Coalescing Droplets in homogeneous isotropic turbulence

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Abstract: This test case concerns the numerical simulation of coalescing droplets suspended in homogeneous isotropic turbulence. The turbulence is predicted by Direct Numerical Simulation (DNS). A forcing scheme is used in order to get statistically steady turbulence. Discrete Particle Simulation (DPS) is coupled with DNS. In DPS, the droplet trajectories are predicted by solving the momentum equation of each droplet by considering that only the drag and gravity act on the droplets. The droplet coalescence is taken into account with a deterministic collision detection algorithm. For the sake of simplicity a pure coalescence regime is considered meaning that the collision of two droplet leads to coalescence only. Several material properties are considered for checking the effect of the turbulence on the coalescence rate.

1 Description

1.1 Fluid flow prediction

The turbulence is predicted by Direct Numerical Simulation of incompressible Navier-Stokes equations:

$$\frac{\partial u_{f,i}}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial u_{f,i}}{\partial t} + u_{f,j}\frac{\partial u_{f,i}}{\partial x_j} = -\frac{1}{\rho_f}\frac{\partial P}{\partial x_i} + \nu_f \frac{\partial^2 u_{f,i}}{\partial x_j \partial x_j} \tag{2}$$

where $u_{f,i}$ is the instantaneous fluid velocity, P the pressure, ρ_f the fluid density and ν_f the kinematic viscosity. The Navier-Stokes equations are discretized using a finite-volume method on a staggered mesh with a second-order centered scheme. The solution is time-advanced using a second order Runge & Kutta scheme and the Poisson equation is solved with a spectral method. The computational domain is a cubic box of length $L_b = 0.128\ m$ with periodic boundary conditions (see Figure 1). Statistically steady turbulence is obtained with a stochastic spectral forcing proposed by [5].

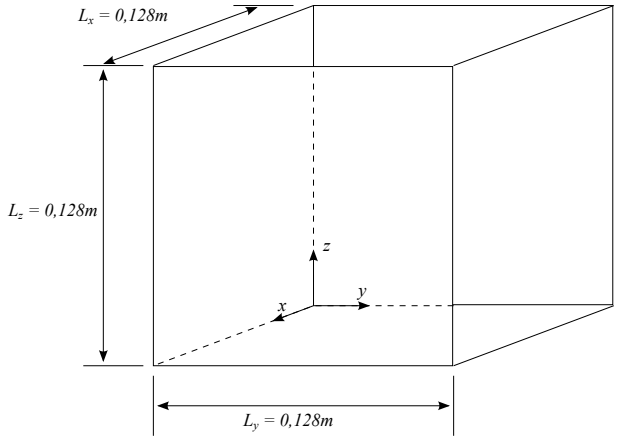

Figure 1: Computational domain.

1.2 Droplet paths

This study is restricted to dispersed phase composed of N_p spherical droplets. According to a large droplet to fluid density ratio, the forces acting on the droplets are only the drag force (the gravity is not taken into account). Then the set of equations for a single droplet write:

$$\frac{dx_{p,i}}{dt} = u_{p,i}, \tag{3}$$

$$\frac{du_{p,i}}{dt} = -\frac{u_{p,i} - u_{f@p,i}}{\tau_p} \tag{4}$$

where $\mathbf{x}_p$ and $\mathbf{u}_p$ are the droplet mass center position and velocity. The droplet response time, τ_p, is given as

$$\tau_p = \frac{\rho_p}{\rho_f}\frac{4}{3}\frac{d_p}{C_d}\frac{1}{|\mathbf{u}_p - \mathbf{u}_{f@p}|}, \tag{5}$$

where $\mathbf{u}_{f@p}(t) = \mathbf{u}_f(t, \mathbf{x}_p)$ is the fluid velocity at the droplet position (locally undisturbed by the particle) also called the fluid velocity seen by the droplet. As the two-way coupling is not taken into account, the undisturbed fluid velocity is the one given by the DNS and evaluated at the droplet position by an interpolation scheme. The drag coefficient, C_d, is given by Schiller & Nauman correlation

$$C_d = \frac{24}{Re_p}\left[1 + 0.15Re_p^{0.687}\right], \tag{6}$$

where the droplet Reynolds number is

$$Re_p = \frac{d_p|\mathbf{u}_p - \mathbf{u}_{f@p}|}{\nu_f}. \tag{7}$$

In (4) is the i^{th} component of the gravity.

1.3 Coalescence

The collision detection algorithm has been detailed in [4]. The algorithm has been validated by comparison with theoretical relation has described by [1]. Here only pure coalescence regime is

taken into account. Then the mass and momentum conservation equations for two undergoing droplets are written as

$$m^* = m_p + m_q \tag{8}$$
$$m^*\mathbf{u}_p^* = m_p\mathbf{u}_p + m_q\mathbf{u}_q \tag{9}$$

where m_p, m_q are the mass of the droplets before coalescence and m^* after. The new diameter is deductible from the mass conservation as the droplet density is constant. The position of the new droplet is given by

$$\mathbf{x}^* = \frac{d_p^{*3}\mathbf{x}_p + d_q^{*3}\mathbf{x}_q}{d^{*3}}\,. \tag{10}$$

2 Test case parameters

2.1 Run organization

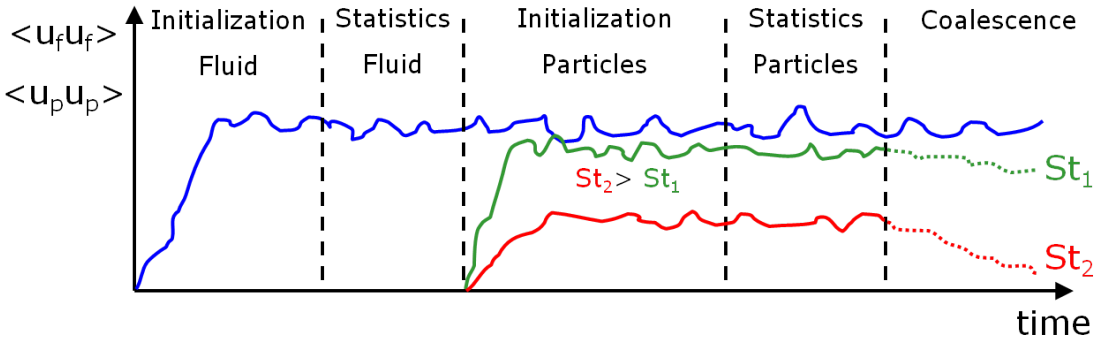

Figure 2: Run organization.

First the steady state of the turbulence is reached. Basically 6-8 times the eddy-turnover timescale are required. Second statistics on fluid phase are gathered. In a third step, the droplets are introduced in the domain with a velocity equal to the fluid velocity at the droplet position. All droplets have the same diameter and the **collision** are taken into account. We emphasized that it is collision (elastic collisions) and not coalescence. After 4-5 droplet response time the droplets reach a steady state corresponding to the Tchen-Hinze theory. The particle statistics are then computed in order to well define the dispersed phase before coalescence. Then the coalescence is activated and time-evolving statistics are computed.

2.2 Parameters and statistics on the turbulence

The Table 1 gives the parameters of the DNS.

The statistics measured for the turbulent fluid flow fields are given in Table 2. The turbulent Reynolds numbers are computed with

$$Re_{L_f} = \frac{L_f\sqrt{2/3q_f^2}}{\nu_f} \quad \text{and} \quad Re_\lambda = \frac{\lambda_g\sqrt{2/3q_f^2}}{\nu_f} \tag{11}$$

A good resolution of the small scales of turbulence is achieved as can be read from the values of $\kappa_{max}\cdot\eta_K$ in Table 2.

Table 1: Simulation parameters for DNS.

Quantity	**Symbol**	**Unit**	**A**	**B**	**C**
Box length	L_b	m	0.128	0.128	0.128
Grid points	N_{grid}	1	80^3	128^3	256^3
Min. resolved wave number	κ_0	$1/m$	49.1	49.1	49.1
Max. resolved wave number	κ_{max}	$1/m$	1914.4	3092.5	6234.0
Fluid density	ρ_f	kg/m^3	1.17	1.17	1.17
Kinematic viscosity	ν_f	m^2/s	$1.47 \cdot 10^{-5}$	$1.47 \cdot 10^{-5}$	$1.47 \cdot 10^{-5}$

Table 2: Turbulent fluid flow statistics.

Quantity	**Symbol**	**Unit**	**A**	**B**	**C**
Box length	L_b	m	0.128	0.128	0.128
Reynolds number integr. scale	Re_{L_f}	–	26.4	61.2	144.3
Reynolds number Taylor scale	Re_λ	–	18.1	32.9	60.5
Integral longit. length scale	L_f/L_b	–	0.0980	0.1056	0.0852
Integral transv. length scale	L_g/L_b	–	0.0511	0.0491	0.0426
Taylor longit. length scale	λ_f/L_b	–	0.0941	0.0805	0.0507
Taylor transv. length scale	λ_g/L_b	–	0.0674	0.0568	0.0357
Kolmogorov length scale	η_K/L_b	–	0.0081	0.0051	0.0023
	$\kappa_{max} \cdot \eta_K$	–	1.98	2.00	1.86
Lagrangian integ. time scale	τ_f^t/T_e	–	0.837	0.704	0.643
Eddy turn over time	T_e	s	0.405	0.203	0.056
Fluid kinetic energy	q_f^2	m^2/s^2	0.0015	0.0067	0.0567
Energy dissipation	ϵ_f	m^2/s^3	0.0028	0.0181	0.3995

2.3 Parameters on the droplets

After the fluid flow reached the state of a homogeneous isotropic turbulence, the droplet phase is added to the system. In the the third step of the fluid-droplet flow field initialization, the droplets may collide, but do not coalesce. Five different droplet classes are defined, such that the Stokes number $St = \frac{\tau_{fp}^F}{\tau_{f@p}^t}$ for each droplet case is the same in the three above introduced flow fields. The droplet fields are parameterized by changing the droplet density ρ_p only. Thus, it is possible to keep parameters such as the droplet number N_p, initial droplet diameter $d_{p,ini}$, droplet volume fraction α_p constant and at the same time vary the Stokes number St constant. Tables 5 to 3 show the statistics of the all the initially monodisperse droplet phases realized.

3 Available data

3.1 Statistics

For the analysis, we introduce τ_{fp}^F the mean particle response time defined as

$$\frac{1}{\tau_{fp}^F} = \left\langle \frac{1}{\tau_p} \right\rangle \tag{12}$$

Table 3: Properties of initially monodisperse for $Re_\lambda = 18.1$.

Symbol	**A1**	**A2**	**A3**	**A4**	**A5**
N_p			100000		
α_p			$8.311\ 10^{-5}$		
$d_{p,ini}$			$1.493\ 10^{-4}$		
ρ_p	500	2000	5000	10000	15000
q_p^2/q_f^2	0.999	0.757	0.529	0.361	0.277
τ_{fp}^F	$3.506\ 10^{-2}$	$1.369\ 10^{-1}$	$3.370\ 10^{-1}$	$6.681\ 10^{-1}$	$9.984\ 10^{-1}$
Re_p	0.086	0.223	0.331	0.380	0.427
$\tau_{f@p}^t$	$3.738\ 10^{-1}$	$4.135\ 10^{-1}$	$3.737\ 10^{-1}$	$3.573\ 10^{-1}$	$3.757\ 10^{-1}$
$St = \frac{\tau_{fp}^F}{\tau_{f@p}^t}$	0.09	0.33	0.90	1.87	2.66
$St_K = \frac{\tau_{fp}^F}{\tau_K}$	0.48	1.88	4.62	9.17	13.70

Table 4: Properties of initially monodisperse for $Re_\lambda = 32.9$.

Symbol	**B1**	**B2**	**B3**	**B4**	**B5**
N_p			100000		
α_p			$8.311\ 10^{-5}$		
$d_{p,ini}$			$1.493\ 10^{-4}$		
ρ_p	226.3	905	2263	4526	6790
q_p^2/q_f^2	1.006	0.764	0.535	0.402	0.310
τ_{fp}^F	$1.563\ 10^{-2}$	$6.022\ 10^{-2}$	$1.469\ 10^{-1}$	$2.889\ 10^{-1}$	$4.305\ 10^{-1}$
Re_p	0.168	0.438	0.657	0.825	0.892
$\tau_{f@p}^t$	$1.639\ 10^{-1}$	$1.664\ 10^{-1}$	$1.545\ 10^{-1}$	$1.752\ 10^{-1}$	$1.792\ 10^{-1}$
$St = \frac{\tau_{fp}^F}{\tau_{f@p}^t}$	0.10	0.36	0.95	1.65	2.43
$St_K = \frac{\tau_{fp}^F}{\tau_K}$	0.55	2.11	5.15	10.13	15.09

Table 5: Properties of initially monodisperse for $Re_\lambda = 60.5$.

Symbol	**C1**	**C2**	**C3**	**C4**	**C5**
N_p			100000		
α_p			$8.311\ 10^{-5}$		
$d_{p,ini}$			$1.493\ 10^{-4}$		
ρ_p	68	272	680	1360	2040
q_p^2/q_f^2	1.010	0.770	0.560	0.380	0.298
τ_{fp}^F	$4.465\ 10^{-3}$	$1.659\ 10^{-2}$	$3.956\ 10^{-2}$	$7.730\ 10^{-2}$	$1.146\ 10^{-1}$
Re_p	0.55	1.37	2.03	2.40	2.59
$\tau_{f@p}^t$	$5.200\ 10^{-2}$	$5.267\ 10^{-2}$	$4.710\ 10^{-2}$	$4.728\ 10^{-2}$	$4.712\ 10^{-2}$
$St = \frac{\tau_{fp}^F}{\tau_{f@p}^t}$	0.11	0.42	1.06	1.63	2.43
$St_K = \frac{\tau_{fp}^F}{\tau_K}$	0.73	2.72	6.49	12.67	18.79

with $\langle\ .\ \rangle$ the particle ensemble average operator. The turbulent Stokes number is defined as

$$St = \frac{\tau_{fp}^F}{\tau_{f@p}^t} \tag{13}$$

where $\tau_{f@p}^t$ is the Lagrangian fluid integral timescale measured along particle trajectories. This fluid-particle interaction timescale is obtained with

$$\tau_{f@p}^t = \int_0^{+\infty} R_{f@p}(\tau) d\tau \tag{14}$$

where the Lagrangian fluid velocity correlation function is

$$R_{f@p}(\tau) = \frac{\langle u_{f@p,i}(t_0) u_{f@p,i}(t_0+\tau)\rangle}{2q_{f@p}^2} \tag{15}$$

with $q_{f@p}^2 = 1/2\left\langle u'_{f@p,i} u'_{f@p,i}\right\rangle$ is the fluid kinetic energy seen by the particles.

4 List of data

From DNS and DPS several statistics have been extracted. As for example:

- Droplet number
- Mean droplet diameter and Sauter diameter: $\langle d_p^3\rangle/\langle d_p^2\rangle$
- Droplet agitation

References

[1] D. Wünsch, P. Fede, O. Simonin. Validation procedure for Discrete Particle Simulation of turbulent two-phase flows with droplet coalescence. In *ERCOFTAC Bulletin 82*, 2010.

[2] D. Wünsch, P. Fede, O. Simonin, P. Villedieu. Numerical Simulation and Statistical Modelling of Inertial Droplet Coalescence in Homogeneous Isotropic Turbulence. *Notes on Numerical Fluid Mechanics and Multidisciplinary Design*, 2009.

[3] D. Wünsch, P. Fede, O. Simonin. DNS/DPS of Inertial Droplet Coalescence in Homogeneous Isotropic Turbulence and Comparison with PDF Model Predictions using the Direct Quadrature Method of Moments. In Proc. *2009 ASME Fluids Engineering Conference, FEDSM2009-78091*, 2009.

[4] D. Wünsch, P. Fede, O. Simonin. Development and Validation of a binary collisions detection algorithm for a poly-dispersed particle mixture. In Proc. *2008 ASME Fluids Engineering Conference, FEDSM2008-55159*, 2008.

[5] V. Eswaran, S. Pope. An Examination of Forcing in Direct Numerical Simulations of Turbulence *Computers & Fluids*, 1988, 16, 257-278.