# Buoyancy driven motion of non-coalescing inertial drops: analysis and modeling of the microstructure kinematic.

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#### Abstract

In this study, we provide a comprehensive analysis of the timescale that govern the droplets' interaction as well as the global microstructure in buoyant emulsions. It is shown in (?) that as predicted by ?, the second moment of the nearest particle pair distribution, noted  $\mathbf{R}$ , has the capability to quantify microstructure's features such as clusters and layers of particles. In this study we propose to analyze the microstructure kinematic through the derivation of a transport equation for  $\mathbf{R}$  within the framework of kinematic theory. We conducted Direct Numerical Simulations (DNS) of statistically steady state mono-disperse buoyant emulsion, over a broad range of Galileo number (Ga), particle volume fraction  $(\phi)$ , and viscosity ratio  $(\lambda)$ . The density ratio and the Bond number are kept constant,  $\zeta = 1.11$  and Bo = 0.2, respectively. By a rigorous theoretical and numerical analysis we could show that : (1) the time of relaxation of  $\mathbf{R}(\mathbf{x},t)$ , is the mean age of interaction of the nearest particles pairs  $\tau_p(\mathbf{x},t)$ ; (2) The particle normal approach velocity scale as  $\tau_p n_p^{1/3}$  with  $n_p$  the number density, and has also a relaxation time of  $\tau_p$ . (3) We could evaluate the different source terms in the transport equation for  $\mathbf{R}$  in terms of the dimensionless parameters. Overall the mean time of interaction  $\tau_p$  seem to be a crucial quantity in the modeling of the particle relative kinematic of dispersed two phase flows.

### 1 Introduction

- 1. We use extensively averaged models in industry
- 2. These models necessitate closure laws. These closure laws are highly dependent on the particles' microstructure.
- 3. In our previous work we performed a *Nearest-particle-statistics* analysis of the microstructure geometry, or the steady state microstructure.
- 4. All the closures in the literature are performed in steady state system. Therefore, in order to be valid in a Euler-Euler averaged context the time scales of the simulation must be greater than the time for the microstructure to reach its steady state. Only then the assumption of quasi steady ness is valid.
- 5. Therefore, in this study we provide a theoritical and numerical analyssi of the timescale that drives the microstructure. Doing so, we demonstrate that the particle interaction time is the main timescale involved in the microstructure relaxation time. We therefor also study the relative kinematic

### 2 Theoretical framework

In the preceding chapter we have seen that the granular temperature could be estimated based on the vector

$$\mathbf{u}_p^{\text{nst}}(\mathbf{x}, \mathbf{r}, t, a) = \frac{1}{P_{nst}(\mathbf{x}, \mathbf{r}, t, a)} \int \sum_{i}^{N_b} \delta(\mathbf{x} - \mathbf{x}_i) \sum_{j \neq i}^{N_b} \delta(\mathbf{x} + \mathbf{r} - \mathbf{x}_j) \delta(t + a - t_c^{ij}) \mathbf{u}_{ij} h_{ij} d\mathscr{P}.$$

the aim of this chapter is therefore to determine the form of  $\mathbf{u}_{n}^{\mathrm{nst}}$ .

In addition to provides physical explanation the field  $\mathbf{u}_p^d = \mathbf{u}_p^r - \mathbf{u}_p$  is of great importance to study the particle phase fluctuation tensor  $\langle \delta_i \mathbf{u}_i' \mathbf{u}_i' \rangle$  which is of crucial importance in multiphase flow modeling. Indeed, it can be shown that

$$\frac{\langle \delta_i \mathbf{u}_i' \mathbf{u}_i' \rangle}{n_p}(\mathbf{x}, t) = \int_{\mathbb{R}^3} \mathbf{u}_p^d \mathbf{u}_p^d P_{nst}(\mathbf{r} | \mathbf{x}, t) d\mathbf{r} + \int_{\mathbb{R}^3} \mathbf{F}(\mathbf{r}, \mathbf{x}, t) d\mathbf{r}$$

where,  $\mathbf{F} = \left\langle \sum_{i} \sum_{j \neq i} \delta_{j} \delta_{i} h_{ij} (\mathbf{u}_{i} - \mathbf{u}_{p}^{nst}) (\mathbf{u}_{i} - \mathbf{u}_{p}^{nst}) \right\rangle$ . Thus, the ensemble averaged particle phase Reynolds stress is the sum of the fluctuation given by  $\mathbf{u}_{p}^{r}$  plus an additional contribution form the others particles fluctuation around the average field  $\mathbf{u}_{p}^{d}$ .

## 3 A transport equation for the nearest particle velocity-included pdf properties

We propose an alternative derivation, to what it is done in ? for the derivation of the nearest particle averaged properties.

The derivation is done by noticing that at the local level we have,

$$\begin{split} \partial_t \delta(\mathbf{x}_i(\mathscr{F},t) - \mathbf{x}) + \mathbf{u}_i(\mathscr{F},t) \cdot \nabla_{\mathbf{x}} \delta(\mathbf{x}_i(\mathscr{F},t) - \mathbf{x}) &= 0 \\ \partial_t \delta(\mathbf{u}_i(\mathscr{F},t) - \mathbf{u}) + \mathbf{a}_i(\mathscr{F},t) \cdot \nabla_{\mathbf{u}} \delta(\mathbf{u}_i(\mathscr{F},t) - \mathbf{u}) &= 0 \\ \partial_t \delta(\mathbf{x}_j(\mathscr{F},t) - \mathbf{x} + \mathbf{r}) + \mathbf{w}_{ji}(\mathscr{F},t) \cdot \nabla_{\mathbf{r}} \delta(\mathbf{x}_j(\mathscr{F},t) - \mathbf{x} + \mathbf{r}) + \mathbf{u}_i(\mathscr{F},t) \cdot \nabla_{\mathbf{r}} \delta(\mathbf{x}_j(\mathscr{F},t) - \mathbf{x} + \mathbf{r}) &= 0 \\ \partial_t \delta(t + a - t_c^{ij}(\mathscr{F})) - \partial_a \delta(t + a - t_c^{ij}(\mathscr{F})) &= 0, \end{split}$$

where we have defined  $\mathbf{w}_{ji} = \mathbf{u}_j - \mathbf{u}_i$  as the relative velocity between particle j and i, and  $\partial_t \mathbf{u}_i = \mathbf{a}_i$  as the acceleration of the particle. For clearly, we note what we call here the *state* function  $\Pi$  as,

$$\Pi(\mathbf{x}, \mathbf{r}, \mathbf{u}, t, a, \mathscr{F}) = \sum_{i} \delta(\mathbf{x}_{i}(\mathscr{F}, t) - \mathbf{x}) \delta(\mathbf{u}_{i}(\mathscr{F}, t) - \mathbf{u}) \sum_{j \neq i} \delta(\mathbf{x}_{j}(\mathscr{F}, t) - \mathbf{x} + \mathbf{r}) \delta(t + a - t_{c}^{ij}(\mathscr{F})) h_{ij}(t, \mathscr{F})$$

Then, one may directly deduce that,  $\Pi$  follows the conservation equation,

$$\partial_t \Pi + \partial_a \Pi + \nabla_{\mathbf{x}} \cdot (\mathbf{u}_i \Pi) + \nabla_{\mathbf{u}} \cdot (\mathbf{a}_i \Pi) + \nabla_{\mathbf{r}} \cdot (\mathbf{w}_{ji} \Pi) = \Pi_S$$
(3.1)

where the source term is explicitly defined by,

$$\Pi_{S} = \sum_{i} \delta(\mathbf{x}_{i}(\mathscr{F}, t) - \mathbf{x}) \delta(\mathbf{u}_{i}(\mathscr{F}, t) - \mathbf{u}) \sum_{j \neq i} \delta(\mathbf{x}_{j}(\mathscr{F}, t) - \mathbf{x} - \mathbf{r})$$

$$\delta(t + a - t_{c}^{ij}(\mathscr{F})) h_{ij}(t, \mathscr{F}) \sum_{l \neq i} \delta(r_{li} - r_{jl}) (\mathbf{n}_{li} \cdot \mathbf{u}_{li} - \mathbf{n}_{ji} \cdot \mathbf{u}_{ji})$$

$$= \prod_{l \neq i} \delta(r_{li} - r_{jl}) (\mathbf{n}_{li} \cdot \mathbf{u}_{li} - \mathbf{n}_{ji} \cdot \mathbf{u}_{ji})$$

such that

$$\iiint \Pi_S d\mathscr{P} dS(\mathbf{r}) da = \iint [\delta(a) P(\mathbf{x}, \mathbf{r}, \mathbf{u}, t, 0) - \frac{P_{\text{nst}}(\mathbf{x}, \mathbf{r}, \mathbf{u}, t, a)}{\tau^{\text{nst}}(\mathbf{x}, \mathbf{r}, \mathbf{u}, t, a)}] dS(\mathbf{r}) da = 0$$

is a source terms related to the inter-changes in nearest neighbors.

Firstly, notice that integrating Equation 3.1 on all configurations yields the same conservation equation as ? for  $P_{\text{nst}}$ . Making our derivation consistent with his.

To derive an equation for  $\mathbf{u}_p^{\text{nst}}$  the process is easy, we simply multiply Equation 3.1 by  $\mathbf{u}_i$  and average on all configurations. It yields,

$$\partial_t \langle \Pi \mathbf{u}_i \rangle + \partial_a \langle \Pi \mathbf{u}_i \rangle + \nabla_{\mathbf{x}} \cdot \langle \mathbf{u}_i \mathbf{u}_i \Pi \rangle + \nabla_{\mathbf{u}} \cdot \langle \mathbf{a}_i \mathbf{u}_i \Pi \rangle + \nabla_{\mathbf{r}} \cdot \langle \mathbf{u}_i \mathbf{w}_{ii} \Pi \rangle = \langle \Pi_S \mathbf{u}_i \rangle + \langle \Pi \mathbf{a}_i \rangle$$

Noticing that,  $\langle \mathbf{u}_i \Pi \rangle = \mathbf{u} P_{\text{nst}}$  we directly obtain the equation for  $\mathbf{u}$ :

$$\begin{split} \partial_t(\mathbf{u}P_{\mathrm{nst}}) + \partial_a(\mathbf{u}P_{\mathrm{nst}}) + \nabla_{\mathbf{x}} \cdot (\mathbf{u}\mathbf{u}P_{\mathrm{nst}}) + \nabla_{\mathbf{r}} \cdot (\mathbf{u}\mathbf{w}_p^{\mathrm{nst}}P_{\mathrm{nst}}) + \nabla_{\mathbf{u}} \cdot (\mathbf{u}\mathbf{a}_p^{\mathrm{nst}}P_{\mathrm{nst}}) \\ &= \mathbf{u} \left[ \delta(a)P(\mathbf{x},\mathbf{r},\mathbf{u},t,0) - \frac{P_{\mathrm{nst}}(\mathbf{x},\mathbf{r},\mathbf{u},t,a)}{\tau^{\mathrm{nst}}(\mathbf{x},\mathbf{r},\mathbf{u},t,a)} \right] + \mathbf{a}_p^{\mathrm{nst}}P_{\mathrm{nst}} \end{split}$$

With our new notation we have shown that we have the exact notation,

$$\langle \delta_i \mathbf{u}_i' \mathbf{u}_i' \rangle = \int \mathbf{u} \mathbf{u} P_{\text{nst}}(\mathbf{x}, \mathbf{r}, \mathbf{u}, a, t) d\mathbf{r} d\mathbf{u} da - \mathbf{u}_p \mathbf{u}_p n_p$$

Thus, we rather derive the previous equation by **u** which gives,

$$\begin{split} \partial_t(\mathbf{u}\mathbf{u}P_{\mathrm{nst}}) + \partial_a(\mathbf{u}\mathbf{u}P_{\mathrm{nst}}) + \nabla_{\mathbf{x}} \cdot (\mathbf{u}\mathbf{u}\mathbf{u}P_{\mathrm{nst}}) + \nabla_{\mathbf{r}} \cdot (\mathbf{u}\mathbf{u}\mathbf{w}_p^{\mathrm{nst}}P_{\mathrm{nst}}) + \nabla_{\mathbf{u}} \cdot (\mathbf{u}\mathbf{u}\mathbf{a}_p^{\mathrm{nst}}P_{\mathrm{nst}}) \\ &= \mathbf{u}\mathbf{u} \left[ \delta(a)P(\mathbf{x},\mathbf{r},\mathbf{u},t,0) - \frac{P_{\mathrm{nst}}(\mathbf{x},\mathbf{r},\mathbf{u},t,a)}{\tau^{\mathrm{nst}}(\mathbf{x},\mathbf{r},\mathbf{u},t,a)} \right] + \mathbf{u}\mathbf{a}_p^{\mathrm{nst}} + \mathbf{a}_p^{\mathrm{nst}}\mathbf{u}P_{\mathrm{nst}} \end{split}$$

integrating Overall age and velocity and relative position gives,

$$\partial_t(n_p \mathbf{F}_p) + \nabla_{\mathbf{x}}(n_p \mathbf{F}_p \mathbf{u}_p + n_p \mathbf{F}^{Re}) = -\frac{n_p \mathbf{F}_p}{\tau_p} + n_p \mathbf{B}_p + n_p \mathbf{D}_p + n_p \mathbf{A}_p$$

with,

$$\begin{split} n_p \mathbf{F}^{Re}(\mathbf{x},t) &= \int_0^\infty \int_{\mathbb{R}^6} \mathbf{u} \mathbf{u} (\mathbf{u} - \mathbf{u}_p) P(\mathbf{x},\mathbf{r},t,a) d\mathbf{r} d\mathbf{u} da, \\ n_p \mathbf{B}(\mathbf{x},t) &= \int_0^\infty \int_{\mathbb{R}^6} \mathbf{u} \mathbf{u} P(\mathbf{x},\mathbf{r},t,0) \delta(a) d\mathbf{r} d\mathbf{u} da, \\ n_p \mathbf{D}(\mathbf{x},t) &= \int_0^\infty \int_{\mathbb{R}^6} \mathbf{u} \mathbf{u} \left[ \frac{1}{\tau_p(\mathbf{x},t)} - \frac{1}{\tau^{\mathrm{nst}}(\mathbf{x},\mathbf{r},t,a)} \right] P_{\mathrm{nst}} d\mathbf{r} d\mathbf{u} da, \\ n_p \mathbf{W}(\mathbf{x},t) &= \int_0^\infty \int_{\mathbb{R}^6} \left[ \mathbf{u} \mathbf{a}_p^{\mathrm{nst}} + \mathbf{a}_p^{\mathrm{nst}} \mathbf{u} \right] P_{\mathrm{nst}} d\mathbf{r} d\mathbf{u} da. \end{split}$$

Which is a global evolution equation for the particle tensor. However, notice how this is pointless since one may directly notice that,

$$\int \int \int \int \mathbf{u} \mathbf{u} \Pi_S d\mathscr{P} dS(\mathbf{r}) da d\mathbf{u} dr = \int \int \mathbf{u} \mathbf{u} \int \int [\delta(a) P(\mathbf{x}, \mathbf{r}, \mathbf{u}, t, 0) - \frac{P_{\mathrm{nst}}(\mathbf{x}, \mathbf{r}, \mathbf{u}, t, a)}{\tau^{\mathrm{nst}}(\mathbf{x}, \mathbf{r}, \mathbf{u}, t, a)}] dS(\mathbf{r}) da dr d\mathbf{u} = 0$$

Indeed, since  $\mathbf{u}$  is not explicitly related to the particle relative position, this is not affected by this source term.. And therefore,

$$\partial_t(n_p \mathbf{F}_p) + \nabla_{\mathbf{x}}(n_p \mathbf{F}_p \mathbf{u}_p + n_p \mathbf{F}^{Re}) = \int_0^\infty \int_{\mathbb{R}^6} \left[ \mathbf{u} \mathbf{a}_p^{\text{nst}} + \mathbf{a}_p^{\text{nst}} \mathbf{u} \right] P_{\text{nst}} d\mathbf{r} d\mathbf{u} da.$$

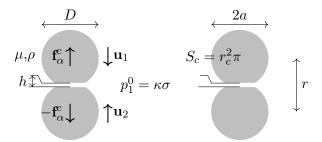


Figure 1: Scheme of two colliding droplets at close contact. Notice the null kurvature in the region of the interface close to the film leading to a capilary force  $\mathbf{f}_{\alpha}^{c} \approx -S_{c}\kappa\sigma\mathbf{r}/|\mathbf{r}|$ .

the inter particle force

$$\mathbf{f}_{ij}^{c} = S_{c}\kappa\gamma\mathbf{r}_{ij}/r_{ij} = \pi r_{c}^{2}\kappa\gamma\mathbf{r}_{ij}/r_{ij} = \pi(a^{2} - r_{ij}^{2}/4)\kappa\gamma\mathbf{r}_{ij}/r_{ij}$$

where the The resultants of these forces on the particle i is therefore the sum of the contact with all particles except the  $j^{\text{th}}$  particle,

$$\mathbf{f}_{i}^{c} = \sum_{j \neq i} \mathbf{f}_{ij} = -\sum_{j \neq i} \pi (a^{2} - r_{ij}^{2}/4) \kappa \gamma \mathbf{r}_{ij} / r_{ij}$$

The relative acceleration might be written as,

$$a_p^{\text{nst}} = \pi (a^2 - r^2/4) \kappa \gamma \mathbf{r}/r$$

where we assume that the force is only due to the only nearest neighbor. Thus,

$$\int_{0}^{\infty} \int_{\mathbb{R}^{6}} \left[ \mathbf{u} \mathbf{a}_{p}^{\text{nst}} \right] P_{\text{nst}} d\mathbf{r} d\mathbf{u} da. = \int_{0}^{\infty} \int_{\mathbb{R}^{6}} \left[ \mathbf{u} \pi (a^{2}/r - r/4) \kappa \gamma \mathbf{r} \right] P_{\text{nst}} d\mathbf{r} d\mathbf{u} da$$

### 3.1 Let remove the condition on $\mathbf{u}_i$ for $\Pi$ .

It gives,

$$\left\langle \delta_i \mathbf{u}_i' \mathbf{u}_i' \right\rangle(\mathbf{x}, t) = \int_{\mathbb{R}^3} (\mathbf{u}_p^{\text{nst}} - \mathbf{u}_p) (\mathbf{u}_p^{\text{nst}} - \mathbf{u}_p) P_{nst}(\mathbf{r}, \mathbf{x}, a, t) d\mathbf{r} + \int_{\mathbb{R}^3} \mathbf{F}(\mathbf{r}, \mathbf{x}, t) d\mathbf{r}$$

where,  $\mathbf{F} = \langle \Pi(\mathbf{u}_i - \mathbf{u}_p^{nst})(\mathbf{u}_i - \mathbf{u}_p^{nst}) \rangle$ .

$$\partial_t \langle \Pi \mathbf{u}_i \rangle + \partial_a \langle \Pi \mathbf{u}_i \rangle + \nabla_{\mathbf{x}} \cdot \langle \mathbf{u}_i \mathbf{u}_i \Pi \rangle + \nabla_{\mathbf{r}} \cdot \langle \mathbf{u}_i \mathbf{w}_{ji} \Pi \rangle = \langle \Pi_S \mathbf{u}_i \rangle + \langle \Pi \mathbf{a}_i \rangle$$

which gives,

$$\begin{split} \partial_t(\mathbf{u}_p^{\text{nst}}P_{\text{nst}}) + \partial_a(\mathbf{u}_p^{\text{nst}}P_{\text{nst}}) + \nabla_{\mathbf{x}} \cdot (\mathbf{u}_p^{\text{nst}}\mathbf{u}^{\text{nst}}P_{\text{nst}} + \mathbf{u}^{Re}) + \nabla_{\mathbf{r}} \cdot (\mathbf{u}_p^{\text{nst}}\mathbf{w}_p^{\text{nst}}P_{\text{nst}} + \mathbf{w}^{Re}) \\ &= \delta(a)\mathbf{u}_p^{\text{nst}}P(\mathbf{x},\mathbf{r},\mathbf{u},t,0) - \frac{\mathbf{u}_p^{nst}(|D)P_{\text{nst}}(\mathbf{x},\mathbf{r},\mathbf{u},t,a)}{\tau^{\text{nst}}(\mathbf{x},\mathbf{r},\mathbf{u},t,a)} + \mathbf{a}_p^{\text{nst}}P_{\text{nst}} \end{split}$$

### Model for the conditioned acceleration based on numerical results

- 4 Numerical methodology
- 5 Results
- 6 Conclusion

### A Numerical validations