Water droplets simulation in a warm cloud like ambient

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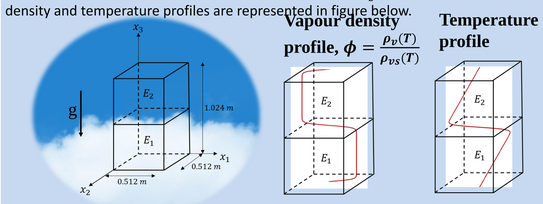
Abstract

Simulations of lukewarm clouds usually assume static and homogeneous conditions on average. However, we are here interested in the unsteady dynamics of the transport through the interface between cloud and the clear air surrounding it. Clouds in fact are fugitive in nature. If one looks for a few seconds, they seem to keep the same form. When looking again, after a minute, one finds that are somewhat changed. Hardly then extended cloud formations can live for more than 2-3 days. Their spatial structure is in-homogenous with continuous changes associated with a large set of coexisting timescales. In our numerical simulation, the cloud interface is modeled through two interacting regions at different turbulent intensity [1]. Different initial conditions reproduce possible local stable or unstable stratification in density and temperature. Currently, our droplet model includes evaporation, condensation, collision and coalescence. The typical water content, associated to an initial condition where drops are 30 microns in diameter, leads to an initial number of drops of 10^{11}in a cloud volume of about 500 cubic meters. A computational grid up to 2048x1024x1024 points is used leads to a Taylor's microscale Reynolds number of 250. The governing equations are NS equations in Boussinesq approximation coupled to equations describing the evolution of water droplets seen as inertial particles, transported by background turbulence and gravity. One aim is the determination of the clustering feature of water droplets inside the shear-less turbulent mixing at the clear air – cloud interface. We compute the distribution of the droplet size and compare the distribution shape with those obtained in a laboratory chamber where turbulent cloud formation is enabled via moist convection [2]. This to deduce information on the possible aerosol/nucleation inputs leading to the local cloud state produced in the simulation.

Introduction

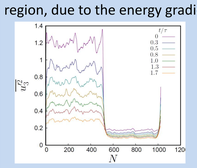
A small portion of the atmosphere in-between a warm cloud and the clear air above, is simulated in a parallelepiped domain. The cloud-clear air interface is modelled as a turbulent shearless mixing in stratified condition. The turbulent shearless mixing is generated by joining two homogeneous and isotropic turbulent field with different turbulent kinetic energy, but with the same integral scale. The initial energy ratio simulated is $\frac{E_1}{E_2} = 6.7$, while the initial water vapour density and temperature profiles are represented in figure below.



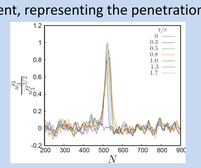
Vapour density profile, $\phi = \frac{\rho_v(T)}{\rho_{vs}(T)}$

Temperature profile

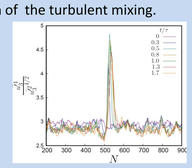
In the figures below the time decay of the mean energy associated with the component u_3 along the x_3 direction is shown together with the normalized third (skewness) and fourth (Kurtosis) single –points moments of the velocity component u_3. Outside the mixing layer the skewness and Kurtosis values agree with a Gaussian distribution (homogeneous and isotropic turbulent fields, $S = 0$ and $K = 3$), while they differ inside the mixing indicating a very large flow intermittency. Furthermore the skewness and Kurtosis maxima move towards the low energy region, due to the energy gradient, representing the penetration of the turbulent mixing.



Energy



skewness



Kurtosis

Two cases are considered: supersaturated case ($Re_\lambda = 43$, $\phi = 1.2$ in cloud region) and saturated case ($Re_\lambda = 53$, $\phi = 1$ in cloud region).

Methods and objectives

1. Introduce nucleation processes into the small-scale direct numerical simulation of local processes
2. study the small-scale local processes in clouds and at the cloud edge
3. check the role of turbulence in nucleation/condensation/collision/coalescence droplet growth processes.

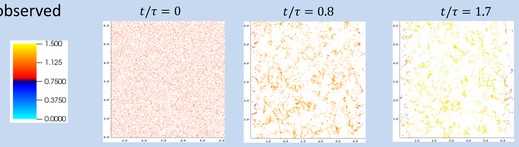
The Navier-Stokes equations in the Boussinesq approximation coupled with the water vapour density advection/diffusion equation are solved by the MPI parallelized DNS code together with the water droplets dynamics equations. Water droplets feedback on the velocity, temperature and water vapour density fields are taken into account.

Concerning the nucleation part, on a lower level, we propose here to introduce a sub-domain feed-back on the direct cloud turbulent fluctuation simulation which is based on the comparison between the size distribution given by classical population balance equation and the distribution deduced from the numerical simulation. In particular, we are thinking to use population balance equations from the nucleation size, about 1nm, to the smallest droplet size we can simulate, about 2.5 μm in radius. The balance equation is parametrized via the initial and boundary conditions which exploit information form laboratory and in-field measurements.

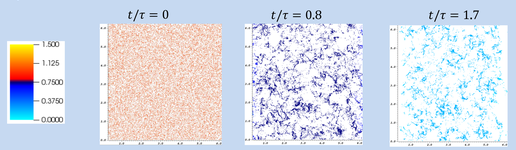
Water droplets dynamics

Water droplets clustering

Preferential drops concentration due to the turbulent transport was observed in both cases. In the supersaturated case an increase in the droplets radius was observed



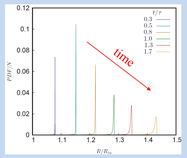
while the opposite trend was observed in the saturated case where a strong drops radius reduction is shown

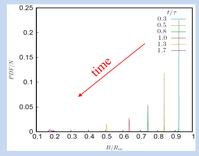


In both case an initial homogeneous and monodisperse droplets distribution is considered with an intial radius of 2.5 μm.

Water droplets size distribution

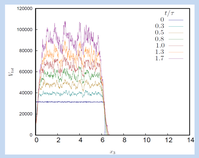
The figures representing the droplets size distribution for the supersaturated case (left panel) and for the saturated case (right panel) show a slight broadening of the drops radius distribution.

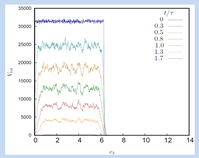




Total liquid water volume distribution

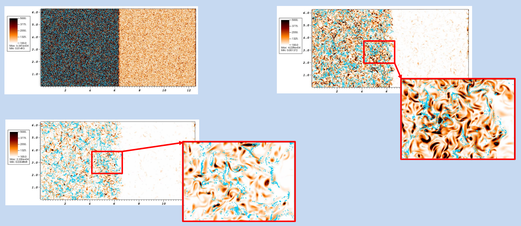
The strong evaporation observed in the saturated case (right panel) shows an almost complete dissolution of the cloud. The figure on the left panel shows instead an important water vapour condensation which increases the liquid water content





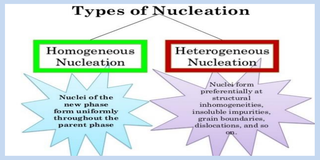
Enstrophy and water droplets concentration

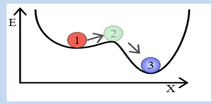
It has been observed that the due to their iniertia, the water particles move towards regions with lower enstrophy.



Nucleation and Growth

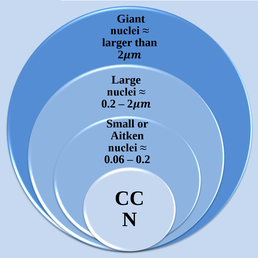
- **What is the nucleation :** Nucleation is the onset of a first-order phase transition by which a metastable phase transforms into a more stable one. Such a phase transition occurs when an initial system initially in equilibrium is destabilized by the change of an external parameter like the temperature or the pressure. If the perturbation is small enough, the system does not become unstable but rather stays metastable. In diffusive transformations, the system then evolves through the nucleation, the growth and the coarsening of a second phase. Such a phase transformation is found in a lot of situations in materials science like condensation of liquid droplets from a supersaturated vapor, precipitation from a supersaturated solid solution.
- **Types of nucleation:**





- **Cloud condensation nuclei(CCN)**

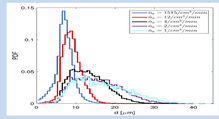
Aerosol particles which are capable of initiating drop formation at the weak super-saturation observed in the atmosphere are called cloud condensation nuclei, CCN. These have been subdivided into three classes of the diameter range, from about 0.06 μm to 2 μm.



Clustering does not mean that water droplets grow very much even if collision-coalescence is strongly enhanced. it has been recently observed in the laboratory [11] that a high particle concentration narrows the drops size distribution spect

In our simulation:

- $N_{collision} = 682$ supersaturated case
- $N_{collision} = 30$ saturated case



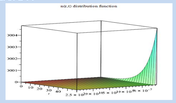
- **population balance equation models**

Model which contains nucleation and the growth of a single particle.(based on Population balance equation PBE) which Considering 3 types of PBE:

1. $\frac{\partial n}{\partial t} + G\frac{\partial n}{\partial r} = 0$ G is constant, no aggregation no nucleation

IC: t=0 , n(r, 0) =$e^{\lambda(-2.27.10^9 r)}$

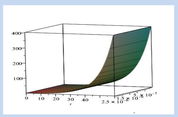
BC: r=10^{-9}m, n(10^{-9}, t) =$e^{\lambda(t-2.27.10^9)}$



2. $\frac{\partial n}{\partial t} + \frac{\partial (G.n)}{\partial r} = 0$ G is not constant, no aggregation no nucleation

IC: t=0 , n(r, 0) =$e^{\lambda(-2.27.10^9 r)}$

BC: r=10^{-9}m, n(10^{-9}, t) =$e^{\lambda(t-2.27.10^9)}$



3. $\frac{\partial n}{\partial t} + G\frac{\partial n}{\partial r} = S(r,t)$ G is constant, no aggregation

Exponential nucleation. **Nucleation source= S(r, t)**

Our aim is to achieve a local dynamical adjusting of the water particle density by killing or breeding water droplets from the simulation threshold size 2.5 μm up to the maximum droplet size reached in the evolving simulation. The sub-domain volume sought for the feedback is one order of magnitude smaller along each linear dimension than the entire domain of the simulation.

Sub-domain

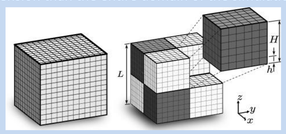
HP: every sub-domain divided by 100 points.

$10*10*10=10^6$ points in each sub domain.

2048/100=20.48 sub-domain we have in each direction.

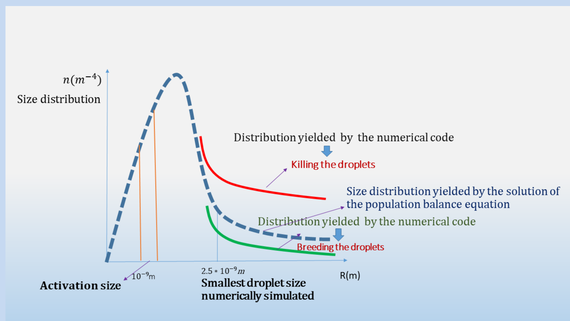
$2*20.48^3=1.7*10^6$

at each time step we will have $1.7*10^6$ G_0



The growth rate is constant in one sub-domain but it will be vary when the droplets shift to other sub-domain.by using FVS for every sub-domain we can obtain the size distribution which is yielded by population balance equation model.

- **Idea for a possible sub-domain feedback from population balance equation models**



If the size distribution which is given by code is laying above than the size distribution which is given by the population model we have a too high concentration, in this case we may consider appropriate to suppress (kill) the droplets in ***surplus***.

Instead if the size distribution which is given by the numerical simulation is laying below than the one which is given by population model we have a too low concentration, so we can consider proper to breed an amount of the droplets compensating the ***deficit***.

Results and conclusion

- In realtively short transients (1 ~2 time scales) where at the initial instant small monodisperse droplets are simulated, the droplets grow/decay mainly by water vapour diffusion:
  - ➢Droplets quickly grow in the supersaturated case
  - ➢Droplets quickly evaporate in the saturated case
- Entrainment of sub-saturated air through the cloud-clear air interface enhance the droplets evaporation
- Significant clustering is observed in both cases, but the collision-coalescence contribution to the droplets growth is negligible unless the long term is reached.
- A slight broadening of the droplets size distribution is observed and the mean droplets radius
  - ➢ Increases in time in the supersaturated case
  - ➢ Decreases in time in the saturated case
- Water droplets concentrate in the low enstrophy regions (low vorticity intensity)

References

[1] D. Tordella and M. Iovieno, Physical Review Letters, 107, 194501 (2011)
[2] K. K. Chandrakar,mW Cantrell, PNAS, Vol 113, n 50, 10.1073 (2016)
[3] S. Ghan et al, JAMES, Vol 3, M10001 (2014)
[4] V. Ruggiero, D. Codoni and D.Tordella, PRACE, white paper, Type C project 2010PA3699 (2018)
[5] J. Curtius et al, The European Physical Journal Conferences, 10.1140 (2009)
[6] B. Kumar and J. Schumacher and R. Shaw, Theory Compute Fluid Dynamic, 10.1007 (2012)
[7] Sh. Qamar and G. Warnecke, Computer and Chemical Engineering, 10.1016 (2007)
[8] B. Kumar and J. Ramkrishna and R. Shaw, Chemical Engineering Science, 4659-4679, (1997)
[9] J. Devenish et al, RMetS, 101002 (2012)
[10] Y. Yin et al. Atmospheric Researcher 53 (2000)
[11] T. Gotoh et al, New Journal Physics. 18, 043042 (2016)
[12] E. Clouet, ASM Handbook, Fundamentals of Modeling for Metals Processing, Vol 22A, pp.203-219 (2009)