Turbulence and droplets in cloud simulator

Conference on Dynamics of Particles in Flows

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Cloud, Cloud, Cloud, and Cloud



Tail of Genji

Aka Fuji (red Mt.Fuji) うろこ雲(cirrocumulus clouds) Hokusai

Ten Chapters in **Turbulence**

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Edited by PETER A. DAVIDSON YUKIO KANEDA KATEPALLI R. SREENIVASAN

La promenade, La femme à l'ombrelle Monet

Vortex cloud

CAMERIDGE



Cloud: dry air, water vapor, water droplets, ice, aerosol,.....

Cloud simulator



Growth of cloud droplets



Goal

Cloud droplets

- How fast do the droplets grow in mean and distribution, and become rain drops?
- What are key processes ?
- What is the spatial distribution of cloud droplets?
- To compute the collision efficiency and the collision kernel

Turbulence

- What is role of turbulence in cloud evolution?
- To what extent is turbulence modified or driven? (energy transfer, scalar variance transfer, intermittency)
- How droplets and scalar are transferred and mixed?

Direct Numerical Simulation of Turbulence and Cloud Droplets

Vaillancourt, P. A., Yau, M. K. & Grabowski, W. W. JAS. 2001 Andfrejczuk et al JAP. 2004 Kumar, Schumacher, Shaw, TCFD 2012

Included

- turbulence + buoyancy
- temperature
- water vapor mixing ratio
- water droplets of radius $10\mu m \sim 20\mu m$
- condensation, evaporation
- Stokes drag + radius dependent relaxation time + gravity

Not included

- Collision of droplets, coagulation
- Nucleation of water droplets
- Rain, ice

Basic Equations

Turbulence (Eulerian) Boussinesq approximation

$$\begin{split} \frac{\partial u}{\partial t} + u \cdot \nabla u &= -\nabla p + \nu \nabla^2 u + e_z B + f, \qquad \nabla \cdot u = 0 \\ \text{buoyancy external force} \end{split}$$

$$\begin{aligned} \frac{\partial T}{\partial t} + u \cdot \nabla T &= \kappa \nabla^2 T + \frac{L}{c_p} C_d \\ \frac{\partial q_v}{\partial t} + u \cdot \nabla q_v &= \kappa \nabla^2 q_v - C_d \end{aligned}$$

$$B = g \left(\frac{T - T_0}{T_0} + \epsilon (q_v - q_{v0}) - q_l \right)$$

High Reynolds number turbulence : Spectral methodScalar transport: Spectral (or hybrid method)

Cloud droplets (Lagrangian)

Collisionless

Vaillancourt *et al.* (2001) Kumar *et al.* (2012, 2013)

$$\begin{split} \frac{dN_j}{dt} &= V_j(t) \\ \frac{dV_j}{dt} &= \frac{1}{\tau_j(t)} \left(u(X_j(t), t) - V_j(t) \right) - ge_3 & \text{Stokes approximation} \\ R_j(t) \frac{dR_j(t)}{dt} &= KS(X_j(t), t) \right), \qquad R_j = \text{droplet radius} & \text{Diffusion process} \\ C_d(x, t) &\equiv \frac{1}{m_{air}} \frac{dm_l(x, t)}{dt} = \frac{4\pi r_l K}{\rho_0 (\Delta x)^3} \sum_{k=1}^{N_\Delta} R_j(t) S(X_j(t), t) \\ Condensation rate \\ S &= \frac{q_v}{q_{vs}(T)} - 1, \qquad \text{supersaturation rate} \\ K^{-1} &= \frac{\rho_l R_v T}{D_v e_{sat}(T)} + \frac{\rho_l L}{\kappa_a T} \left(\frac{L}{R_v T} - 1 \right) \end{split}$$

PIC

dX

Interpolation of velocity and scalar fields at particle position Redistribution of cloud properties onto grid points



Initial Condition

Turbulence

Temperature fluctuation

Droplets



Water vapor mixing ratio $q_{\rm v}$

$$q_v(x,t=0) = (q_v^{\max} - q_{v0}) \exp(-Az^6) + q_{v0}$$

$$q_v^{\text{max}} = 1.02 q_{vs}$$
 $q_{v0} = 0.90 q_{vs}$
 $q_v = q_{vs}$ at $z = \pm L_{\text{B}} / 6$ Kumar *et al.* (2012, 2013)

Isotropic Steady turbulence

- θ : 275 K + zero fluctuation
- Random in space in the range $-L_{\rm B}/6 \leq z \leq L_{\rm B}/6$
- No. of droplets : $2^{21} = 2 \times 10^{6}$ $2^{27} = 1.3 \times 10^8$
- No. density of droplets 31~125/cm³
- Initial radius : $10 \sim 20 \,\mu m$



Run	Α	В	C'	C "	С	D(A)	E(B)	Obs.
N ³	128 ³	128 ³	128 ³	128 ³	1024 ³	1024 ³	1024 ³	
N _p	2 ²¹	2 ²¹	2 ²²	2 ¹⁹	2 ²⁵	2 ²⁷	2 ²⁷	
n _p [cm ⁻³]	125	125	250	31	31	125	125	100~600
q_v	Decay	Grow	Grow	Grow	Grow	Decay	Grow	
θ'	0	0	0	0	0.05K	0	0	
ε[cm ^{2 -3}]	68.3	68.3	68.3	68.3	138	138	138	1~100
R_{λ}	92	92	92	92	252	252	252	3~4x10 ⁴
K_{max} η	1.2	1.2	1.2	1.2	2.1	2.1	2.1	
r(0) [µm]	20	20	15	15	15	20	20	
St(0)	0.068	0.068	0.068	0.068	0.10	0.18	0.18	
								Siebert et al JAS (2006)

$$\begin{array}{lll} \mathsf{Grow} & M_{\mathrm{vs}} \leq M_{\mathrm{v}} + M_{\mathrm{l}} \Longleftrightarrow \rho_{\mathrm{a}} \int_{V} q_{\mathrm{vs}} \mathrm{d}V \leq \rho_{\mathrm{a}} \int_{V} q_{\mathrm{v}}(x,t) \mathrm{d}V + \frac{4}{3} \pi \rho_{\mathrm{l}} \sum_{j=1}^{N_{\mathrm{p}}} r_{j}^{3} \\ \\ \mathsf{Decay} & M_{\mathrm{vs}} \geq M_{\mathrm{v}} + M_{\mathrm{l}} \end{array}$$



R_{λ} =92 (Run C')

- Periodic boundary condition
- e(t=0): 68.3 cm²/s³
- No. droplets: 4×10^{6}
- No. density droplets: 250/cm³
- No. visualized droplets: 10⁵
- r(0): 15 µm
- color : droplet radius
 red ⇒grow, blue⇒decay
- time : 0s~4s

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R_{λ} =252 (Run E)

- Periodic boundary condition
- ε (t=0)=138 cm²/s³
- No. droplets: 1.3×10^8
- No. density droplets: 125/cm³
- No. visualized droplets: 10⁵
- r(t=0): 20 µm
- color : droplet radius
 red ⇒grow, blue⇒decay
- time : 0s~6s

Radial distribution function of cloud droplets

$$g(R) = rac{G(R)}{4\pi R^2 n_d}$$

 $G(R)\Delta R$: No. of particles within spherical shell between R and ΔR n_d : Average number density



Power low $g(R) \propto R^{-\alpha}$







r [µm]

20.4

20.6

Run B (R_{λ} =92) and E(R_{λ} =252)









Stronger intermittency in vertical acceleration







 $oldsymbol{ heta}$

Turbulence modulation (spectrum)

Turbulence spectrum

Homogeneous, axially symmetric

$$\begin{split} \frac{1}{2} \left\langle u^2 \right\rangle &= \int_0^\infty \!\!\! E^v(k) \, \mathrm{d}k = \frac{1}{2} \int \left\langle u(k) \cdot u(-k) \right\rangle \, \mathrm{d}k = \frac{1}{2} \int_0^\infty \!\!\! \int_{-1}^1 2\pi k^2 Q^v(k,\mu) \, \mathrm{d}k \, \mathrm{d}\mu, \\ \left\langle \theta^2 \right\rangle &= \int_0^\infty \!\!\! E^\theta(k) \, \mathrm{d}k = \int \left\langle \theta(k) \cdot \theta(-k) \right\rangle \, \mathrm{d}k = \int_0^\infty \!\!\! \int_{-1}^1 2\pi k^2 Q^\theta(k,\mu) \, \mathrm{d}k \, \mathrm{d}\mu, \\ \left\langle q^2 \right\rangle &= \int_0^\infty \!\!\! E^q(k) \, \mathrm{d}k = \int \left\langle q(k) \cdot q(-k) \right\rangle \, \mathrm{d}k = \int_0^\infty \!\!\! \int_{-1}^1 2\pi k^2 Q^q(k,\mu) \, \mathrm{d}k \, \mathrm{d}\mu, \end{split}$$

Expansion in terms of Legendre polynomial

$$Q^lpha(k,\mu) \;=\; \sum_{l=0}^\infty Q^lpha_{2l}(k) P_{2l}(\mu), \qquad \mu = \cos heta$$

$$E^v_{2l}(k,t)=2\pi k^2 Q^v_{2l}(k,t), \quad E^ heta_{2l}(k,t)=2\pi k^2 Q^ heta_{2l}(k,t), \quad E^q_{2l}(k,t)=2\pi k^2 Q^q_{2l}(k,t).$$

Turbulence modulation (spectrum)



 $E_0^v(k,t) \propto k^{-\gamma}, \quad \gamma = 2.92 \pm 0.05 \quad {\rm for} \ \ 200 < k < 350$

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Kinetic energy transfer function

$$R_{\lambda} = 252$$



$$= T_{B\theta}(k,t) + T_{Bq_v}(k,t) + T_{Bq_l}(k,t).$$

Contribution of buoyancy force

 $\mathsf{T}_{\mathsf{B}\theta},\,\mathsf{T}_{\mathsf{B}q},\,\mathsf{T}_{\mathsf{B}\mathsf{I}}\,[\mathsf{cm}^3/\mathsf{s}^3]$



Z.

Spectrum of anisotropic sector

$$\begin{aligned} Q^{\alpha}(k,\mu) &= \sum_{l=0}^{\infty} Q^{\alpha}_{2l}(k) P_{2l}(\mu), \qquad \alpha = v, \ \theta, \ q \qquad \mu = \cos \theta \end{aligned}$$
$$E^{v}_{2l}(k,t) &= 2\pi k^{2} Q^{v}_{2l}(k,t), \quad E^{\theta}_{2l}(k,t) = 2\pi k^{2} Q^{\theta}_{2l}(k,t), \quad E^{q}_{2l}(k,t) = 2\pi k^{2} Q^{q}_{2l}(k,t). \end{aligned}$$



 $|E_l^{lpha}(k,t)| = 2\pi k^2 |Q_l^{lpha}(k,t)| \propto k^{-5/3 - l/3}, \qquad {
m for} \quad l=0,2,4$

Droplet Collision



condensation

~30µm

collision / coalescence

two or many body collision

collision scheme perfect or imperfect coalescence

conservation mass, momentum, energy

DNS

Navier Stokes

$$\nabla \cdot \boldsymbol{u} = 0$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \boldsymbol{u} + \boldsymbol{f}$$

External force

$$\widehat{\boldsymbol{f}}(\boldsymbol{k},t) = \begin{cases} a(t)\widehat{\boldsymbol{u}}(\boldsymbol{k},t) & \text{for } 1 \leq |\boldsymbol{k}| \leq 2 \\ 0 & \text{otherwise} \end{cases} \quad a(t) = \frac{\epsilon}{\sum_{1 \leq |\boldsymbol{k}| \leq 2} < |\boldsymbol{u}(\boldsymbol{k})|^2 > \epsilon}$$

• Particles

$$\frac{d\boldsymbol{x}_j}{dt} = \boldsymbol{v}_j$$
$$\frac{d\boldsymbol{v}_j}{dt} = -\frac{1}{\tau_p} (\boldsymbol{v}_j - \boldsymbol{u}(\boldsymbol{x}_j, t))$$

DNS parameters

Np	: No. of particles	3 × 2 ¹⁸	Φ	: volume fraction	4×10^{-3}
σ	: particle diameter	1.35×10^{-2}	E _{in}	: kinetic energy input	0.5

For St number dependence

R_{λ}	50	80	120		
Ν	64 ³	128 ³	128 ³		
Δt	2.0×10^{-3}	8.0×10^{-4}	5.0×10^{-4}		
ν	1.0×10^{-2}	4.0×10^{-3}	2.0×10^{-3}		
η	0.0376	0.0189	0.0112		
$ au_\eta$	0.141	0.089	0.063		
St	0.04 , 0.1 , 0.4 , 1.0 , 2.0 , 4.0 , 8.0				

$$S_t = \frac{\tau_p}{\tau_\eta}$$

$$N_C = \frac{C}{L_{box}{}^3\Delta t}$$

Turbulence statistics



Shiotsu and Watanabe (2014)

Collision frequency



Droplet collision

Condition

$$r = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2} \le r_i + r_j$$

•Momentum cons. *N*

•Mass cons.

$$M_p \boldsymbol{V}_p = M_i \boldsymbol{V}_i + M_j \boldsymbol{V}_j \longrightarrow \boldsymbol{V}_p = \frac{M_i \boldsymbol{V}_i + M_j \boldsymbol{V}_j}{M_p}$$



 $M_p = M_i + M_j$

Collision

 $r_{p}^{3} = r_{i}^{3} + r_{j}^{3}$



Efficiency : coalescence or separation

Collision of droplets in air by LBM (D3Q15)



Yoshino et al 2014

Collision of droplets in air by LBM (D3Q15)



Yoshino et al 2014



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Collision of stretching separation B = 0.5, We = 79.6

We – B diagram



Development of Fast Time-reversible (FT) method

FT method

Y.Kajima et al., J. Chem. Phys. 136 (2012) 234105.

- Fastest algorithm for molecular dynamics of water molecules of submicron meter
- ${\scriptstyle \odot}$ Time reversal symmetry in translational and angular momentum evolution
- ${\hfill \circ}$ Use of 4 arithmetic operations (+,-,x,/) alone and 1/3 of the conventional computation
- Total energy is well conserved for larger time step width

O(N) code for large scale computation of the water molecules by combined use of FT method and fast multi-pole expansion

O(N) computation of the Coulomb force

O(N)個の遠方微細セルを中心とした多重極係数セットに 関するO(N)の階層的計算:



Quasi-Liquid Layers on Ice Crystal Surfaces

Т

Sazaki et al. (2012)

laser confocal microscopy combined with differential interference contrast microscopy

Skating Thunder Snow flake Freezing of food and organ



図1 氷結晶の六角底面上で生成する2種類の表面液体相。

Large scale MD simulation of submicron ice crystal



Melting of ice crystal at (T_c-1) K

~ 0.08µm

Kajima et al. 2014

displacement

Summary

- Reynolds number effects (no collision) may be small on growth rate of the average particle radius broaden PDF of particle radius
- Average growth of cloud droplets governed by diffusion process is very slow Needs for particle collision process Needs for uniform gradient source of temperature and vapor (updraft)
- Turbulence modulation begins at small scales due to the cloud droplets and the anisotropic modulation is inversely transferred to large scales
- LBM simulation of the cloud droplet collision in air is successful. Detailed data of the collision process will be obtained in the near future.
- MD simulation of the micro ice crystal found that the melting process (two step stage at the temperature near the melting point) is consistent with the experimental observation

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