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Particle migration modeling in solid propellants

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Abstract. This work presents the development of an OpenFOAM solver to predict the migration of solid particles in concentrated suspensions under non-uniform shear flow. The solver modifies the *pimpleFoam* solver by implementing the conservation equation for particle volume fraction. It adapts the equation of motion for non-Newtonian flows and establishes a model for the viscous field using Krieger's correlation. The code is successfully validated by the experimental results from literature.

Introduction

Solid Rocket Motors (SRM) are commonly used in space propulsion. They provide additional thrust in the first phase of flight, either in conjunction with liquid engines (Ariane 5 and 6) or as the main thrust system (Vega C). While numerical modelling has considerably advanced [1, 2], there are still complex phenomena and uncertainties that make comprehensive performance descriptions challenging [3, 4]. Consequently, expensive testing is necessary to design and certify each SRM. The burning rate of the propellant plays a crucial role in predicting flight performance [2, 6, 7], affected by factors such as grain shape, particle orientation, air bubbles, and more [5, 8-14]. Manufacturing processes also impact ballistic performance [15-17], with macroscopic and microscopic phenomena potentially altering thrust profiles [18, 19]. One notable phenomenon is particle migration and segregation caused by the casting process, which gives rise to grain heterogeneity. All these aspects produce the so-called Hump effect, and its empirical evaluation is typically incorporated into internal ballistic simulations. However, a complete understanding and reliable prediction method for the Hump effect have not yet been achieved.

This study focuses on designing a CFD code using OpenFOAM [20] to simulate and describe particle migration. A bidimensional channel flow case is examined, and the simulation results are compared and validated against literature data. The validated approach can then be applied to simulate segregation phenomena in a motor. The paper is divided into two sections, one describing the developed model and the other presenting the results and validation using experimental data [21].

Theoretical model for particle migration

During the past few decades, it has become common knowledge that initially uniformly distributed particles will assume extremely nonuniform concentration distribution when subjected to a nonuniform shear flow. This non-homogeneous distribution is the result of a migration process which occurs at small values of particle Reynolds number ($\sim 10^{-4}$), so that the importance of inertial effects can be precluded. In general, solid particles will move from regions characterized by a higher shear rate to the neighbouring areas where lower values are measured.

The diffusive-flux model for the prediction of particle distribution ($\boldsymbol{\phi}$) resulting from shear-induced migration, has been developed by Phillips et al. [22]. In particular, two separate contributions to the segregation process are present, the first being related to the frequency of impacts between solid particles while the other depending mainly on the non-uniform viscosity field.

The conservation equation for solid particles in the Eulerian frame may be written as:

$$\frac{D\phi}{Dt} = a^2 K_c(\phi^2\nabla\dot{\gamma} + \phi\dot{\gamma}\nabla\phi) + a^2 K_\eta \nabla\cdot(\dot{\gamma}\phi^2\nabla \ln\eta(\phi)) \tag{1}$$

where $\dot{\gamma} = (2\mathbf{D}:\mathbf{D})^{1/2}$ (D being the deformation rate tensor) is the local value of the shear rate, K_c and K_η are two empirical constants, a is the solid particle diameter, and η is the viscosity.

The mathematical model for the viscosity is set following the work performed by Krieger in [23] through empirical observations.

$$\eta(\phi) = \eta_0\left(1 - \frac{\phi}{\phi_m}\right)^{-c} \tag{2}$$

where *c* is obtained by fitting the experimental data. The original fitting was performed for volume fractions in the range $0.01 < \phi < 0.5$, however, for the sake of simplicity, many papers assume the model to be verified on a wider range, that is $0.01 < \phi < 0.68$. The asymptote in correspondence of the volume fraction ϕ_m is due to the fact that, beyond such limit, usually referred to as maximum packing fraction, the dispersed particles will create a rigid structure, and the fluid will cease to flow. The maximum packing fraction is evaluated as a function of the geometry of the solid particles and the microstructure that they form within the fluid, the value for a monomodal packing of rigid spheres is usually set to 0.63, while for poly-dispersed packing, values are usually higher (up to $0.75 \div 0.80$). In this paper the chosen value for ϕ_m is 0.68 (in accordance with [24]).

Solver validation

The simulation of the bidimensional channel flow has been carried out for the duration of 12 seconds (time estimated for the reaching of steady conditions). The simulated channel is 35 mm and 1.7 mm wide. The time assumption shall be directly verified by considering the value of the variation of the volume fraction ($\Delta\phi$).

Considering the section of the channel at the position $L = 0.238$ m, i.e., where the data for the validation are going to be gathered, and the time t = 12 s, the maximum recorded value amounts to:

$$max\{|\Delta\phi|\}_L \cong max\left\{\left|\frac{\partial\phi}{\partial t}\right|\right\}_L \Delta t \cong 5.2\cdot 10^{-7} \tag{3}$$

It is evident how the variation has not achieved a zero value yet, however, since the order of magnitude is considerably narrow, and the profile peak is already close to the maximum value of packing, it is realistic to assume that the steady condition has been reached. It is hence possible to compare the results produced by OpenFOAM with the two references.

This comparison is performed in Fig. 1; with respect to the set of experimental data measured by Lyon & Leal [21] and the 1D and 2D models introduced by Ilyoung Kwon et al. in [24].

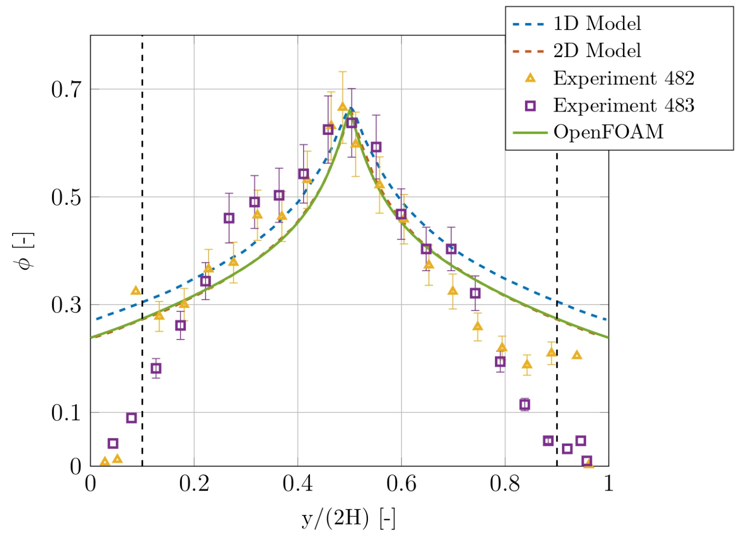

Figure 1: Comparison between OpenFOAM results and literature data of the particle distribution across the section of the channel (L = 0.238 m, t = 12 s). The 1D and 2D have been developed in [24], while the experimental data are measured in [21].

As it can be noticed, the OpenFOAM results emulate in a quite precise manner the behaviour of the 2D model. The global trend of the experimental data is respected, as the peak of the volume fraction is reached at the midpoint of the channel according to the theory and the observations. Furthermore, the right part of the curve, in the proximity of the centreline, appears to be quite close to the values of the two experiments. Adversely, on the left side, the situation is different, nonetheless, the reason may be also related to the precision of the measurements. Approaching the walls, the observed volume fraction diverges from the one predicted via CFD, the motivation might be due to the inaccuracy of the method adopted (i.e., LDV), which had the tendency to underestimate the particle concentration due to the drop of the signal-to-noise ratio caused by the solid boundaries.

Conclusion

The aim of this work was the development of an OpenFOAM solver aimed at correctly predicting the migration phenomenon that is experienced by the solid particles in concentrated suspensions when subjected to non-uniform shear flows. In order to simulate such behaviour, the conservation equation expressing the time variation of the particle volume fraction has been implemented in OpenFOAM. The chosen preexisting solver that has been modified is *pimpleFoam*, which discretizes the Navier-Stokes system of equation through the PIMPLE algorithm. As a first step, the formulation of the equation of motion has been adapted to correctly solve non-Newtonian flows. Successively, the model for the viscous field was established. The code implements the Krieger's correlation to include the viscosity variation over the domain due to the heterogeneity of the particle spatial distribution. Subsequently, the iterative cycle for the solution of the migration equation has been included within the time loop.

The above-mentioned code has been successfully validated by taking into account the measured data provided by the experiment of Lyon & Leal [21] and the results of the CFD code developed by Ilyoung Kwon et al. [24]. The flow that has been simulated in order to verify the capacity of the solver to approach the migration problem is a 2D channel flow. From the comparison between the results produced via OpenFOAM, with the finite volume discretization, and the data from literature it has been verified that the particles volume fraction ϕ is predicted in a quite satisfactory way. The various operations that compose the solver *migrationPimpleFoam* are suitable for a 3D flow; therefore, more complex scenarios might be simulated.

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