An Eulerian-Lagrangian approach for coupling CFD and population balance equation

Etienne Chantoiseau, A. Plana-Fattori, F-T Ndoye, C Doursat, D. Flick

An Eulerian-Lagrangian approach for coupling CFD and population balance equation

E. Chantoiseau[a,b], A. Plana-Fattori[a,b], F-T. Ndoye[c], C. Doursat[a,b], and D. Flick[a,b]

[a] *AgroParisTech, UMR1145 Ingénierie Procédés Aliments, F-91300 Massy, France (etienne.chantoiseau@agroparistech.fr, planafattori@agroparistech.fr)*
[b] *AgroParisTech, UMR1145 Ingénierie Procédés Aliments, F-91300 Massy, France (doursat@agroparistech.fr, flick@agroparistech.fr)*
[c] *Cemagref, Refrigeration Processes Engineering Research Unit, Parc de Tourvoie, BP 44, F92163 Antony, Cedex, France (fatou-toutie.ndoye@cemagref.fr)*

ABSTRACT

A new approach is proposed here to ensure a complete resolution of the population balance equation (PBE) coupled with the fluid flow equations, which splits the determination of the fluid flow on an Eulerian frame from the PBE resolution along the Lagrangian trajectories of a set of fluid parcels. Knowing the size distribution of the particles aggregates, the viscosity of the overall product can be determined and used for the flow estimation. The coupling of the two types of model is allowed thanks to an iterative procedure until the stability of the calculated viscosity field. The numerical scheme is here described as a proof of concept for a continuous isothermal aggregation process in a pipe with likely parameters. This method allows the description of the aggregation process, and especially the size distribution determination, for the entire domain using a size class method. It was observed notably a high difference of aggregation state for the product flowing near the axis of the pipe and near the wall due to the differences between the shear rate histories of the two parts of the domain. The reconstruction of the bulk output product exhibit that the product properties dispersion is in large part due to the differences of product histories. The versatility of the numerical scheme presented here allows investigating a wide range of transformation.

Keywords: Complex fluid; Mathematical modelling; Computational fluid dynamics; Population balance; Lagrangian particles tracking.

INTRODUCTION

In some continuous processes involving complex liquid products, the transport and thermal properties (viscosity, conductivity) depend sharply on the transformation state. This is especially the case for processes involving aggregation (e.g. whey proteins) or fragmentation (e.g. emulsification) described by population balance equations. Indeed, the viscosity of the products depends on the size of the aggregates and the total volume fraction occupied by them. A proper determination of the aggregate size distribution is thus of great interest for the proper modelling of the process unit, especially in the case of continuous processing. However, classical coupling of the population balance with CFD involves simplifying the set of equation in order to limit the computational cost, as performed by the method of moment.
In order to achieve a precise description of the aggregation for a continuous and isothermal aggregation in a pipe, the present work presents a new numerical approach. The CFD is calculated using an Eulerian finite element method on an Eulerian grid, whereas the PBE is solved on a set of fluid parcels trajectory, allowing the determination of the product state, and thus its viscosity. The two-way coupling of the aggregation and flow models is performed by repeating the two calculations until convergence of the calculated viscosity field.

MATERIALS & METHODS

General numerical approach

The proposed Eulerian-Lagrangian approach is based on an iterative algorithm depicted on figure 1. The first step is the Eulerian calculation of the flow at 353 K using the water viscosity ($\eta_{w\ (T=353K)}$=3.55 10^{-4} Pa.s) on the whole equipment in order to determine the velocity and the shear rate fields.
The second step is the calculation of the trajectories of a number of representative fluid parcels using the velocity field obtained from the previous CFD calculation. The shear rate is retrieved along the trajectories.

The third step is the determination of the transformation state (size distributions of the particles) along each trajectory using the shear rate history. Once the transformation state was calculated along all the fluid parcels trajectories, the viscosity is deduced on those positions knowing the relation between the product state and the viscosity.
Finally, the next step of the algorithm is the interpolation of the viscosity on the whole domain for the next Eulerian calculation of fluid flow.

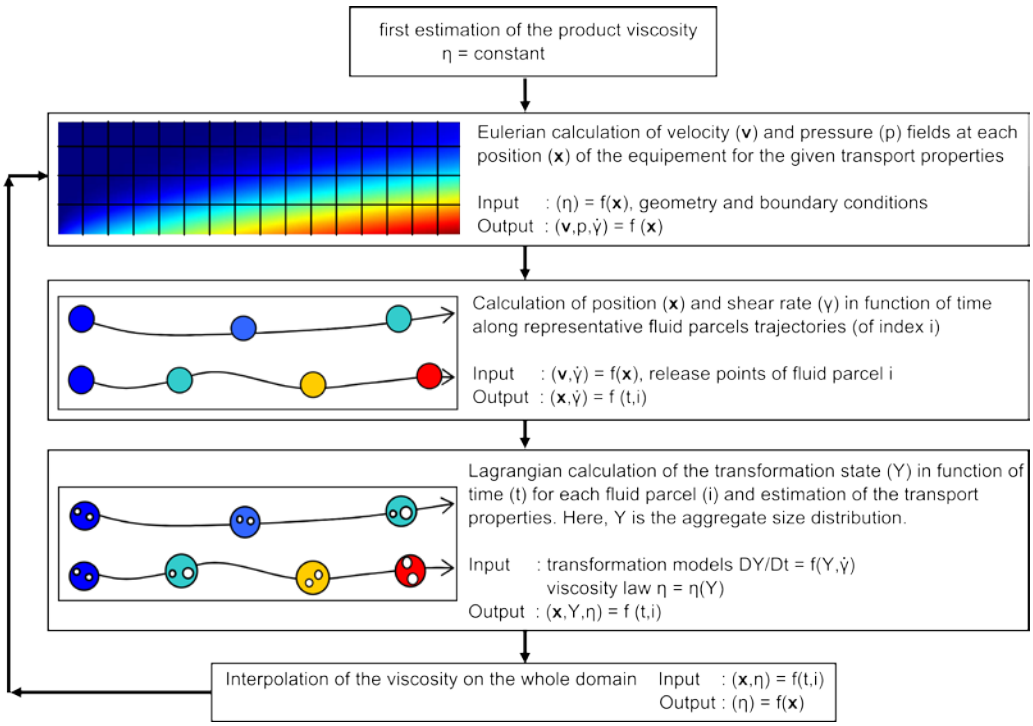

Figure 1. Iterative procedure

The iterations are stopped when the relative difference between two consecutive viscosity fields is less than 0.1% on the entire domain.

CFD calculation

A suspension of small particles (monomers) in water with a concentration of 1% (v/v) was considered. Because of its high content of water, the suspension was assumed to behave as a Newtonian liquid; its density was approximated by pure water behaviour.
The coupled phenomena under consideration are investigated inside a tubular pipe whose length is 1 m and radius is 5 mm. For a feed flow of 5.55 10^{-6} $m^3.s^{-1}$ (20 L/h), the input Reynolds number is 884 indicating a laminar flow.
The flow was determined by solving the Navier-Stokes equations with boundary condition described on figure 2. The mesh was constituted of 200 000 rectangular cells (100 on the pipe radius by 2000 on its length), finer near the wall boundary. The flow determination was conducted using COMSOL Multiphysics 3.5a.

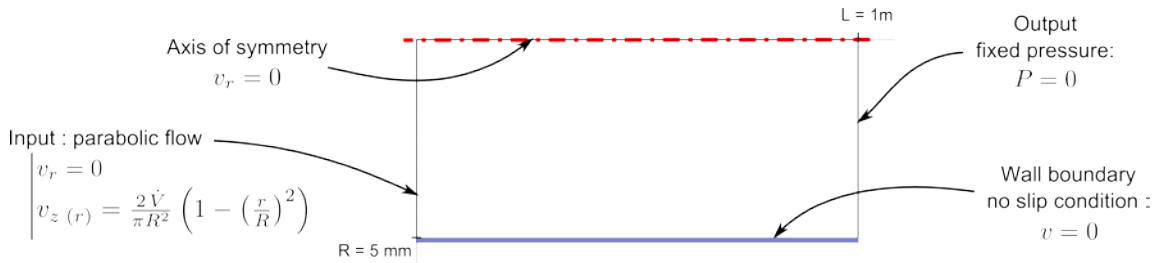

Figure 2. Numerical domain and attached boundary condition

Population balance modelling

In order to describe the aggregation of the dispersed phase, the population balance equation proposed by von Smoluchowski was used. If the aggregates breakage is neglected, the evolution of the concentration of particles containing i monomers, noted N^i, is given for time t by equation 1:

$$\frac{d\,N^i_{(t)}}{dt} = \sum_{j=1}^{i-1} \frac{k_{i-j,j}}{W} \frac{N^j_{(t)}\, N^{i-j}_{(t)}}{2} - N^i_{(t)} \sum_{j=1}^{n} \frac{k_{i,j}}{W} N^j_{(t)} \tag{1}$$

where $k_{i,j}$ is the kernel of aggregation, denoting the aggregation frequency of particles containing respectively i and j monomers; and W is the Fuchs stability factor denoting the particles stability and its influences on aggregation.

The kernel of aggregation is a function of the temperature T and continuous phase viscosity η_w that are constant. It also depends on the shear rate $\dot{\gamma}$ and the size of the involved aggregates (denoted a_i and a_j), as depicted by equation 2 [1], and thus must be calculated for each size couple and time step.

$$k_{i,j} = \frac{2\,k_B\,T}{3\,\eta_w} \cdot \frac{(a_i + a_j)^2}{a_i \cdot a_j} + \frac{4}{3} \cdot \dot{\gamma} \cdot (a_i + a_j)^3 \tag{2}$$

where k_B is the Boltzmann constant ($1.38\ 10^{-23}$ $J.K^{-1}$). The radius a_i of an aggregate containing i monomers can be calculated knowing the monomer radius (a_0=10 10^{-9} m), using the fractal dimension, referred as D [2] and which takes into account its microstructure, by:

$$a_i = a_0\ i^{1/D} \tag{3}$$

The aggregates volume fraction Φ was calculated from the aggregates size distribution by equation 4 and was used to determine the relative viscosity (i.e. η / η_W) by equation 5 [3].

$$\Phi = \frac{4\pi}{3} \cdot \sum_{i=1}^{n} N^i \cdot a_i^3 \tag{4}$$

$$\eta = \eta_w \cdot \left(1 + 2.5\,\Phi + 10.05\,\Phi^2 + 0.00273\,\exp\{16.6\,\Phi\}\right) \tag{5}$$

The PBE was here solved using MATLAB 2009b thanks to the size class method described by Kumar & Ramkrishna [4] involving the discretization of the aggregates population into K classes regrouping particles by number of monomers. A geometric discretization was chosen, with class k (ranging from 1 to K) regrouping particles containing around 2^k monomers. In this work K=30, as a higher number of class doesn't significantly change the results (the last largest possible aggregate contains $1.07\ 10^9$ monomers).

The aim of the study is to exhibit the feasibility of the numerical approach. Thus, the parameters have been chosen in order to describe a general aggregation process with typical values more than to depict a specific product transformation. The table 1 lists the numerical values used for the simulations.

Table 1. Aggregation parameters used for the studie.

Constant	Notation	Value
Fuchs stability factor	W	50
Fractal dimension	D	2.5
Initial aggregate volume fraction	$\Phi_{t=0}$	0.01 m^3/m^3

The simulation has been conducted with 160 trajectories whose initial positions are evenly distributed on the inlet boundary. In order to ensure that the wall boundary condition is properly taken into account, another

trajectory has been added near the boundary. Starting at 10^{-5} m from the wall, its radial velocity is neglected, that is a reasonable assumption at such a distance from the wall. As this trajectory is linear it allows having a consistent wall boundary condition regardless of the flow behaviour.

The iterative procedure (CFD + transformation) was performed 21 times before the maximum relative difference between the last two calculated viscosity fields fell below 0.1% and thus reaches the convergence criterion.

RESULTS & DISCUSSION

The aggregate concentration of the output product is presented on figure 3 and its cumulative size distribution on figure 4. In each case, the results are presented for the bulk product as well as for two fluid parcels: the one starting from the pipe axis and the other from 1 mm from the wall (r_0=4 mm). As presented on figure 3, the total number of particles by unit volume is lower near the wall than on the axis denoting a higher aggregation rate near the wall. Indeed, as the large particles contain a higher number of monomers, the overall number concentration of the suspension decreases with aggregation.

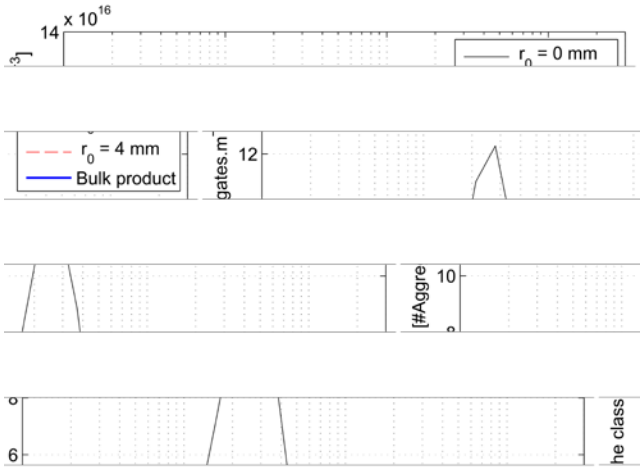

Figure 3. Output concentration of the aggregates by size classes for bulk product and for two fluid parcels.

The lower aggregation at the pipe axis is confirmed on figure 4 which shows that the cumulative size distribution for r_0=4 mm is shifted toward the larger aggregate sizes. As expected, the output bulk product, which is a blend of the output product of each trajectory, has a size distribution comprised between the ones of the two displayed trajectories.

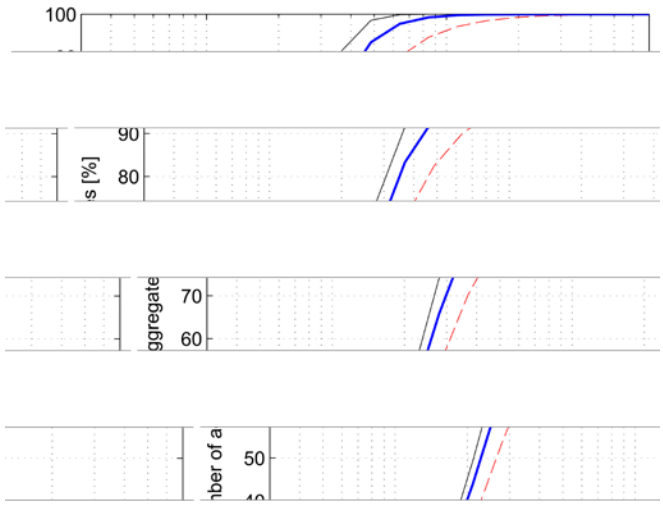

Figure 4. Output aggregates cumulative size distribution for bulk product and for two fluid parcels.

The difference on the product composition is reflected in the viscosity field that is displayed on figure 5. As larger particles are formed, the total particle fraction increases. Indeed, for a fractal dimension lower than 3, when two particles aggregate, the new particle has a higher volume than the total volume of two initial particles. As the aggregation occurs, the total particle volume fraction hence increases, and so does the viscosity.

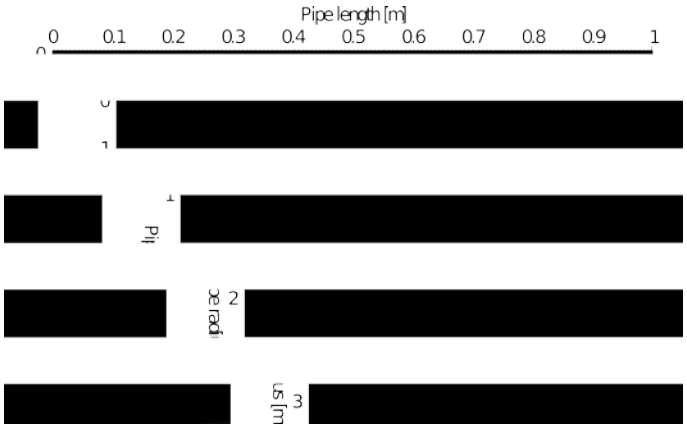

Figure 5. Viscosity fields in the pipe. Flow from left to right

Figure 6 and 7 present the velocity and the shear rate fields. At the inlet parabolic flow is assumed, as for a fully developed laminar flow of constant viscosity. Maximum shear rate is then observed at the wall. But further downstream the liquid near the wall is less sheared than the one at an intermediate radius. This is due to the presence of a growing part of the domain where the product is very viscous so that velocity decreases in this zone and so does also the velocity gradient.

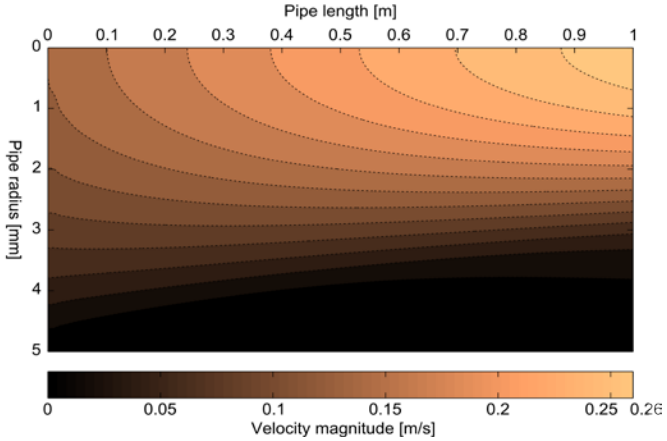

Figure 6. Velocity magnitude in the pipe. Flow from left to right

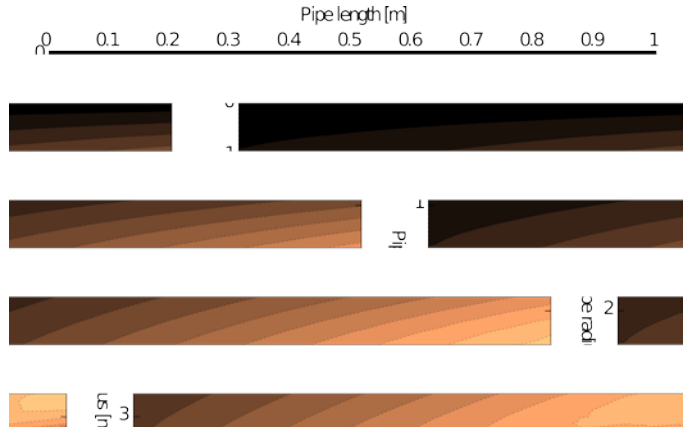

Figure 7. Shear rate fields in the pipe. Flow from left to right

Such behaviour can be explained by the history of the fluid parcels involved, as depicted on figure 8 with the example of a fluid parcel entering the domain at r_0=4.75 10^{-3} m.

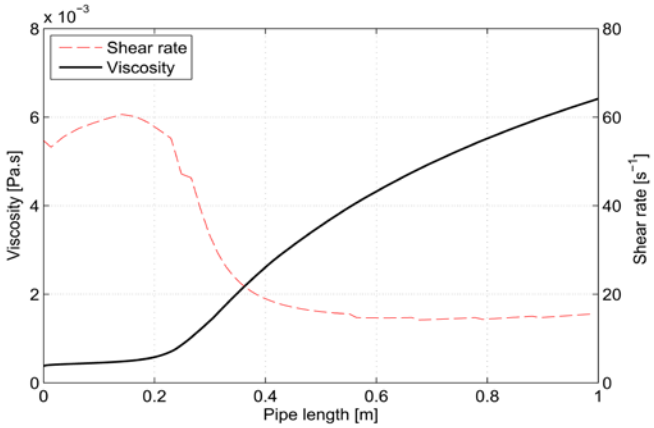

Figure 8. Viscosity and shear rate along the fluid parcel trajectory starting at r_0=4.75 10^{-3} m.

At the pipe entrance, the product is subjected to relatively high shear rate that enhance aggregation and leads to an increase of the viscosity. As the fluid parcel flows into the pipe, its viscosity reaches a critical value leading to the decrease of velocity and shear rate.

In the second part of the fluid parcel trajectory starting at a pipe length of about 0.25 m, the shear rate is limited and thus aggregation rate is lower. But aggregation goes on, so that the viscosity continues to increase (until about 6 10^{-3} Pa.s).

Such history is repeated for each fluid parcel, and can explain the low velocity and low shear rate near the pipe wall that are depicted on figure 6 and 7. This is particularly important as this behaviour explains that a large part of the product flows very slowly in the pipe and thus has a large residence time, explaining the output product properties dispersion.

CONCLUSION

The present work shows the feasibility and the interest of the Eulerian-Lagrangian approach for the modeling of fluid flow coupled with complex transformations. The transformation model can be easily improved, for example by including the effects of aggregates breakage, allowing a better prevision of the output product properties for a moderate numerical cost.
The proposed approach allows a complete description of the aggregation process. The size class distribution of the output product can be precisely determined without the need to use simplified PBE expression, as with the method of moments, which is mandatory with classical purely Eulerian method. Indeed, in the case proposed here, the PBE is evaluated on fluid parcels trajectories; and thus, the transformation doesn't have to be solved together with the Navier-Stokes equations, allowing the use of any pertinent transformation model.

ACKNOWLEDGEMENTS

The research leading to these results has received funding from the European Community's Seventh Framework Program (FP7/ 2007-2013) under the grant agreement n° FP7-222 654-DREAM.

REFERENCES

[1] Atteia, O. (1998). Evolution of size distributions of natural particles during aggregation: modelling versus field results. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 139(2), 171-188.
[2] Bremer, L.G., Bijsterbosch, B.H., Schrijvers, R., van Vliet, T., & Walstra, P. (1990). On the fractal nature of the structure of acid casein gels. Colloids and Surfaces, 51, 159-170.
[3] Thomas, D.G. (1965). Transport characteristics of suspension: VIII. A note on the viscosity of Newtonian suspensions of uniform spherical particles. Journal of Colloid Science, 20(3), 267-277.
[4] Kumar, S. & Ramkrishna, D. (1996). On the solution of population balance equations by discretization--I. A fixed pivot technique. Chemical Engineering Science, 51(8), 1311-1332.