22	0.219983	0.219804	300.995
2	2	1.86539	366.44	0.103209	0.22	0.219983	0.21967	301.041
3	3	2.07415	376.35	0.0817965	0.22	0.219982	0.219508	301.043
4	4	2.22368	341.77	0.0678687	0.22	0.219982	0.219398	301.046
5	5	2.35489	331.84	0.0580685	0.22	0.219982	0.219264	301.04
6	6	2.43815	305.35	0.0501234	0.22	0.219984	0.219194	301.051

3) It's done!

…

Droplet size standard deviation

CCN concentration

Average droplet size (μm)