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

Timeline

Dec, 2019	**Announcements & invitations**
Jan 30th, 2020	**Confirmation of participation**
May 15th, 2020	**Results received from the participants**
Before Jul 20th	**Data post-processing & communication with participants**
Jul 27th-31, 2020	**International cloud modeling workshop**

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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 process 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

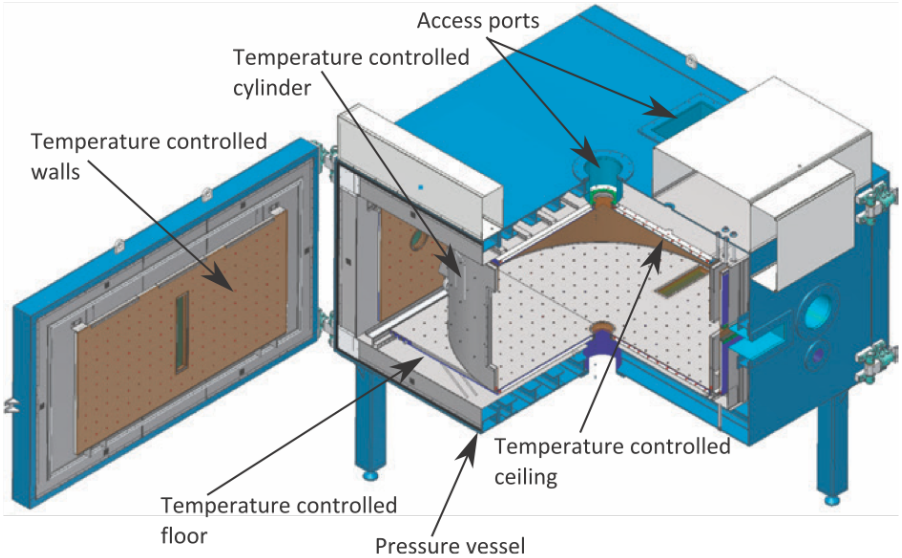

FIG. 1. A cutaway schematic of the cloud chamber with one door open and the cylindrical thermal panel in place.

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

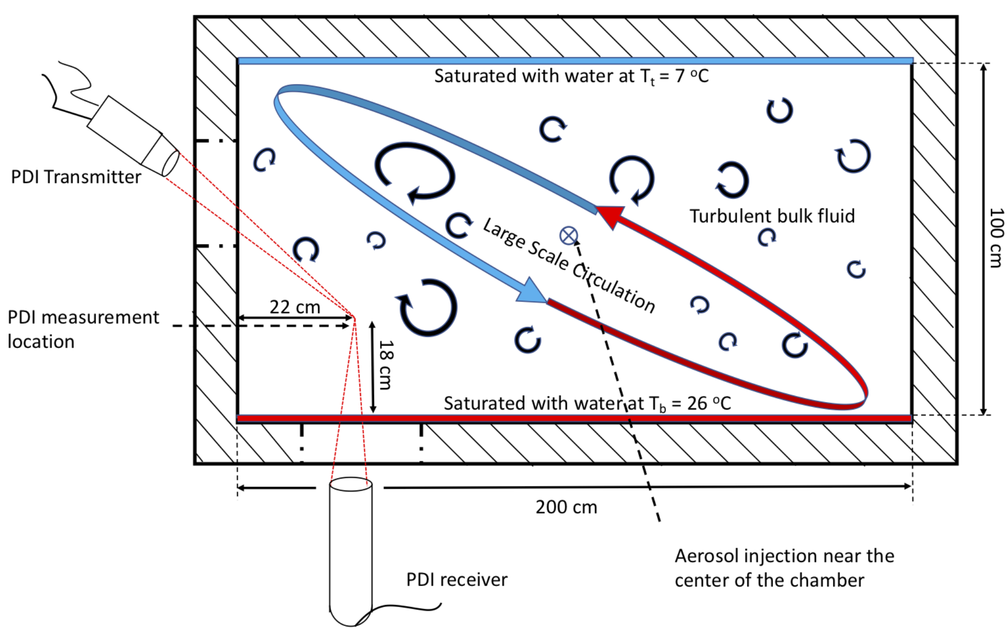

Fig. 2: Vertical cross-section of the PI Chamber (Chandrakar et al., 2019 QJRMS)

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.

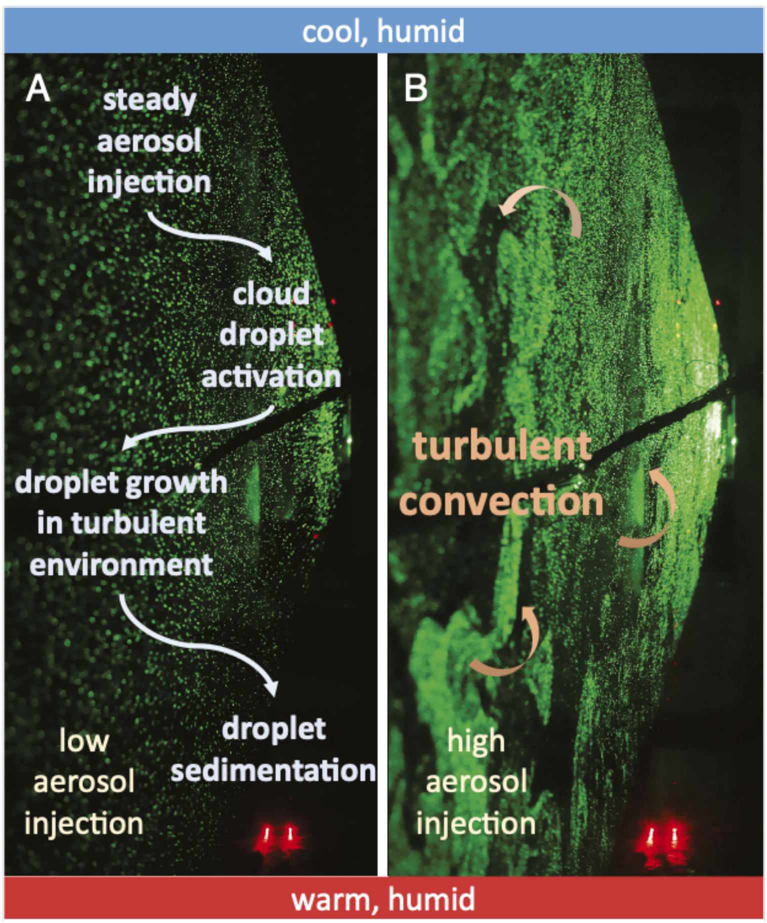

Fig. 3. Snapshot inside the PI Chamber with aerosols injected (Chang et al. 2016 BAMS)

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.

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 are required.**

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.

1) Model configuration for the steady state case

For base cases, there is no droplet collision-coalescence, only condensational growth.
We mainly provide the model.

1.1) DNS simulating the core region of the chamber

Assume homogenous 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 model**, one may use forcing in the low wavenumber band to maintain the fluctuations of the **v**, T, and Qv fields. For more information on forcing T and Qv in the DNS, one may refer to the method in Saito et al. (2019) or Paoli & Shariff (2009).

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 LES configurations in (1.2)).

<table>
<tr><td colspan="2">variables</td><td>methods/calculations</td><td>values</td></tr>
<tr><td colspan="2">Initial mean T, Qv, and p in the core region</td><td>Derived from the flux balance model (*) (Thomas et al. 2019)</td><td>$\bar{T}_0 =$ 287.25K
$\bar{Q}v_0 = 0.0104126 kg/kg$
$P = 1000hPa$</td></tr>
<tr><td colspan="2">Diagnostic mean and standard deviation of supersaturation</td><td>The diagnostic statistics are calculated based on the local T and Qv in the domain</td><td>$\bar{S}$ =3.11%
$\sigma s = 1.4\%$</td></tr>
<tr><td rowspan="2">Forcing on the fluctuations and means of the scalars (T, Qv).</td><td>Apply the external forcing to the fluctuation fields to maintain steady-state σT & σQv</td><td>The intensity of the forcings are determined based on the observed steady-state σT and σQv in the case without droplets.
The same forcing intensities will then be applied to the case when aerosols are injected.
As σT and σQv will respond to the condensation/evaporation of droplets, their values are expected to change accordingly.</td><td>$\sigma T = 0.5633K$
$\sigma Qv =$
$0.4775 \times 10^{-3} kg/kg$</td></tr>
<tr><td>Nudge the mean T & Qv to approach $\bar{T}_0$ and $\bar{Q}v_0$</td><td>Nudge the mean with the relaxation timescale τ (eqn (28-29) in Saito et al. 2019):
$$\frac{\partial \bar{T}}{\partial t} = -\frac{1}{\tau}(\bar{T}(t) - \bar{T}_0) + \frac{L}{Cp}\bar{C}d$$
$$\frac{\partial \bar{Q}v}{\partial t} = -\frac{1}{\tau}(\bar{Q}v(t) - \bar{Q}v_0) - \bar{C}d$$
The last term on the RHS of both eqns is the condensation term</td><td>$\tau = 60s$</td></tr>
<tr><td colspan="2">Turbulence level</td><td>Mean eddy dissipation rate ϵ</td><td>$\epsilon = 0.001 m^2/s^3$</td></tr>
<tr><td colspan="2">Spatial resolution Δx</td><td colspan="2">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 $\Delta x < \eta$</td></tr>
<tr><td colspan="2">Initial wind velocity mean</td><td></td><td>$\bar{U}_0 = \bar{V}_0 = \bar{W}_0 = 0m/s$</td></tr>
<tr><td colspan="2">(Minimum) simulated time duration after reaching steady-state</td><td></td><td>$T_{tot} = 5min$</td></tr>
<tr><td colspan="2">Domain size</td><td></td><td>$Lx = Ly = Lz =$
$20cm \times 20cm \times 20cm$</td></tr>
</table>

Footnotes:

(*): flux balance model (use temperature 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 $\hat{A} \approx \frac{A_s}{A} = \frac{4LH}{2L^2} = \frac{2H}{L} = 2$ is the chamber geometry parameter defined by the area ratio between the side wall and the top/bottom walls. A rectangular geometry is assumed, L is the side length of the top/bottom walls, H is the height of the chamber. In the PI Chamber, H=L

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

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

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 $T = T_s = 287.25K$

1.2) **LES/DNS** of the entire chamber environment

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

Note that for **DNS aiming to simulate the entire chamber**, 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	$\Delta T = 19K$ (299K bottom and 280K top)	$T_t = 280K$ $T_b = 299K$ $T_s = 285K$
Pressure	Standard atmospheric pressure	P=1000hPa
Water vapor mixing ratio at the walls	For the top and bottom, set to saturated Qv based on T_t, T_b And assume RH=82% at the side wall ($Qv_s \approx 82\% Qv_{sat}(Ts)$)	$Qv_t = 6.1562 \times 10^{-3} kg/kg$ $Qv_b = 0.0215865 kg/kg$ $Qv_s = 7.1183 \times 10^{-3} kg/kg$
Initial vertical T & Qv profile in the chamber	A linear (unstable) profile of T and Qv between the top and	$T(z) = 299K - 19K \times \frac{z}{H}$

	bottom walls	$Qv(z) = 0.0216 - 0.0154 \times \frac{z}{H}$ $[kg/kg]$
Geometry of the chamber and grid spacing	Rectangular shape ($2m \times 2m \times 1m$)	H=1m (z direction) Lx=Ly=2m $\Delta x = 3.125cm$ with $N = 64 \times 64 \times 32$
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 $z_0 = 0.000035m$
Total simulation time and time step		$T_{tot} = 2hr$ $\Delta t = 0.02s$ to satisfy CFL condition
Initial wind profile		U= V= W= 0m/s

1.3) How to include droplet & aerosol processing

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	$d_{dry} = 125nm$
Chemical composition		NaCl
Aerosol injection	Inject aerosols (in a small region or throughout the domain) at rates to produce N_{drop} (activated droplet number concentrations) ranging from 10 to 3000 cm^{-3}. (Suggested number concentrations = 10, 30, 100, 300,1000, 3000 cm^{-3}) See Fig.4 below for the observed DSD in the Pi Chamber.	
Droplet removal / sedimentation	Drop gravitational settling velocity (Rogers & Yau, 1989): $v_{drop} = k_1 * r^2 m/s$ $k_1 = 1.233 \times 10^8 m^{-1} s^{-1}$	**DNS**: remove at a constant rate based on the Stokes settling: Use random droplet removal based on the probability of droplet fallout during certain time interval Δt, which is

		$v_{drop}/H\,\Delta t = k_1 r^2/H\,\Delta t, H = 1m$, where $k_1 r^2$ is the Stoke's Law droplet terminal velocity.
		LES: remove droplets when contacting the walls
Droplet growth	Grow by condensation (in base cases, droplet collision-coalescence is not considered)	

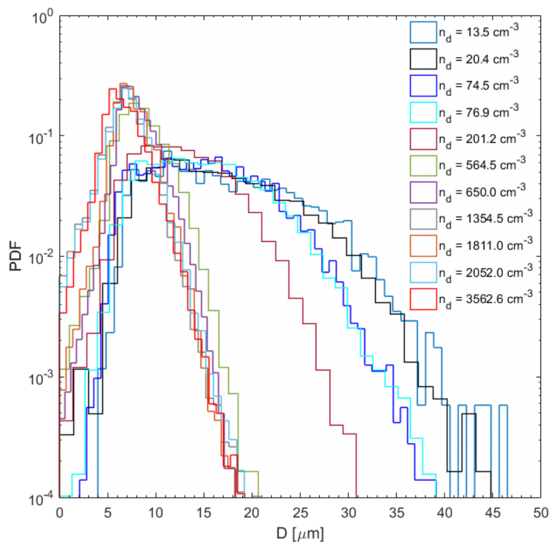

Fig. 4: Observed steady-state droplet size distribution in the Pi Chamber corresponding to different aerosol injection rates. n_d is the droplet number concentration (Fig. 1 in the supplementary material of Chandrakar et al. 2018 JAS)

1) (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) Output: Time series of domain average statistics

Frequency: every **1s**.

For LES, the domain average excludes regions within **12.5 cm (=4 grid points)** from the walls, i.e., grid points [5:60, 5:60, 5:28] in x, y, z direction.

Output variables	Output format	units
{time} - Time t		s
{T} - temperature		K
{Qv} - water vapor mixing ratio		g/kg
{RH} - relative humidity		%
{LWC} - liquid water content		g/kg
{N_drop} - Droplet number concentration N_{drop}		cm^{-3}
{N_aerosol} - aerosol number concentration		cm^{-3}
{N_removal} - droplet removal rate		$s^{-1}cm^{-3}$
{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
{r_mean2} - droplet effective mean radius	$= \frac{\Sigma r^3 n(r)}{\Sigma r^2 n(r)}$	μm
{Sigma2_S} - variance of supersaturation σ_S^2		
{Sigma2_T} - variance of		

temperature σ_T^2		
{Sigma2_Qv} - variance of water vapor mixing ratio σ_{Qv}^2		
{epsilon} - eddy dissipation rate ϵ		$m^2 s^{-3}$
*The above time series of variables can be saved in a single file, filename: **AAA_Nxxx_1D**, AAA is model name (DNS or LES); xxx is the injection rate (e.g, 100, 200...)*		
Droplet size distribution at **steady-state** in response to different injection rates	Bins of droplet size from 0-50 μm in **radius** with a bin width of 0.2 μm *Saved in a separate file* *filename: **AAA_Nxxx_dsd**,* *AAA is model name (DNS or LES);* *xxx is the injection rate (e.g, 100, 200...)*	μm

1.2) **(optional output)** For LES & DNS that simulate the entire chamber, we also ask for time series of the variables **near the walls** at <u>every 1s</u> (wall average separately for top, bottom and side)

{time} - time		s
{T_s} - sidewall temperature $T_s(t)$		K
{T_b} - bottom temperature $T_b(t)$		K
{T_t} - top temperature		K
{Qv_s} - sidewall Qv		kg/kg
{Qv_t} - top Qv		kg/kg
{Qv_b} - bottom Qv		kg/kg
{RH_s} - sidewall relative humidity		%
{RH_t} - top relative humidity		%
{RH-b} - bottom relative humidity		%

{qv_flux_t} - moisture flux at the top		$kgkg^{-1}ms^{-1}$
{qv_flux_b} - moisture flux at the bottom		$kgkg^{-1}ms^{-1}$
{qv_flux_s} - moisture flux at the sidewall		$kgkg^{-1}ms^{-1}$
{H_flux_t} - heat flux at the top		Wm^{-2}
{H_flux_b} - heat flux at the bottom		Wm^{-2}
{H_flux_s} - heat flux at the sidewall		Wm^{-2}
The above time series of variables can be saved in a single file, filename: ***AAA_Nxxx_1D_wall*** *AAA is model name (DNS or LES); xxx is the injection rate (e.g, 100, 200...)*		

1.3) For LES (optional) Time series of instantaneous values of S, T, Qv at the center of the domain.

2) 2D data (For LES and DNS that simulate the entire chamber)

2.1) time series of the mean vertical profile data **at every 30s**. The value is averaged over the horizontal plane (also excluding 4 points or 12.5cm from the wall) and at a thickness of every **dz=1cm**

{time} - time		s
{T} - temperature $T(z,t)$		K
{Qv} - $Qv(z,t)$		kg/kg
{RH} - $RH(z,t)$		%
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 or LES); xxx is the injection rate (e.g, 100, 200...);* *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.*		

2.2) Distribution of instantaneous T and Qv near the walls at every 1min
*Filename: **AAA_Nxxx_2D_wall** for **netcdf**.*
***AAA_Nxxx_2D_var_wall** for **ASCII files**.*

3) 3D data (for all models)

A few 3D snapshots of the T, Qv, and S at steady-state (and at transient-state if available)
*Filename: **AAA_Nxxx_3D (in figure format or netcdf)***

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
$Qv_{sat}(T) = eps\frac{e_{sat}(T)}{(P - e_{sat}(T))}$	Qv at saturated water vapor pressure $e_{sat}(T) = 2.53 \times 10^{11} exp(\frac{-5.42 \times 10^3}{T})$ is the saturated water vapor pressure $eps \approx 0.61$	kg/kg
T_b, T_t, T_s	Temperature at the top and bottom, and side wall	K
$\Delta T = 19$	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	

	$S = \frac{Qv}{Qv_{sat}(T)} - 1$	
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
N_{inj}	Aerosol injection rate	$s^{-1}cm^{-3}$
N_{drop}	Droplet number concentration	cm^{-3}
e_{sat}	Saturated water vapor pressure	hPa
$\bar{C}_d$	Mean condensation rate	$kg \cdot kg^{-1}s^{-1}$

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