DYNAMICS AND DISPERSION IN 3D UNSTEADY EULERIAN-EULERIAN SIMULATIONS OF TWO-PHASE FLOWS

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Abstract

Particle-laden flows are of great interest since they occur in a variety of industrial applications, such as chemical reactors or internal combustion engines in which either solid or liquid particles are injected in a gas flow. These two-phase flows are characterized by a high level of dynamic coupling, heat and mass transfer between the phases. Other complex phenomena of these flows are linked to the size of the particles, depending on the formation process, heterogeneous chemical reactions, coalescence and break-up.
Commonly used Lagrangian particle tracking techniques are able to handle most of these complex physical processes. However they are also known to be numerically expensive, as they require a high particle number density to reach a minimum level of accuracy. For unsteady simulations of practical applications of turbulent industrial flows in complex geometries, Lagrangian methods can not be efficiently used today.
As an alternative a three dimensional unsteady Eulerian-Eulerian approach is proposed to simulate dispersed two-phase flows. In this approach the dispersed phase is treated as the continuous gas phase, through an averaging operator that leads to a system of conservation equations very similar to the ones for the gas. The main advantage is therefore that the gas phase algorithm may be used on the dispersed phase with the same numerical accuracy and computational efficiency. However this averaging operation introduces unclosed terms [15] in the equations that need to be modeled. These terms are the nonlinear term in the transport operator and other terms related to the unresolved part of the particle velocities.
The Eulerian-Eulerian approach has already been successfully applied to Reynolds-Averaged Simulation (RANS) of turbulent flows. The objective of the present work is to extend this approach to unsteady three dimensional simulations of complex flows. Long term objective is to extend this method to an approach comparable to Large Eddy Simulation (LES) as being used in aerodynamics or recently in reactive flows. LES has become a

very attractive tool and has proven to be very efficient on inert turbulent flows. Its use for reactive flows is quite recent and its extension to two phase flow needs specific developments.
In the present paper a model for the unclosed non-linear terms of the dispersed phase equations is proposed. This term has a direct impact on the particles transport and concentration and is crucial in order to capture dynamics and dispersion. It controls the segregation effects, that in turn control many other physical processes like mass and heat transfer or particle-particle interactions.
The proposed model is based on an additional stress term in the dispersed phase momentum equation, as described in the first section of the paper. Two different approaches to calculate this stress term may be used. One is tested in the case of homogeneous isotropic decaying turbulence, computed in a quasi Direct Numerical Simulation (DNS) mode, and compared to an Eulerian-Lagrangian (DNS) reference solution. In this case it is possible to derive analytical relations for several integral quantities that are very usefull to cross-check the Eulerian and Lagrangian approaches.

1 The Eulerian model

Eulerian equations for the dispersed phase may be derived by several means. A popular simple way consists of volume filtering of the the separate, local, instantaneous phase equations accounting for the inter-facial jump conditions [3]. Such an averaging approach is very restrictive, because particle sizes and particle distances have to be smaller than the smallest length scale of the turbulence.

A different, not totally equivalent way is the statistical approach in the framework of kinetic theory. In analogy to the derivation of the Navier-Stokes equations by non-equilibrium statistics [1], a point probability density function (pdf) $f_p^{(1)}(\mathbf{c}_p; \mathbf{x}_p, t)$ may be defined. This gives the local instantaneous probable number of particles with the given translation velocity $\mathbf{u}_p = \mathbf{c}_p$. This function obeys a Boltzmann-type kinetic equation, which accounts for momentum exchange with the carrier fluid and for the influence of external forces such as gravity and inter-particle collisions. Reynolds-averaged transport equations of the first moments (such as particle concentration, mean velocity and particle kinetic stress) may be derived directly by averaging from the pdf kinetic equation [13].

For the sake of simplicity in this feasibility study, interaction forces are limited to drag, considering non-evaporating particles in absence of gravity. The extension to evaporating flows, gravity force, turbulence corrections in the drag force and other interaction forces is not in conflict with the presented derivation of the Eulerian field equations. In the presented approach the gas is presumed undisturbed by the dispersed phase. Therefore passage from one-way to two-way coupling is more delicate.

1.1 Conservation Equations for particle properties

To derive local instantaneous Eulerian equations in dilute flows (without turbulence modification by the particles), Février et al. [5], [6], [15] propose to use an averaging over all dispersed-phase realizations conditioned by one carrier-phase realization. Such an averaging procedure leads to a conditional velocity pdf for the dispersed phase,

$$\tilde{f}_p^{(1)}\left(\mathbf{c}_p; \mathbf{x}, t, H_f\right) = \left\langle W_p^{(1)}\left(\mathbf{c}_p; \mathbf{x}, t\right) | H_f \right\rangle . \tag{1}$$

$W_p^{(1)}$ are the realizations of position and velocity in time of any given particle [11] and H_f is the unique carrier flow realization. With this definition one may define a local instanta-

neous particulate velocity field, which is here named "mesoscopic Eulerian particle velocity field". This field is obtained by averaging the conditioned velocity pdf over all particle-flow realizations.

$$\tilde{u}_p\left(\mathbf{x},t,H_f\right)=\frac{1}{\tilde{n}_p}\int \mathbf{c}_p\tilde{f}_p^{(1)}\left(\mathbf{c}_p;\mathbf{x},t,H_f\right)d\mathbf{c}_p. \tag{2}$$

Here

$$\tilde{n}_p=\int \tilde{f}_p^{(1)}\left(\mathbf{c}_p;\mathbf{x},t,H_f\right)d\mathbf{c}_p \tag{3}$$

is the "mesoscopic" particle-number density and

$$\langle\tilde{\Phi}\rangle_p=\frac{1}{\tilde{n}_p^{(1)}}\int \tilde{f}_p^{(1)}\Phi d\mathbf{c}_p \tag{4}$$

stands for any ensemble averaged quantity.
For simplicity, the dependence of the above variables on H_f is not shown explicitly. Application of the conditional-averaging procedure to the kinetic equation governing the particle pdf leads directly to the transport equations for the first moments of number density and mesoscopic Eulerian velocity,

$$\frac{\partial}{\partial t}\tilde{n}_p+\frac{\partial}{\partial x_i}\tilde{n}_p\tilde{u}_{p,i}=0 \tag{5}$$

$$\tilde{n}_p\frac{\partial}{\partial t}\tilde{u}_{p,i}+\tilde{n}_p\tilde{u}_{p,j}\frac{\partial}{\partial x_j}\tilde{u}_{p,i}=-\frac{\tilde{n}_p}{\tau_p}\left[\tilde{u}_{p,i}-u_i\right]-\frac{\partial}{\partial x_j}\tilde{n}_p\delta\tilde{\sigma}_{p,ij} \tag{6}$$

Here $\delta\tilde{\sigma}_{p,ij}$ is the mesoscopic kinetic stress tensor of the particle Quasi-Brownian velocity distribution discussed in section 1.2. One of the current objectives is to show that this term is non-negligible for inertial particles in turbulent flow. Due to the very small droplet Reynolds number value measured in the simulation, the particle relaxation time τ_p is defined as the relaxation time for Stokes drag.

$$\tau_p=\frac{\rho_p d^2}{18\mu} \tag{7}$$

1.2 The stress tensor of Quasi-Brownian Motion (QBM)

The stress term in eq. 6 arises from an ensemble average of the nonlinear term in the transport equation for particle momentum,

$$\begin{aligned}\tilde{n}_p\delta\tilde{\sigma}_{p,ij} &= \int\left(c_{p,i}-\tilde{u}_{p,i}\right)\left(c_{p,j}-\tilde{u}_{p,j}\right)\tilde{f}_p^{(1)}\left(\mathbf{c}_p;\mathbf{x},t,H_f\right)d\mathbf{c}_p &(8)\\ &= \tilde{n}_p\langle\delta u_{p,i}\delta u_{p,j}\rangle_p. &(9)\end{aligned}$$

When the Euler or Navier-Stokes equations are derived from kinetic gas theory the trace of $\langle\delta u_{p,i}\delta u_{p,j}\rangle_p$ is interpreted as temperature (ignoring the Boltzmann constant and molecular mass) and related to pressure by an equation of state. In the case of the Euler or Navier-Stokes equations temperature is defined as the uncorrelated part of the kinetic energy. Here the uncorrelated part of the particulate kinetic energy is defined as

$$\delta\tilde{\theta}_p=\frac{1}{2}\langle\delta u_{p,i}\delta u_{p,i}\rangle_p. \tag{10}$$

In analogy to the Euler or Navier-Stokes equations a Quasi-Brownian Pressure (QBP) may be defined by the product of uncorrelated kinetic energy and particle number density, as

$$\tilde{P}_{QB}=\tilde{n}_p\frac{2}{3}\delta\tilde{\theta}_p \tag{11}$$

When the particle number distribution becomes nonuniform, as in the case of a compressible gas, this pressure term tends to homogenize particle number density.

The non-diagonal elements of the stress tensor can be identified, in analogy to the Navier-Stokes equations, as a viscous terms due to shear. The diagonal part of the stress tensor is then proportional to one third of the trace of the tensor and an eventual deviation such that ($\tilde{n}_p \delta\tilde{\sigma}_{p,ij} = P_{QB}\delta_{ij} - \delta\tilde{\tau}_{p,ij}$). The momentum-transport equation (6) becomes

$$\tilde{n}_p \frac{\partial}{\partial t}\tilde{u}_{p,i} + \tilde{n}_p \tilde{u}_{p,j}\frac{\partial}{\partial x_j}\tilde{u}_{p,i} = -\frac{\tilde{n}_p}{\tau_p}\left[\tilde{u}_{p,i} - \tilde{u}_{f,i}\right] - \frac{\partial}{\partial x_i}\tilde{P}_{QB} + \frac{\partial}{\partial x_j}\delta\tilde{\tau}_{p,ij} \tag{12}$$

In analogy to the derivation of the Navier-Stokes equations from kinetic gas theory the stress term can be related to the gradients of the first moments based on the Onsager relations [7]. Making some assumptions on symmetry and isotropy the stress term can be modeled as detailed below:

$$\tilde{n}_p\langle\delta u_{p,j}\delta u_{p,i}\rangle_p = P_{QB}\delta_{ij} - \xi_{QB}\frac{\partial\tilde{u}_{p,k}}{\partial x_k}\delta_{ij} - \mu_{QB}\left(\frac{\partial\tilde{u}_{p,i}}{\partial x_j} + \frac{\partial\tilde{u}_{p,j}}{\partial x_i} - \frac{2}{3}\frac{\partial\tilde{u}_{p,k}}{\partial x_k}\delta_{ij}\right) \tag{13}$$

The dynamic viscosity related to Quasi Brownian Motion can be estimated by $\mu_{QB} = 1/3\tilde{n}_p\tau_p\delta\tilde{\theta}_p$ [15] where τ_p is the relaxation time related to Stokes drag. This expression can be obtained using the transport equation for the complete stresses $\langle\delta u_{p,i}\delta u_{p,j}\rangle$ and supposing isotropic behavior in shear flow [1]. In incompressible flow it is common use to ignore the volume viscosity and to use the Stokes relation. In the present simulations the volume viscosity has been retained following the approach of Truesdell of a "Stokesian" fluid [17] in which the volume viscosity is function of the divergence itself. Since compressibility effects increase with the Stokes number the volume viscosity is modeled heuristically as $\xi_{QB} = \tilde{n}_p B\tau_p\left|\partial\tilde{u}_{p,k}/\partial x_k\right|$. Here B is a constant with the units of an ordinary viscosity. In the present simulation it was chosen as five times the gaseous viscosity ($B = 6\nu$). The present model requires the knowledge of $\delta\tilde{\theta}_p$ which is developed in the next section.

1.3 The equation for quasi brownian energy (QBE)

To calculate the QBE, two approaches are presented; the first one assumes a quasi isentropic behavior of the dispersed phase leading to an algebraic expression for $\delta\tilde{\theta}_p$.

$$\delta\tilde{\theta}_p = A\tilde{n}_p^{2/3} \tag{14}$$

A is the residual mean kinetic energy of the particles averaged over the computational domain pondered by moments of the particle distribution. In order to define A it is necessary to introduce some definitions. Spatial averages (over the computational domain) are defined by $\langle\phi\rangle_V = 1/V\int_V \phi dV$. Particle pondered averages are defined by $\langle\phi\rangle_p = \langle\tilde{n}_p\phi\rangle_V/\langle\tilde{n}_p\rangle_V$. This allows to define $A = \langle\tilde{n}_p\rangle_V\delta q_p^2/\langle\tilde{n}_p^{5/3}\rangle_V$. The mean residual particle kinetic energy is defined as $\delta q_p^2 = \langle\delta\tilde{\theta}_p\rangle_p$. The expression in eq. 14 relates therefore the local residual particle kinetic energy to the mean residual particle kinetic energy. It can be obtained using the conservation equation for number density (eq. 5) and the lowest order conservation equation for quasi brownian energy (QBE) in the Chapman-Enskog expansion [1]:

$$\frac{\partial}{\partial t}\tilde{n}_p\delta\tilde{\theta}_p + \frac{\partial}{\partial x_j}\tilde{n}_p\tilde{u}_{p,j}\delta\tilde{\theta}_p = -\frac{2}{3}\tilde{n}_p\delta\tilde{\theta}_p\frac{\partial\tilde{u}_{p,j}}{\partial x_j} \tag{15}$$

It is then sufficient to multiply eq. 5 by $-\frac{2}{3}\tilde{n}_p^{-5/3}\delta\tilde{\theta}_p$ and to add the resulting expression to eq. 15 times $\tilde{n}_p^{-2/3}$ to achieve a transport equation for $\tilde{n}_p^{-2/3}\delta\tilde{\theta}_p$ with a zero right hand side. Lagrangian simulations performed by P. Février [6] in stationary homogeneous isotropic turbulence suggest that the mean residual kinetic energy δq_p^2 depends on the resolved dispersed phase kinetic energy $\tilde{q}_p^2 = 1/2\langle\tilde{u}_{p,k}\tilde{u}_{p,k}\rangle_p$, the fluid-particle correlation $q_{fp} = \langle\tilde{u}_{p,k}u_k\rangle_p$ where u_k is the carrier phase velocity, and the carrier phase kinetic energy pondered by the particle presence $q_{f@p}^2 = 1/2\langle u_k u_k\rangle_p$. This expression is given by

$$\delta q_p^2 = \tilde{q}_p^2\left(1 - \frac{\left(q_{fp}^2\right)^2}{4\tilde{q}_p^2 q_{f@p}^2}\right) \tag{16}$$

The second approach uses the full transport equation for quasi brownian energy [15]

$$\begin{aligned}\frac{\partial}{\partial t}\tilde{n}_p\delta\tilde{\theta}_p + \frac{\partial}{\partial x_j}\tilde{n}_p\tilde{u}_{p,j}\delta\tilde{\theta}_p = &-2\frac{\tilde{n}_p}{\tau_p}\delta\tilde{\theta}_p \\ - &\left[P_{QB}\delta_{ij} - \xi_{QB}\frac{\partial\tilde{u}_{p,k}}{\partial x_k}\delta_{ij} - \mu_{QB}\left(\frac{\partial\tilde{u}_{p,i}}{\partial x_j} + \frac{\partial\tilde{u}_{p,j}}{\partial x_i} - \frac{2}{3}\frac{\partial\tilde{u}_{p,k}}{\partial x_k}\delta_{ij}\right)\right]\frac{\partial\tilde{u}_{p,i}}{\partial x_j} \\ + &\frac{\partial}{\partial x_j}\left[k_{QB}\frac{\partial}{\partial x_j}\delta\tilde{\theta}_p\right]\end{aligned} \tag{17}$$

in which the third order correlation is modeled as a diffusive flux like thermal diffusion in the Navier-Stokes equations. The diffusivity constant for quasi brownian energy is estimated by $k_{QB} = 5/3\tilde{n}_p\tau_p\delta\tilde{\theta}_p$. This is the equivalent of the Fick's law for the heat flux in the Navier-Stokes equations.

2 Numerical implementation

The Eulerian equations for the dispersed phase have been implemented into the Navier-Stokes Solver AVBP [12]. It is based on a 2D/3D finite Volume/ finite Element method for unstructured, structured and hybrid meshes. The carrier phase conservation equations for density, mass fractions, velocities and total energy (kinetic + internal) ($w = (\rho, \rho Y_k, \rho u, \rho v, \rho w, \rho E)$) are presented in the compact form

$$\frac{\partial}{\partial t}w_i + \frac{\partial}{\partial x_j}F_{ij} = S_i \tag{18}$$

where S_i are source terms in the case of reactive flow and two way coupling. The fluxes F_{ij} are then divided into a non viscous part, the Euler fluxes F_{ij}^I, and a viscous part F_{ij}^V. The inviscid fluxes are defined as

$$F_{ij}^I = \begin{pmatrix} \rho u & \rho v & \rho w \\ \rho Y_k u & \rho Y_k v & \rho Y_k w \\ \rho u^2 + P & \rho uv & \rho uw \\ \rho uv & \rho v^2 + P & \rho vw \\ \rho uw & \rho vw & \rho w^2 + P \\ (\rho E + P)u & (\rho E + P)v & (\rho E + P)w \end{pmatrix} \tag{19}$$

where P is the thermodynamic pressure given by the ideal gas law $P = \rho r T$ and E is the total (kinetic + internal) energy. The viscous fluxes are defined as

$$F_{ij}^V = \begin{pmatrix} 0 & 0 & 0 \\ J_{x,k} & J_{y,k} & J_{z,k} \\ -\tau_{xx} & -\tau_{xy} & -\tau_{xz} \\ -\tau_{yx} & -\tau_{yy} & -\tau_{yz} \\ -\tau_{zx} & -\tau_{zy} & -\tau_{zz} \\ -(u\tau_{xx} + v\tau_{xy} + w\tau_{xz}) + q_x & -(u\tau_{yx} + v\tau_{yy} + w\tau_{zx}) + q_y & -(u\tau_{zx} + v\tau_{zy} + w\tau_{zz}) + q_z \end{pmatrix} \tag{20}$$

where $J_{j,k}$ are the species fluxes due to species diffusion, τ_{ij} is the stress tensor and q_j are the fluxes due to thermal diffusion. The stress tensor for the carrier phase is modeled as the trace free tensor of the velocity gradients with the dynamic viscosity μ.

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \tag{21}$$

The transported moments of the dispersed phase are number density, mesoscopic particle velocity fields, and quasi brownian energy (QBE). $w_{p,i} = \left(\tilde{n}_p, \tilde{n}_p \tilde{u}_p, \tilde{n}_p \tilde{v}_p, \tilde{n}_p \tilde{w}_p, \tilde{n}_p \delta\tilde{\theta}_p \right)$. The conservations equations are then as in the case of the Navier-Stokes equations

$$\frac{\partial}{\partial t} w_{p,i} + \frac{\partial}{\partial x_j} F_{p,ij} = S_{p,i} \tag{22}$$

where $S_{p,i}$ are source terms as drag force and production of quasi brownian energy (QBE). Again the fluxes $F_{p,ij}$ are then divided into the non viscous part, the Euler fluxes $F_{p,ij}^I$, and the viscous part $F_{p,ij}^V$. The inviscid fluxes are defined as

$$F_{p,ij}^I = \begin{pmatrix} \tilde{n}_p \tilde{u}_p & \tilde{n}_p \tilde{v}_p & \tilde{n}_p \tilde{w}_p \\ \tilde{n}_p \tilde{u}_p^2 + P_{QB} & \tilde{n}_p \tilde{u}_p \tilde{v}_p & \tilde{n}_p \tilde{u}_p \tilde{w}_p \\ \tilde{n}_p \tilde{u}_p \tilde{v}_p & \tilde{n}_p \tilde{v}_p^2 + P_{QB} & \tilde{n}_p \tilde{v}_p \tilde{w}_p \\ \tilde{n}_p \tilde{u}_p \tilde{w}_p & \tilde{n}_p \tilde{v}_p \tilde{w}_p & \tilde{n}_p \tilde{w}_p^2 + P_{QB} \\ \tilde{n}_p \delta\tilde{\theta}_p \tilde{u}_p & \tilde{n}_p \delta\tilde{\theta}_p \tilde{v}_p & \tilde{n}_p \delta\tilde{\theta}_p \tilde{w}_p \end{pmatrix} \tag{23}$$

The viscous fluxes for the dispersed phase are defined as

$$F_{p,ij}^V = \begin{pmatrix} 0 & 0 & 0 \\ -\tilde{\tau}_{p,xx} & -\tilde{\tau}_{p,xy} & -\tilde{\tau}_{p,xz} \\ -\tilde{\tau}_{p,yx} & -\tilde{\tau}_{p,yy} & -\tilde{\tau}_{p,yz} \\ -\tilde{\tau}_{p,zx} & -\tilde{\tau}_{p,zy} & -\tilde{\tau}_{p,zz} \\ +q_{p,x} & +q_{p,y} & +q_{p,z} \end{pmatrix} \tag{24}$$

where $q_{p,i}$ are the fluxes of QBE by diffusion.
The source term $S_{p,i}$ includes drag and production of QBE by mean gradients.

$$S_{p,i} = \begin{pmatrix} 0 \\ \frac{\tilde{n}_p}{\tau_p} \left(u_i - \tilde{u}_{p,i} \right) \\ \frac{\tilde{n}_p}{\tau_p} \left(v_i - \tilde{v}_{p,i} \right) \\ \frac{\tilde{n}_p}{\tau_p} \left(w_i - \tilde{w}_{p,i} \right) \\ \left(-P_{QB} \delta_{ij} \xi_{QB} \frac{\partial \tilde{u}_{p,k}}{x_k} \delta_{ij} + \mu_{QB} \left(\frac{\partial \tilde{u}_{p,i}}{x_j} + \frac{\partial \tilde{u}_{p,j}}{x_i} - \frac{2}{3} \frac{\partial \tilde{u}_{p,k}}{x_k} \delta_{ij} \right) \right) \frac{\partial \tilde{u}_{p,i}}{x_j} - \frac{2\tilde{n}_p}{\tau_p} \delta\tilde{\theta}_p \end{pmatrix} \tag{25}$$

The conservative variables w are then advanced using a standard finite Volume cell-vertex Lax-Wendroff approach [12]. The code AVBP is parallel and based on the COUPL library using MPI for communication. Simulations have been performed on COMPAQ α machines (CEA,CERFACS) using up to 16 processors and excellent speed-up was obtained [1].

3 Description of the numerical test case

Homogeneous isotropic turbulence is one of the classical cases where dynamics and dispersion of particle laden flows can be studied. This has been done extensively using the Lagrangian formalism and encouraging results and insight are obtained by such methods. Comparison of Lagrangian particle tracking in decreasing homogeneous isotropic turbulence [4] with experimental measurements of particle dispersion in grid generated turbulence [16] show that essential features of the particle dynamics can be captured. Preliminary computations with a simplified Eulerian formalism of this test case gave encouraging results [8]. In the case of tracer particles (small Stokes number limit) Eulerian methods are well suited to describe the dynamics [3]. With increasing Stokes number the particle velocities become decorrelated from the gaseous carrier phase velocity. Inertia effects become important and segregation occurs for Stokes numbers about unity. The subject of the study is therefore not only the development of an adequate numerical tool but the validity of the Eulerian approach for Stokes numbers from the tracer limit ($St \to 0$) to unity.

3.1 Initialization of the test case: The gaseous velocity field

The gaseous carrier phase is initialized with a divergence free velocity field obeying a Passot-Pouquet spectrum for the kinetic energy:

$$E(k) = C \left(\frac{k}{k_e} \right) e^{-2(k/k_e)^2} \tag{26}$$

Here k is the wave length and k_e corresponds to the most energetic wave length. The initial gaseous solution is then numerically advanced over a characteristic time scale of the turbulence in order to establish a physical spectrum and velocity field that is solution of the Navier-Stokes equations.

The Reynolds number $Re = u'l/\nu$ based on the integral length scale l and u' is $Re = 18$. The spatial resolution of the Eulerian simulations are 64^3 and 128^3 equidistant nodes. After a non dimensional time of $t = 4.23$ the Reynolds number of the carrier phase is $Re = 14$. This flow field is taken as the initial flow field for the carrier phase for all test cases.

3.2 Initialization of the test case: The dispersed phase velocity field

Several options exist to initialize the dispersed phase although there does not exist a natural way. Here particles are considered equally distributed throughout the computational domain when computation of the dispersed phase is started. Special attention is taken for the initialization of the dispersed phase velocity. Three principal possibilities exist:

1. **Dispersed phase velocity equals carrier phase velocity:** In the case of relaxation times small compared to the characteristic time scales of the carrier phase, the particles have a velocity field close to the carrier phase velocity field. In this case it is physical

[1] see *http://www.cerfacs.fr*

to initialize the dispersed phase velocity field with the gaseous velocity field and to initialize the quasi brownian energy field with a value close to zero. The QBE field can not be initialized with zero since shear viscosity and QBE flux coefficients are directly linear in QBE.

2. **Dispersed phase velocity equals zero:** When relaxation times are large compared to the characteristic time scales of the carrier phase, there is much more QBE than kinetic energy in the mesoscopic particle velocity field. In this case it might be more physical to initialize the dispersed phase velocity field with zero and to initialize the quasi brownian energy field with some fraction of the gaseous kinetic energy.

3. **Dispersed phase velocity is partially correlated to the carrier velocity:** In the intermediate case the most physical approach is to initialize the dispersed phase velocity field with a fraction of the carrier phase velocity field and the quasi brownian energy field with the complement of the carrier phase kinetic energy.

Here the two extreme positions, 1 and 2 , are considered. Furthermore simulations are placed in the unfavorable case of a Stokes number ($St = \tau_p/T_f$) close to unity leading to maximal segregation effects. $T_f = \lambda/u'$ is the turnover time and λ is the integral length scale of the carrier phase.

4 Computation of the Lagrangian reference solution

The Lagrangian particle tracking method is a well understood tool for the numerical investigation of particle laden turbulence. In the case of Stokes drag the particle coordinate and velocities are advanced in time with the following set of differential equations.

$$\frac{\partial}{\partial t} X_i^{(k)} = V_i^{(k)} \tag{27}$$

$$\frac{\partial}{\partial t} V_i^{(k)} = \frac{1}{\tau_p} \left(u_i(X_i^{(k)}, t) - V_i^{(k)} \right) \tag{28}$$

In realistic applications particle numbers are so large that it is not possible to track all particles individually and particles are advanced as "numerical" particles that are supposed to represent a large number of "physical" particles. In order not to bias the result by such a procedure here all particles are computed individually. Special care is taken to evaluate the gaseous velocity u_i at the particle location for the drag force by using high order interpolation methods [18]. The spatial resolution of the gaseous phase is 64^3 and an average of 40 particles are computed per gaseous node. This corresponds to a total of 10.48 million individual particles. This high particle number ensures convergence when averaged fields are computed from the discrete particle distribution. The averaged fields are sensitive to the numerical procedure used. With the high number of particles used the error can be shown to be smaller then 3%. Initially, as for the Eulerian simulation, particle velocities are either initialized with the gaseous velocities or zero.

5 Dynamics of dispersed two phase flows in homogeneous isotropic turbulence

Integral properties of decaying homogeneous isotropic turbulence can be summarized to a simple set of ordinary differential equations of the integral kinetic energy,

$$q_f^2 = \frac{1}{V}\frac{1}{2}\int u_k u_k dV \tag{29}$$

and the dissipation of kinetic energy

$$\varepsilon = \frac{1}{V}\frac{\nu}{2}\int \frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j} dV \tag{30}$$

where ν is the kinematic viscosity.

$$\frac{\partial}{\partial t} q_f^2 = -\varepsilon \tag{31}$$

$$\frac{\partial}{\partial t}\varepsilon = -C_2\frac{\varepsilon^2}{q_f^2} \tag{32}$$

Those equations can be obtained from the Navier-Stokes equations with some assumptions on the properties of the flow [2] satisfied in incompressible decaying homogeneous turbulence. Using the Lagrangian equations of particle transport with Stokes drag (eqs. 27,28) a corresponding set of ordinary differential equations for the fluid particle correlation,

$$q_{fp} = \frac{1}{V}\frac{1}{N}\sum_{k=1}^{N}\int u_i V_i^k dV \tag{33}$$

and the particle kinetic energy,

$$q_p^2 = \frac{1}{V}\frac{1}{N}\sum_{k=1}^{N}\int V_i^k V_i^k dV \tag{34}$$

can be obtained for the dispersed phase [9]:

$$\frac{\partial}{\partial t} q_{fp} = -\frac{q_{fp}}{\tau_{fp}^t} - \frac{1}{\tau_p}\left[q_{fp} - 2q_{f@p}^2\right] \tag{35}$$

$$\frac{\partial}{\partial t} q_p^2 = -\frac{1}{\tau_p}\left[2q_p^2 - q_{fp}\right] \tag{36}$$

Here τ_{fp}^t corresponds to the turbulence time scale that governs the dissipation of fluid particle correlation. Eq. 35 can then be used to calculate this dissipative time scale a posteriori.

$$\tau_{fp}^t = -\frac{q_{fp}}{\frac{\partial}{\partial t} q_{fp} + \frac{1}{\tau_p}\left[q_{fp} - 2q_{f@p}^2\right]} \tag{37}$$

The time scale for the dissipation of the carrier phase $\tau^+ = q_f^2/\varepsilon$ and the relaxation time of the particles τ_p can then be compared to the dissipative time scale of fluid particle correlation.

6 Measurement of particle dispersion

Particle dispersion is usually measured in Lagrangian simulations by tracking individual particle path and calculating the variance of the relative displacement

$$\left\langle X^2(t) \right\rangle = \frac{1}{N} \sum_{j=1}^{N} \left[X^j(t) - X^j(t_0) \right]^2 . \tag{38}$$

Particle dispersion can then be related to the time derivative of this quantity (see [10]),

$$D_p^L(t) = \frac{1}{2} \frac{d}{dt} \left\langle X^2(t) \right\rangle . \tag{39}$$

In Eulerian simulations individual particle paths are not available. Particle dispersion can still be measured by a semi-empirical method [10]. Defining a subset of particles called colored particles, a transport equation is written for the ratio of these colored particles to total particles ($\tilde{c} = \tilde{n}_c / \tilde{n}_p$). This transport equation is similar to the transport equation for particle number density (eq. 5):

$$\frac{\partial}{\partial t} \tilde{c} \tilde{n}_p + \frac{\partial}{\partial x_i} \tilde{c} \tilde{n}_p \tilde{u}_{p,i} = \frac{\partial}{\partial x_i} \tilde{c} \tilde{n}_p \left(\tilde{u}_{p,i} - \tilde{u}^c_{p,i} \right) \tag{40}$$

Here, $\tilde{u}^c_{p,i}$ is the mesoscopic velocity of colored particles. Since only the velocity of the total droplet number is resolved, a supplementary term arises on the right-hand side of (eq.40). This term takes into account the slip velocity between colored particles and the mesoscopic velocity of the particle ensemble. Comparing the above equation to the Navier-Stokes equations, this term is the equivalent of molecular diffusion in a species equation. Since the slip velocity can arise only from uncorrelated movement of the particles, this term can be modeled as a diffusion related to the quasi-Brownian motion.

If the ensemble-averaged mean number-density fraction of colored particles $\langle \tilde{n}_p \rangle \mathcal{C} = \langle \tilde{n}_p \tilde{c} \rangle$, such that $(\tilde{c} = \mathcal{C} + c')$ is uniformly stratified, say in the k-direction, and fluctuations are assumed periodic with respect to the computational domain, the fluctuating number density of colored particles $c' \tilde{n}_p$ can be extracted from the total colored number density and a transport equation for the fluctuations of colored-particle concentration is obtained:

$$\frac{\partial}{\partial t} c' \tilde{n}_p + \frac{\partial}{\partial x_i} c' \tilde{n}_p \tilde{u}_{p,i} = -\tilde{n}_p \tilde{u}_{p,k} \frac{\partial}{\partial x_k} \mathcal{C} + \frac{\partial}{\partial x_i} \tilde{c} \tilde{n}_p (\tilde{u}_{p,i} - \tilde{u}^c_{p,i}) \tag{41}$$

Averaging the colored number-density equation (eq. (40)) one obtains a Reynolds-averaged transport equation,

$$\frac{\partial}{\partial t} \langle \tilde{n}_p \rangle \mathcal{C} + \frac{\partial}{\partial x_i} \langle \tilde{n}_p \rangle \mathcal{C} \langle \tilde{u}_{p,i} \rangle_p = -\frac{\partial}{\partial x_i} \langle \tilde{n}_p c' u_{p,i} \rangle + \frac{\partial}{\partial x_i} \left\langle \tilde{c} \tilde{n}_p \left(\tilde{u}_{p,i} - \tilde{u}^c_{p,i} \right) \right\rangle . \tag{42}$$

Eq. 41 has been solved neglecting the quasi Brownian motion term. This is equivalent to neglecting species diffusion due to molecular exchange in a transport equation for species.

Particle dispersion can be derived by making a gradient assumption: $(\langle c' \tilde{n}_p \tilde{u}_{p,k} \rangle = \langle \tilde{n}_p \rangle D^t_{p,k} \frac{\partial}{\partial x_k} \mathcal{C})$ A semi-empirical diffusion coefficient is defined by:

$$D^t_{p,k} = \frac{\langle \tilde{n}_p c' u_{p,k} \rangle}{\langle \tilde{n}_p \rangle \frac{\partial}{\partial x_k} \mathcal{C}} \tag{43}$$

This dispersion coefficient is comparable to the Lagrangian dispersion coefficient (39) in the long-time limit of stationary turbulence. Nevertheless simulations neglecting the quasi-Brownian motion are likely to underestimate the Lagrangian dispersion. This is due to the fact that only turbulent dispersion of the resolved velocity field is taken into account in the Eulerian framework. This can be compared to the molecular and turbulent diffusion of species.

7 Numerical results

Numerical computations are performed using the initialization procedure described in section 3. Numerical results are presented for the two extreme initialization procedures (1 and 2).
The temporal development of the integral values for kinetic energies and fluid particle correlation are presented for the first initialization procedure in fig. 1 The numerical results of the Eulerian computation (lines) are compared to the numerical results of the Lagrangian reference computation (symbols). In the Eulerian computation the total kinetic energy of the particles q_p^2 is obtained from the sum of the resolved kinetic energy $\tilde{q}_p^2$ and the QBE δq_p^2. The open triangles give the QBE estimated with the values with the equilibrium formula (eq. 16). This shows that the Eulerian simulation is able to capture the dynamics of the dispersed phase. In fig. 4 the time scales from the Eulerian simulations are compared. Initially the relaxation time of the particles (line) is about half the dissipative time scale of the carrier phase (dashed line). This corresponds to as Stokes number of about 0.5. In the decreasing homogeneous isotropic turbulence the dissipative time scale increases slowly and thus leads to a decreasing Stokes number (about 0.3 at the end of the Eulerian computation). The dissipative time scale of the fluid particle correlation is initially close to the dissipative time scale of the carrier phase and decreases in time such as to reach a level where it is about half the dissipative time scale of the carrier phase. This matches results from theoretical considerations [14].

Numerical results for the second initialization procedure are presented in fig. 3. The Eulerian result is compared to the Lagrangian equivalent. The Eulerian simulations tends to underestimate fluid-particle correlation and to underestimate the correlated dispersed phase kinetic energy since the QBE is comparable. The open triangles give the QBE estimated by the equilibrium formula 16. In fig. 4 the dissipative times scales are again compared to the relaxation time of the particles. Here the dissipative time scale of the fluid-particle correlation is initially zero since the fluid particle correlation is initially zero. After about one particle relaxation time the time it shows qualitatively the same behavior as with the other initialization procedure.

Results of the dispersion measurement are given in fig.5. The turbulent carrier phase dispersion is given as a reference by the continuous line with crosses. The value of measured dispersion coefficient depends on the initialization procedure: When the dispersed phase has initially the velocity field of the carrier phase, dispersion is bigger as found by Lagrangian computations. When particle velocities are initially zero turbulent mixing is not as important and the dispersion coefficient is significantly smaller.

Fig. 6 shows the temporal development of the particle segregation in the Eulerian simulation with the two initialization procedures (lines) and the Lagrangian reference solution for the $u_{p,i} = u_i$ initialization (triangles). The measurement of the Eulerian segregation is smaller than the corresponding Lagrangian segregation. Furthermore segregation is smaller when particles are initially at rest since the carrier phase needs to accelerate the dispersed

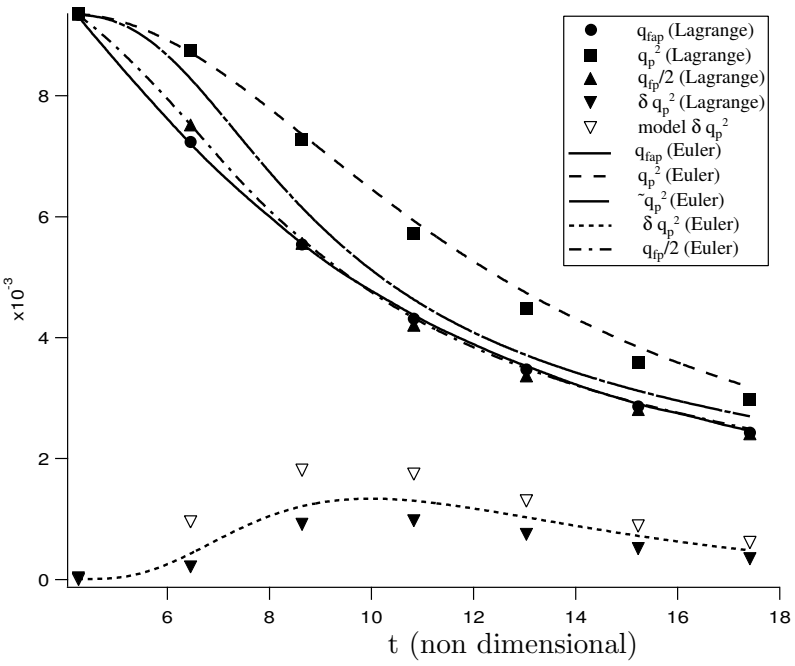

Figure 1: Comparison of Lagrangian results (symbols) to Eulerian results (lines). For Eulerian-Eulerian approach the total particle kinetic energy q_p^2 computed as the sum of the kinetic energy due to correlated motion $\tilde{q}_p^2$ and the quasi brownian energy δq_p^2.

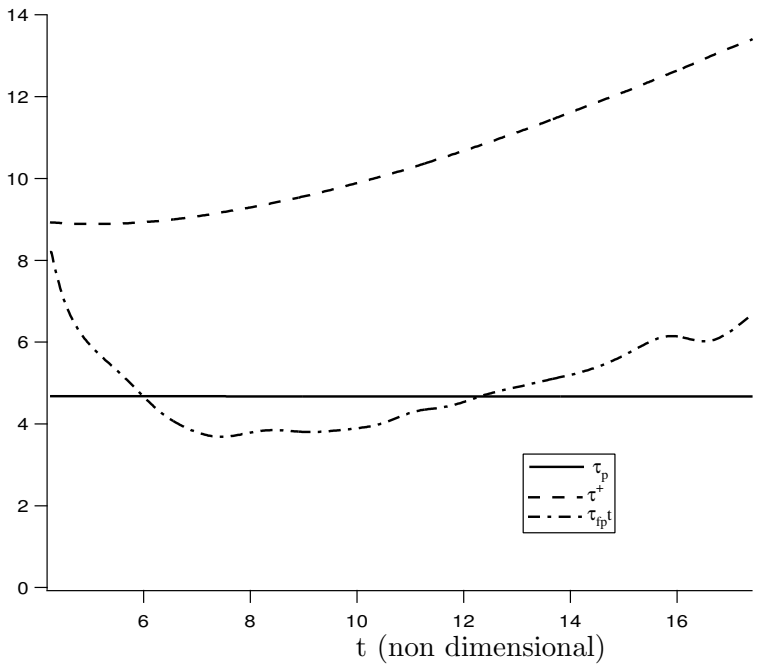

Figure 2: Comparison of the dissipative time scale of the carrier phase τ^+ with the relaxation time of drag τ_p and the dissipative timescale of fluid particle correlation τ_{fp}^t.

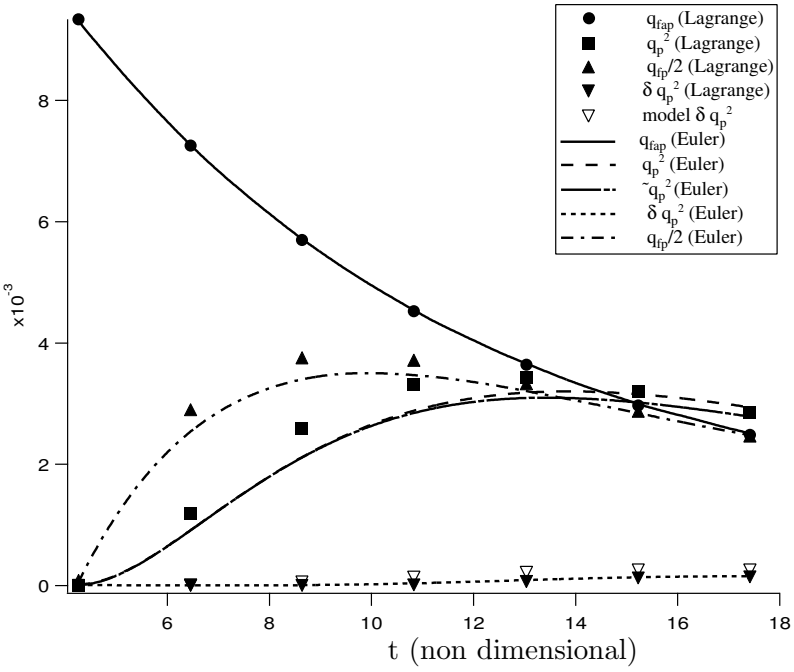

Figure 3: Comparison of Lagrangian results (symbols) to Eulerian results (lines). For Eulerian-Eulerian approach the total particle kinetic energy q_p^2 computed as the sum of the kinetic energy due to correlated motion $\tilde{q}_p^2$ and the quasi brownian energy δq_p^2.

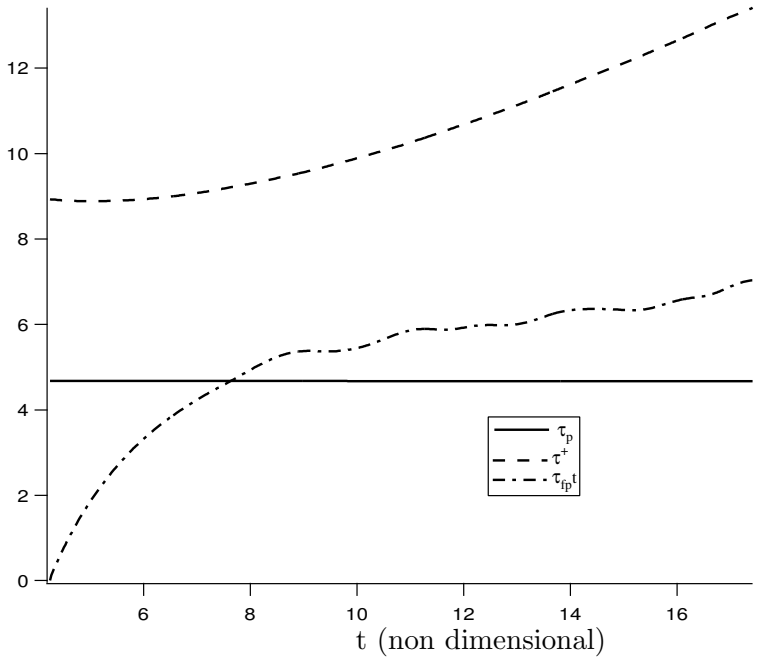

Figure 4: Comparison of the dissipative time scale of the carrier phase τ^+ with the relaxation time of drag τ_p and the dissipative timescale of fluid particle correlation τ_{fp}^t.

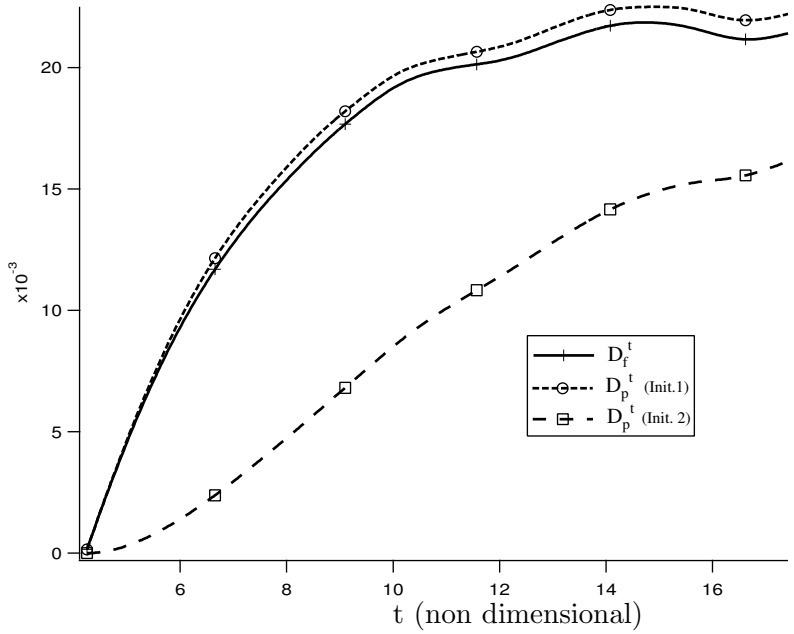

Figure 5: Temporal development of the dispersion coefficient. The carrier phase dispersion coefficient is given as a reference (continuous line with crosses, the dispersion coefficient is bigger than the carrier phase dispersion coefficient when the dispersed phase is initialized with the carrier phase velocity.

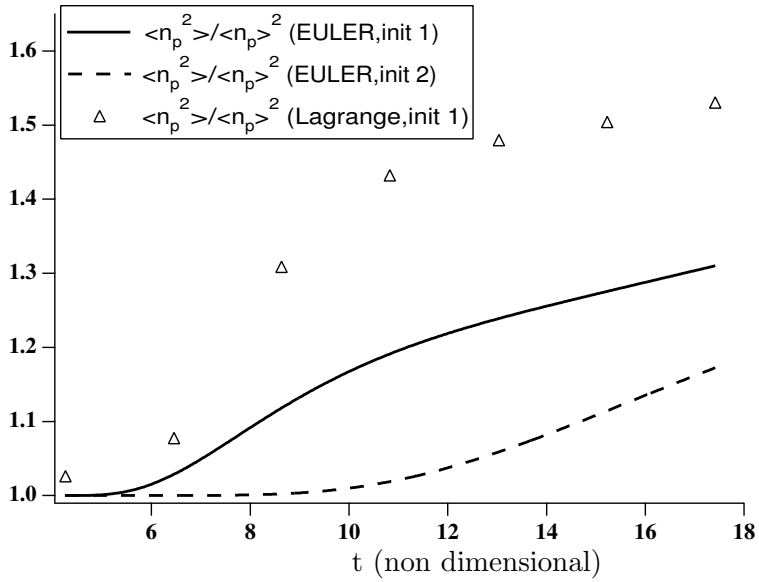

Figure 6: Temporal development of particle segregation. Segregation in Eulerian computations is underestimated compared to Lagrangian segregation.

phase before compression and dilatation can occur.

We have experienced that the Eulerian simulations are very sensible to spatial resolution. This sensibility is contributed to the segregation effects. The heuristically introduced volume viscosity tends to render the spatial particle number distribution more uniform. Without this volume viscosity calculations can currently not be carried out: particle segregation and enstrophy become too big. An important remaining question is therefore whether the volume viscosity has a physical justification due to the non-equilibrium of the particle velocity distribution, or is a "numerical trick" needed to render the computation stable or to account for subgrid effects. In the first case, this viscosity should be independent of the numerical scheme and of the mesh size and should be related to the local particulate phase properties. This point is under current investigation.

8 Conclusion

The presented study shows the capacity of Eulerian formalism to capture the dynamics of particles even in the vicinity of unity Stokes numbers. Simulations were performed at very small Reynolds numbers since simulations with higher Reynolds numbers of the carrier phase showed deficiencies in the spatial resolutions of the dispersed phase. Therefore tests have to be extended to higher Reynolds numbers and it would be interesting to develop a subgrid model for the dispersed phase. This would lead to Large Eddy Simulations in an Eulerian framework which are very interesting for the unsteady computations of industrial applications with a high number of particles or droplets. Concerning dispersion measurements it is interesting to extend the simulations by taking gravity into account and to test whether the crossing trajectory effect is captured in such an Eulerian framework.

Numerical computation of the Eulerian simulations were performed on the COMPAQ supercomputers of CEA and CERFACS . The Lagrangian reference solution was obtained with numerical simulations performed at computing center IDRIS using the Eulerian-Lagrangian version of *NTMIX*.
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