PARTICLE AGGLOMERATION IN TURBULENT FLOWS

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RESUME

Nous présentons ici un modèle permettant de mieux simuler l'agglomération de particules dans un écoulement complexe. Ce modèle couple plusieurs approches: un calcul Eulérien pour le fluide porteur, un suivi Lagrangien stochastique des inclusions et une approche de type "Equilibre de population" pour l'agglomération. Un raffinement du modèle est introduit pour discrétiser le domaine en présence d'inhomogénéités dans la répartition spatiale des particules. Les performances et la précision de ce nouveau modèle sont évaluées par rapport à un calcul direct.

ABSTRACT

Here, we present a model for the simulation of particle agglomeration in complex flows. This model couples several approaches together: an Eulerian calculation of a fluid flow, a stochastic Lagrangian tracking of particles and a model for agglomeration based on PBE (Population Balance Equation). We have further refined this model to discretize the simulation domain depending on the presence of inhomogeneities in the spatial repartition of particles. The accuracy and efficiency of this model are evaluated by comparing it to direct simulations of agglomeration.

MOTS-CLÉS : particule, agglomération, quantification d'incertitutes / **KEYWORDS:** particle, agglomeration, uncertainty quantification

1. INTRODUCTION & CONTEXT

Particle agglomeration is the process whereby particles in a suspended flow interact together to form bigger particles. As described in numerous reviews/books (see e.g. Elimelech et al. (1995), Maximova (2006)), the agglomeration process is at play in a number of atmospheric applications (formation of droplets in clouds, volcanic fallout due to the agglomeration of particles together), oceanographic issues (formation of river delta or formation of chains of diatoms in the ocean) and industrial application (flocculation of un-desired particles in waste-water treatment facilities).

One of the key challenges related to particle agglomeration comes from the wide range of scales and mechanisms involved which makes it hard to model and simulate numerically. Agglomeration involves indeed various physical elementary objects (such as bubbles, droplets, solid inorganic particles, organic or biological particles) as well as different physico-chemical conditions (laminar or turbulent flows, electrolytes with or without polymers, etc.). It is thus a multi-disciplinary topic involving both hydrodynamics (for the transport of particles in a flow), interface chemistry (for the adhesion of particles to form clusters/aggregates).

The aim of this study is to come up with a more accurate simulation tool to capture the agglomeration of particles in complex flows. In particular, this study focusses on the main sources of errors in the simulation of particle agglomeration and tries to quantify the uncertainties related to these sources.

2. METHOD & RESULTS

The process of particle agglomeration encompasses two phenomena: aggregation (i.e. formation of larger particles) and fragmentation (i.e. breakup of large aggregates into smaller fragments).

The method used in the present study couples tools for the simulation of a fluid flow, particle motion and agglomeration. The turbulent fluid flow is simulated resorting to an Eulerian calculation and using standard turbulence models (here a RANS approach). Particle dynamics is then solved using a stochastic Lagrangian approach, i.e. by tracking a large number of particles in the flow (assuming that drag forces, gravity and Brownian motion are the leading terms in the particle equation of motion). Particle agglomeration is solved using Population Balance Equation (PBE), which describes the evolution of a population of particles in a given volume with time. In PBE formulations, particles are classified in terms of their size (usually a cluster labelled 'i' corresponds to an aggregate of 'i' particles).

The main difficulties that arises from the use of a PBE approach are the following: the particles are first assumed to be homogeneously distributed in the given volume and, second, an agglomeration kernel needs

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to be provided (it describes the frequency of agglomeration events between particles of a given size per unit time and unit volume).

Here, we quantify the uncertainties related to the use of such models on the accuracy of the results. For that purpose, numerical results are compared to direct simulations in simple cases where the agglomeration kernel is known (and by changing its value to assess the influence of this parameter on the results).

Besides, a new grid generation method is proposed in order to distinguish areas of high density from areas of low density, and therefore dividing the domain of study into several regions where, in each one, particles are distributed almost uniformly. This grid generation method is based on the PDF of the spatial distribution of particles to locate and separate regions of high/low densities. Then, applying PBE for each region, one can get a much more precise result. To quantify the error without such grid refinement techniques, we quantify the deviation from uniformity of the initial sample of particles. Results show that the method allows to correctly identify inhomogeneities in the spatial repartition of particles (see Figure 1). Besides, the precision of the numerical results obtained with this refinement seems to be inversely proportional to the number of particles (provided that $Np < 10^3$) and converges quickly (see Table 1).

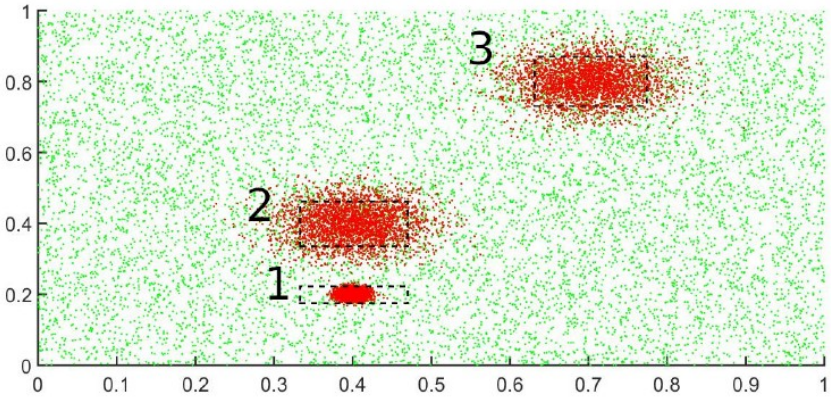

Figure 1. Identification of regions with higher densities of particles using the new grid generation method.

Table 1. Deviation of the results from the results from the theoretical value for a set of particles with 3 clusters (see Figure 1).

Number of particles	Mean score	Number of cells identified
10^2	0.02010	0.6
10^3	0.002740	1.4
10^4	0.001090	4.7
10^5	0.001070	2.9

3. CONCLUSION & PERSPECTIVES

This new grid generation method can help reduce the error made in the simulation of particle agglomeration in hydrid Euler/Lagrange approaches.

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