PI Chamber Simulation Case: Modeling Aerosol-Cloud-turbulence Interactions in the Cloud Chamber

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Timeline

Dec, 2019	**Announcements & invitations**
Feb, 2020	**Confirmation of participation**
Oct 12, 2020	**Results received from the participants**
Oct-Nov, 2020	**Data post-processing & communication with participants**
21:00-24:00 UTC Nov 16, 2020	**Online workshop for current participants**
Post online workshop	**Report summarizing the case**
Feb 2021	**deadline for new registrations**
April 2021	**Updates & call for new data**
July 1 2021	**Data submission deadline**
July 26-30 2021	**International Cloud Modeling Workshop**
Post workshop	**Paper summarizing the case**

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Case overview

Motivation

- Cloud-aerosol-turbulence interactions in fine scales are not well-understood. Cloud modeling contains a large uncertainty from microphysical parameterizations.
- Due to the chaotic nature of clouds, in-situ measurement of cloud microphysics properties often comes with large uncertainty and the condition during measurement is often not controllable. Therefore, finding a good case based on measurements to compare with model results is challenging.
- Measurements for creating and evaluating parameterizations are sparse, boundary conditions are often poorly constrained, and atmospheric systems are rarely statistically stationary.
- Therefore, a turbulent mixed-layer formed within a cloud chamber provides an ideal environment for comparing measurements to simulations. Many of the thermodynamic, turbulence and microphysical properties in the Pi Chamber are comparable to those observed in stratocumulus clouds. The experiments also have reasonably well-characterized boundary conditions and achieve a statistical steady-state, and the detailed aerosol, cloud, and thermodynamic properties are available.
- On the other hand, high-resolution modeling provides alternative tools to look at small-scale cloud processes unresolved by traditional cloud models.
- In the long run, comparing the results of high-resolution models to laboratory measurements helps to verify physics in the model. And the well-validated model in return can be used to better understand the details of physical processes that are challenging to measure with existing instruments.

Objective

- The objectives of the base cases in this case study are to answer:
    - What are the key processes/parameters that impact the shape of the droplet size distribution (DSD), e.g., turbulence, fluctuation of supersaturation, mean supersaturation, aerosol number concentration, droplet sedimentation and fall out, and the interactions of the above processes?
    - How do the size distribution properties vary as the aerosol injection rate is changed? Do they capture the observed dispersion indirect effect?
    - Can simulations qualitatively or quantitatively capture the steady-state cloud droplet size distribution with realistic properties?
- The objectives of the variation cases are to determine:
    - How sensitive are the model results to the variation/perturbation of the initial conditions/model configurations?
    - What is the model uncertainty due to the level of uncertainty in the measurements?
- By model comparisons, we aim to figure out:
    - What are the key differences in the results of different models when imposing the same set of constraints from laboratory measurements? What causes the differences?

    - How can we justify/mitigate the divergence between the model results.
    - What are the implications for model parameterization/development at sub-grid scales?
- Out of this case study, we will formulate a test case for future model development & verification.

Introduction to the Pi chamber facility

What is the PI Chamber?

The Pi chamber is a turbulent, multiphase reaction chamber developed at Michigan Technological University. The cloud chamber is capable of generating and sustaining cloud formation in simulated tropospheric conditions for minutes to days.

Chamber schematics & capacity

Schematics of the PI Chamber structure are illustrated below (Figure 1 and Figure 2). The pressure shell is rectangular. The internal volume is 1 m high and 2 m wide. Two front-opening hinged doors give full access to the internal workspace. The thermal panels, which regulate the temperature within the chamber, are controlled on three separate circuits, corresponding to the top, bottom, and sidewall sections of the chamber internal workspace. All panels are capable of maintaining thermostatic conditions. For more detailed technical specification, see Chang et al. (BAMS 2016) https://journals.ametsoc.org/doi/full/10.1175/BAMS-D-15-00203.1

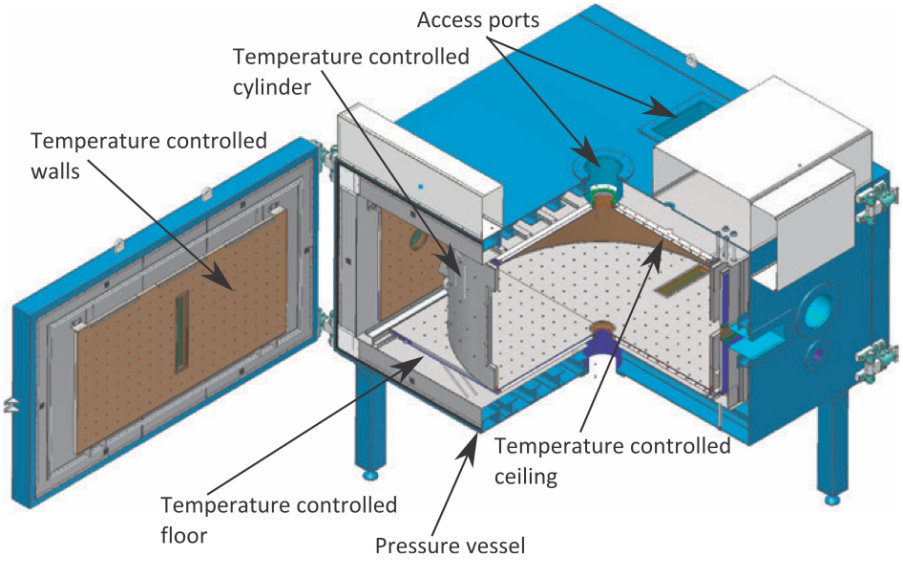


FIG. 1. A cutaway schematic of the cloud chamber with one door open and the cylindrical thermal panel in place.

Fig.1: Cutaway view of the PI Chamber (Chang et al., 2016)

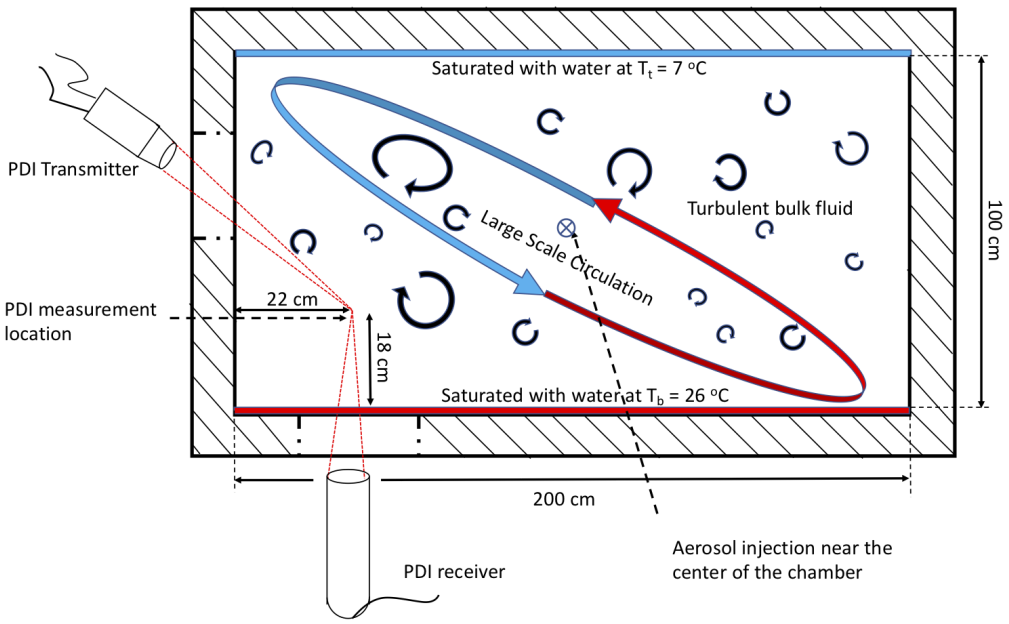


Fig. 2: Vertical cross-section of the PI Chamber (Chandrakar et al., 2019 QJRMS)

The chamber is also accompanied by a suite of instrumentation allowing for the generation and characterization of aerosol and cloud particles, measurement of thermodynamic and turbulence conditions, and sampling of particles for subsequent chemical and morphological analysis.
The research problems that can be addressed with this facility range from aerosol formation and optical properties to turbulent clouds and ice nucleation. Fig. 3 illustrates the spatial structures of aerosol and cloud drop distribution inside the chamber corresponding to different aerosol injection rates.

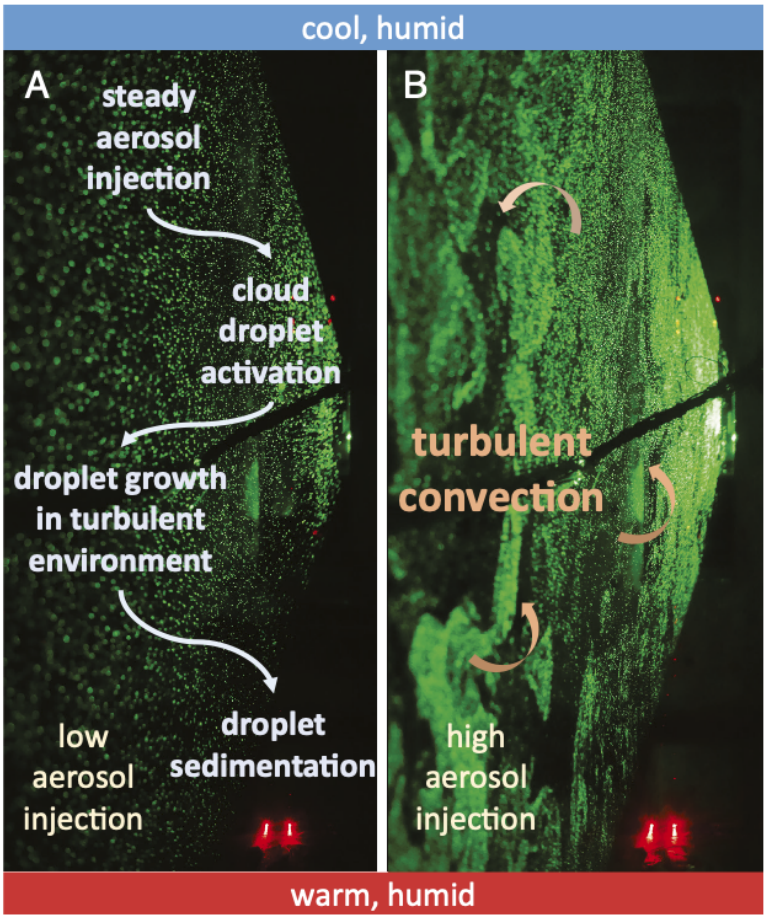


Fig. 3. Snapshot inside the PI Chamber with aerosols injected (Chang et al. 2016 BAMS)

Case description

The cases proposed here are focused on cloud-aerosol-turbulence interactions in a warm cloudy environment, i.e., no ice particles. Modeling results from DNS, LES, and other numerical/theoretical models are all welcome.

Two **base cases** are provided, with an emphasis on the steady state.

1) Steady-state case (primary emphasis)
Aerosols are constantly injected with a prescribed injection rate to form a steady-state droplet size distribution (DSD) in a steady-state thermal and turbulent environment, given the thermostatic wall conditions, i.e., fixed wall temperature and near wall humidity. The detailed numerical configurations are listed in the Section of "*Model configuration for the steady state case*"

2) Transient state case (optional)
Aerosol injection is switched off after the steady-state is achieved. The boundary condition and turbulent intensity, i.e., any forcing will remain the same except for the aerosol injection is switched off.

3) We also highly recommend that the participants perform some **variation cases** to look at **the response/sensitivity to various processes/conditions within each model**:
Examples of variations/perturbations in the configuration/parameters are turbulence intensities, $\bar{Q}v, \bar{T}$, Qv', T', aerosol size/composition, switch on/off collision-coalescence, model resolution, microphysics schemes (bin, bulk, and Lagrangian particles), with/without droplet losses due to contacting the side walls, and results on DSDs with/without the sidewall, etc.

Results from the two base cases will be used to do inter-model comparisons. For the attendants presenting in the workshop, **model results of the steady-state case are required.**

1) Model configuration for the steady state case

No droplet collision-coalescence in the base cases (both steady-state case and transient case), and droplets grow by condensation only. We mainly provide the configurations for DNS and LES models. Attendants may adjust configurations for other types of models accordingly.

Spin up and steady-state definitions:

For all models, allow for a dynamic spin-up before injecting aerosols. i.e., run simulations without aerosols to let the turbulence develop (until T and Qv reach steady-state).

After the spin-up, inject aerosols and run simulations until microphysics are in steady-state. We define that the simulation is in steady-state if both mean N_drop and R_drop reach steady-state.

1.1) **Models simulating the core region of the chamber**

Assume homogeneous and isotropic turbulence in the core region of the PI chamber. This assumption is ideal for the spectral DNS models due to their requirement for periodicity of the boundary conditions.

For **spectral DNS models**, one may use forcing in the low wavenumber band to maintain the fluctuations of the **v**, T, and Qv fields, see table below for detail.

For **DNS with a finite difference scheme**, we strongly encourage participants to construct the full geometry of the PI chamber with explicit wall boundary conditions (see configurations in table (1.2)).

variables		methods/calculations	values
Initial mean T, Qv, and p in the core region		Derived from the flux balance model (*) (Thomas et al. 2019)	$\bar{T}_0 = 287.25\ K$ $\bar{Qv}_0 = 0.0104126\ kg\ kg$ $P = 1000.0\ hPa$
Diagnostic mean and standard deviation of supersaturation		The diagnostic statistics $\bar{S}$ are calculated based on $\bar{T}_0$ and $\bar{Q}_{v0}$: $S \approx Qv/Qv_{sat} - 1.$ $Qv_{sat} = eps\frac{e_{sat}}{(P-e_{sat})}, eps \approx 0.615.$ $e_{sat} = 2.53 \times 10^{11} exp(-5.42 \times 10^3/T)$. cf. equation (2.12) in Rogers & Yau (1989).	$\bar{S} = 3.11\%$ $\sigma S = 1.4\%$
Forcing on the fluctuations and the mean of the scalar fields (T, Qv).	External forcing on fluctuations to maintain steady-state σT & σQv	The intensity of the forcings are determined in the *case **without particles** (i.e., before aerosols are injected into the chamber).* The participants shall first conduct the simulation without injecting aerosols to determine the forcing intensity to obtain the desired standard deviation (σ) of T and Qv fields (listed on the right).	$\sigma T = 0.5633\ K$ $\sigma Qv = 0.4775 \times 10^{-3} kg$

		The same forcing intensity should be applied to the *case when aerosols are injected*. Forcing schemes on scalar fields are similar to forcing on the turbulence. cf. Saito et al. (2019) or Paoli & Shariff (2009) for detail.	
	Nudge the mean T & Qv to approach $\bar{T}_0$ and $\bar{Qv}_0$	Nudge the mean value with the relaxation timescale τ (eqn (28-29) in Saito et al. 2019): $\frac{\partial \bar{T}}{\partial t} = -\frac{1}{\tau}(\bar{T}(t) - \bar{T}_0) + \frac{L}{C_p}\bar{C}_d$ $\frac{\partial \bar{Qv}}{\partial t} - \frac{1}{\tau}(\bar{Qv}(t) - \bar{Qv}_0) - \bar{C}_d$ The last term on the RHS of both eqns is the condensation term	$\tau = 60\ s$
Turbulence level		Constrain the mean eddy dissipation rate ϵ	$\epsilon = 0.001\ m^2 s^{-3}$
Spatial resolution Δx		The grid size is required to resolve the smallest turbulence scale (Kolmogorov length-scale, η), i.e., $k_{max}\eta > 1$. k_{max} is the maximum resolvable wavenumber. Or$\Delta x < \eta$	
Initial wind velocity mean			$\bar{U}_0 = \bar{V}_0 = \bar{W}_0 = 0\ m/s$
Model spin-up time	**Dynamic spin-up**	Spin up the model to reach steady-state in T and Qv before aerosols are injected	
	Microphysical spin-up	Reach steady-state in N_drop and R_drop. If steady-state is not observed, then at least 1min of spin-up time is required.	
(**Minimum**) simulated time duration **after spin-up**			$T_{tot} > 5min$
Domain size			$L_x = L_y = L_z =$ $20\ cm \times 20\ cm \times 20\ cm$

Footnotes:

(*): flux balance model (use the evolution of the mean temperature, T, as an example)

The evolution of the mean temperature T inside the chamber is determined by the fluxes at the top/bottom boundaries (T_t and T_b) and the side wall T_s.

$\frac{dT}{dt} = -\frac{1}{\tau}[2(T - T_0) + \hat{A}(T - T_s)]$,

here $T_0 = \frac{T_t + T_b}{2}$ and $\hat{A} = \frac{A_s}{A} = 2$ is the chamber geometry parameter defined by the area ratio between the side wall and the top/ bottom plates. A cuboidal geometry is assumed. The side length of the top/bottom walls = 2m, and the height of the chamber = 1m.

Assuming $\frac{dT}{dt} = 0$ in steady state, we then obtain

$T = \frac{\hat{A}T_s + 2T_0}{2 + \hat{A}}$ $T = \frac{\hat{A}T_s + 2T_0}{2 + \hat{A}}$

Plug in $T_s = 285K$, $T_0 = \frac{T_b + T_t}{2} = \frac{280K + 299K}{2} = 289.5K$, and $\hat{A} = 2$,

we get $T = \frac{(T_s + T_0)}{2} = 287.25K$

1.2) **Models** simulating the entire chamber environment

Note that for **DNS**, the same boundary and initial conditions as listed in the table below are applied, but some parameters and conditions such as dx and dt will be different to meet their specific CFL conditions, and for resolving more detailed dynamics and microphysics.

variables	method	values
Top, bottom, and side wall temperature	$\Delta T = 19K$	$T_t = 280K$, $T_b = 299K$, $T_s = 285K$
Pressure	Standard atmospheric pressure	P=1000hPa
Water vapor mixing ratio at the walls	For the top and bottom, set to saturated Qv (RH=100%). Adjust the sidewall Qv or RH or adjust the sink term (if no sidewall) in order to get the domain mean (including near wall region) supersaturation =**3%**	$Qv_t = 6.1562 \times 10^{-3} kg/kg$ $Qv_b = 0.0215865\ kg/kg$ $Qv_s = 7.1183 \times 10^{-3} kg/kg$ (Qv_s is adjustable based on the $\bar{S} = 3\%$ assumption).
Initial vertical	A linear (unstable) profile	$T(z) = 299K - 19K \times z/H$ [K]

T & Qv profile in the chamber	of T and Qv between the top and bottom walls	$Qv(z) = 0.0216 - 0.0154 \times z/H\ [kg/kg]$
Geometry of the chamber, grid spacing, and timestep	Rectangular shape $(2m \times 2m \times 1m)$	H=1m (z direction) Lx=Ly=2m $\Delta x = 3.125\ cm$ $N = 64 \times 64 \times 32$ $\Delta t = 0.02\ s$
Boundary conditions	For **LES**: By providing T and Qv at the walls, we imply that fluxes are computed using some kind of similarity conditions	No-slip boundary conditions preferred. Roughness length for LES $z_0 = 0.000035\ m$
Model spin-up time	**Dynamic spin-up** Spin up the model to reach steady-state in T and Qv before aerosols are injected	
	Microphysical spin-up Reach steady-state in N_drop and R_drop. If steady-state is not observed, then at least 1min of spin-up time is required.	
minimum simulation time after spin-up		For LES, $T_{tot} > 1\ hr$ For DNS, $T_{tot} > 30\ min$
Initial wind profile		U= V= W= 0m/s

Detailed information can be found in the LES study of Thomas et al. (2019): https://doi.org/10.1029/2019MS001670

1.3) How to include droplet & aerosol processing

Definition of droplet, aerosol, particle:

Aerosols are referred to those not activated (i.e., for NaCl particle with $d_{dry} = 125\ nm$, r_{wet} below the critical radius of r = 1.5μm).

The estimated critical droplet radius of the NaCl particle for $d_{dry} = 125\ nm$ *is estimated around* $r_{critical} = 1.5\ \mu m$ *(cf. Rogers and Yau, 1989, p.88-89)*

Droplets are defined as those over r=1.5μm.

Particles include both aerosols and droplets.

Mean & fluctuation scalar fields (T & Qv)	For DNS, same forcing for mean and fluctuations as described in (1.1)

	For LES, same boundary conditions applied as in (1.2)	
Size of aerosol (dry)	Monodisperse r	$d_{dry} = 125\ nm$ (diameter)
Chemical composition		NaCl
Aerosol injection	A uniform aerosol injection on every grid box instead of in the center is encouraged, though not required if it is too difficult to implement. Keep the injection rate constant over time. Inject aerosols at rates to produce N_{drop} (r>1.5μm) ranging from 10 to 3000 cm^{-3}. We will not target for an exact droplet number concentration, which is impractical and time consuming for modelers. We suggest you at least try 5 injection rates in the range of $N_{inj} = 1 - 1500\ cm^{-3} min^{-1}$ (suggested rates: $1, 10, 50, 100, 500, 1000, 1500\ cm^{-3} min^{-1}$). One can then adjust the range up/down, if needed, to get it closer to the desired range of droplet number concentrations ($N_{drop} = 10 - 3000\ cm^{-3}$) See Fig.4 below for the observed DSD in the Pi Chamber.	
Droplet removal / sedimentation 2 options	Drop gravitational settling velocity (Rogers & Yau, 1989): $k_1 = 1.233 \times 10^8\ m^{-1} s^{-1}$ $v_{drop} = k_1 r^2\ m\ s^{-1}$	
	Simulation of the core region without walls: remove based on the Stokes settling: Use random droplet removal based on the probability of droplet fallout during certain time interval Δt, which is $v_{drop}/H\Delta t = k_1 r^2/H\Delta t, H = 1\ m$, where $k_1 r^2$ is the Stoke's Law droplet terminal velocity.	
	Full chamber simulations: remove droplets when contacting the walls	
Droplet growth	Grow by condensation (in base cases, droplet collision-coalescence is not considered)	

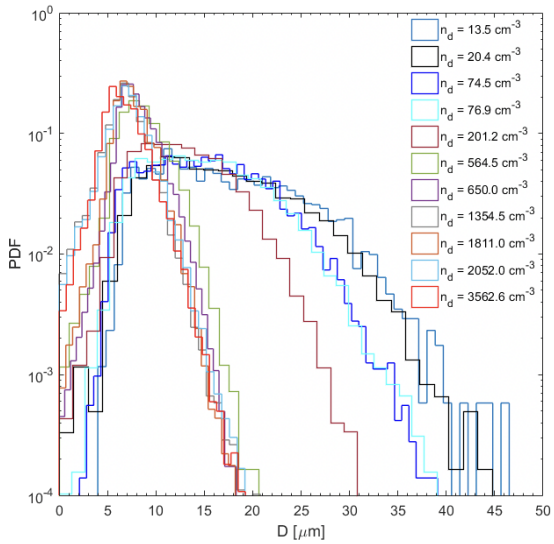


Fig. 4: Observed steady-state droplet size distribution in the Pi Chamber corresponding to different aerosol injection rates. n_d is the droplet number concentration (Fig. 1 in the supplementary material of Chandrakar et al. 2018 JAS)

2) (Optional) Model configuration of the transient case

Use the same condition as the steady-state case, but turn off the aerosol injection after reaching the steady-state. Measurements are taken after the aerosol injections are switched off. Simulated time for the transient period = 30 min for LES & 10 min for DNS.

Model output

1. Data Format

The model output should be submitted in **NetCDF** format, or **ASCII file** with code (in Fortran, python or matlab) to read the file(s) or with reading instructions. The output variables are listed in the tables below with the given **units**.

For the base cases, output from each aerosol injection scenario is required to be saved in separate files.

2. Output Variables

1) 1D data (for all models):

1.1) Time series of domain average statistics (Please include the spin-up periods)

Frequency: every **1s**.

Please INCLUDE the ENTIRE DOMAIN for calculating the domain average.

Output variables	Output format	units

{time} - Time t		s
{T} - temperature		K
{Qv} - water vapor mixing ratio		kg/kg
{RH} - relative humidity		%
{S_drop} - supersaturation at droplet locations	How to calculate the mean supersaturation at droplet locations: For Lagrangian particle method, it's the average of the supersaturation over all droplet locations; for bin-scheme, it's the average of the supersaturation at each grid cell weighted by the number of droplets in that grid cell.	
{LWC} - liquid water content	defined as mass of liquid water per unit **volume** of dry air	gm^{-3}
{N_drop} - Droplet number concentration N_{drop}	Droplets are defined as the one grow beyond its critical radius, i.e., $r_{aerosol} > r_{critical}$, where $r_{critical}$ is the critical radius, here we set $r_{critical} = 1.5\ \mu m$	cm^{-3}
{N_aerosol} - aerosol number concentration	Defined as the number of aerosols which are unactivated: $r_{aerosol} < r_{critical}$	cm^{-3}
{N_removal} - droplet removal rate		$cm^{-3}min^{-1}$
{disp_r} - relative dispersion of droplet size distribution	Defined as ratio between the standard deviation of droplet size distribution and the mean droplet size $= \frac{\sqrt{\Sigma(r-\bar{r})^2/N_{drop}}}{\bar{r}}$	
{r_mean1} - droplet mean radius	$= \Sigma r/N_{drop}$	μm
{Sigma2_S} - spatial variance of supersaturation$\sigma^2 S$		
{Sigma2_T} - spatial variance of		

temperature$\sigma^2 T$		
{Sigma2_Qv} - spatial variance of water vapor mixing ratio$\sigma^2 Qv$		
{Sigma2_S_drop} - variance of supersaturation at droplet locations		
{epsilon} - eddy dissipation rate ϵ		$m^2 s^{-3}$
The variables below are required for models of entire chamber		
{TKE}	TKE of the entire domain	$m^2 s^{-2}$
{H_flux_t} - heat flux at the top	Fluxes near the top and bottom walls	Wm^{-2}
{H_flux_b} - heat flux at the bottom		Wm^{-2}
{qv_flux_t} - moisture flux at the top		$kg\ kg^{-1} ms^{-1}$
{qv_flux_b} - moisture flux at the bottom		$kg\ kg^{-1} ms^{-1}$
*The above time series of variables can be saved in a single file, filename: **AAA_Nxxx_1D**, AAA is model name (DNS, LES, etc); xxx is the injection rate (e.g, 001, 010, 100...)*		

1.2) DSD (number concentration of each bin, time) at the end of the simulation.

{dsd} - $DSD(r,t)$	The first dimension of the array contains the number concentration of each droplet size bin; The second dimension is time. You may include several DSDs if there is no steady-state DSD established in your simulations.	cm^{-3}(number concentration in each bin)
	DSD output bin resolution: Bin width is 0.2μm, from 0 - 50μm	
Saved in a separate file *filename: **AAA_Nxxx_dsd**,* *AAA is the model name (DNS, LES, etc); xxx is the injection rate (e.g, 001, 010, 100...)*		

2) 2D data (**height z, time t**) for models that simulate the entire chamber

2.1) mean vertical profile **at every 30s**. The value is averaged over the horizontal plane (also INCLUDES the near wall region).

Output variables	Output format	units
{time} - time		s
{z} - height	Distance from the bottom lid, please **DO NOT** exclude near wall region (z=**0-1m**)	m
{T} - temperature $T(z,t)$		K
{Qv} -$Qv(z,t)$		kg/kg
{RH} - $RH(z,t)$	relative humidity	%
{Sigma2_S}	Profile of spatial variance of supersaturation $\sigma^2 S$ as a function of height	
{S_drop}- the mean supersaturation at droplet locations	How to calculate the mean supersaturation at droplet locations: For Lagrangian particle method, it's the average of the supersaturation over all droplet locations; for bin-scheme, it's the average of the supersaturation at each grid cell weighted by the number of droplets in that grid cell.	
{Sigma2_S_drop} - the variance of the supersaturation at droplet locations		
{N_drop} - Droplet number concentration N_{drop}	Number concentration of droplets at each height.	cm^{-3}
{r_mean1} - droplet mean radius	$= \Sigma r / N_{drop}$ at each vertical level	μm

*For **netcdf** output, the above time series of variables can be saved in a single file, filename: **AAA_Nxxx_2D,** AAA is model name (DNS, LES, etc); xxx is the injection rate (e.g, 001, 010, 100...);*

*For **ASCII files**, each variable is saved in one file.*
*Filename: **AAA_Nxxx_2D_var**, var is the name of the variable*

Data is saved in the following format: each row represents the profile at one time point, and each column is the time series at a given z location.

2.3) Optional, so far we do not need the near-wall 2D field for model inter-comparison. Therefore, for now we suggest only calculating average & variances of the near-wall field (we will only need the top and bottom walls), which is already part of the profile data in (2.1)

Spatial distribution of instantaneous T and Qv near the top/bottom walls at every 1min
Filename: ***AAA_Nxxx_2D_wall*** *for* ***netcdf****.*
AAA_Nxxx_2D_var_top *and* ***AAA_Nxxx_2D_var_bottom*** *for* ***ASCII files****.*

3) Simple plots for quick checkup and comparison (**for all models**)

We encourage people to provide simple plots for quick checkup and comparison. Please include them along with the datasets (plot examples are attached at the end):

3.1) 1D time series for each variable

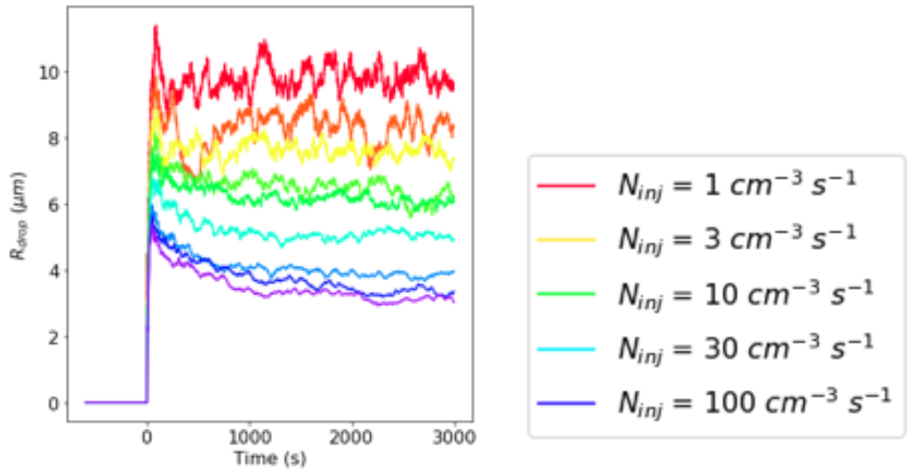
3.2) 2D vertical profile plots for each variable (one profile at the end of the dynamic spin-up, one at 30s after the aerosol injection, one at the end of the simulation)

3.3) DSD at the end of simulation for each injection rate.

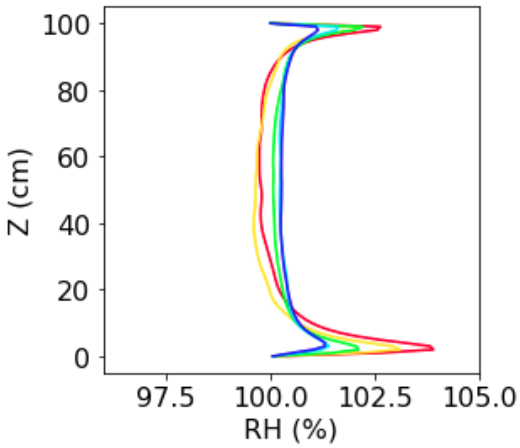
Filename: ***AAA_Nxxx_1D***, ***AAA_Nxxx_2D***, ***AAA_Nxxx_dsd*** (in any readable ***figure*** format)

Example plots (taken from UND's simulation):

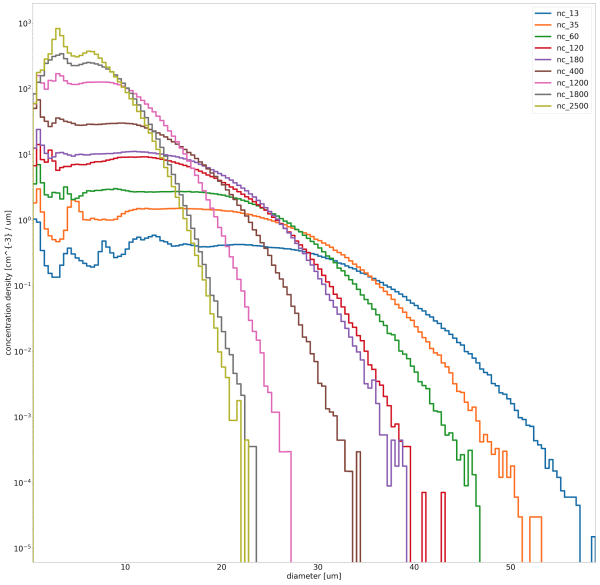
1D time series:



2D vertical profile:



DSDs (from Piotr's plot)



List of symbols:

Symbol	Name of variable	Unit
Qv	Water vapor mixing ratio	kg/kg
Qv_t, Qv_b, Qv_s	Qv at the top, bottom, and side wall	kg/kg

$Qv_{sat}(T) = eps\frac{e_{sat}(T)}{P-e_{sat}(}$	Qv at saturated water vapor pressure $e_{sat} = Ae^{-B/T}$ is the saturated water vapor pressure. (eq. (2.12) in Rogers & Yau, 1989) A=2.53e8 kPa, B=5.42e3 K $eps \approx 0.615$	kg/kg
T_b, T_t, T_s	Temperature at the top and bottom, and side wall	K
$\Delta T = 19K$	Temperature difference of the top and bottom walls	K
P	Pressure inside the chamber	hPa
H=1	Height of the chamber	m
Lx, Ly=1	Width of the chamber in horizontal direction	m
dx, dz	Size of the grid box	m
σQv, σT	Standard deviation of Qv and T	
S	Supersaturation ratio $S = \frac{e}{e_{sat}} - 1 \approx \frac{Qv}{Qv_{sat}(T)} - 1$	
d_{dry}	Diameter of the dry aerosol	μm
r	Droplet radius	μm
ϵ	Eddy dissipation rate	$m^2 s^{-3}$
U, V, W	Wind speed in x, y, z direction	$m\ s^{-1}$
N_{inj}	Aerosol injection rate	$cm^{-3} min^{-1}$
N_{drop}	Droplet number concentration	cm^{-3}
e_{sat}	Saturated water vapor pressure	hPa
$\bar{C}_d$	Mean condensation rate	$kgkg^{-1}s^{-1}$

References

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