Modelling and numerical simulations of instabilities and mass transfer at interfaces in the acoustic resonance mixing process

2-year post-doctorate at I2M Bordeaux, from January 2024

Context

Many industrial sectors, such as pharmaceuticals or civil and military aeronautics, require the use of raw materials made from mixtures of constituents that are as homogeneous as possible to ensure the efficiency of the raw material. The most common industrial mixers are intrusive because they use rotating blades or a grid and require relatively long process times. To reduce mixing times, a new, non-intrusive technology using acoustic resonance (RAM) has been developed, based on vertical oscillation of the container containing the components. This induces both macroscopic convective movements and vortex micro-movements. The latter are generated throughout the volume to be mixed, unlike intrusive technologies where they are only present in areas close to the rotating blades, which improves mixing and enables a homogenous mixture to be obtained very quickly. As part of an ANR ASTRID project (SINRAM), a liquid (binder) and particles (fillers) are mixed in a tank partially filled with air at low pressure. The tank is set in oscillation, which generates complex physical phenomena: instabilities at the interface between the air and the binder, vortex micro-movements, collisions of solid particles with each other, variable rheology, viscous dissipation, and so on.

Objectives

The aim of this 2-year post-doctorate is to propose a 3D numerical simulation code for the RAM mixer, which will be used to understand the physical phenomena, to design highly homogeneous mixtures and to optimise the sizing of the mixer. More specifically, it will take into account: i) the effects of air compressibility, ii) instabilities at the air/binder interface (without particles and then in monodisperse solution), iii) the anisothermal conditions of the flow, and iv) the degassing kinetics taking into account the transport of air trapped in the binder and its transfer to the interface (but without interaction with the particles). All of this work will be carried out using the free and open source Notus code (https://notus-cfd.org). More specifically, the proposed work will focus on 2 aspects:

1) Compressible/incompressible two-phase solver

The simulation of the process must be able to take into account the non-negligible effects of compressibility in air and the incompressibility of the binder. Initially, we propose to continue the work developed in the laboratory [1] on a class of pressure correction type methods [2,3], based on the pressure evolution equation [4] and leading to the solution of a Poisson equation similar to that which would be solved for an incompressible flow, but including terms and specific coefficients relative to the compressibility of the flow. The proposed formulation will be compatible with the Volume-of-Fluid two-phase approach, and the interface between the binder and the air will be reconstructed linearly in the mesh using Weymouth's VOF-PLIC method [5]. Surface tensions will be taken into account by the Continuum Surface Force model and curvature by the height function method [6]. A non-Newtonian rheology of the binder could be considered, as well as heat transfer in the flow. In a second phase, the Philips model [7] and Krieger's law [8], which have already been implemented, will also be used to take account of the particles in the binder. Together, these methods will make it possible to simulate the tank containing the binder in vibration for different air pressures, and thus to reproduce the instabilities of the interface and the temperature increase of the mixture.

2) Outgassing and transfer at interfaces

In order to take account of the outgassing phenomenon in numerical simulations, it is necessary to develop suitable physical models that deals with the mechano-chemical coupling of air transport in the binder and its transfer to the binder/air interface, while respecting the concentration jump at the interface in accordance with thermodynamic equilibrium. At this stage, we will consider air as a dissolved entity in order to solve the transport and transfer at the interfaces using a single macroscopic advection/diffusion equation [9,10]. The 1-fluid model described in the previous paragraph will therefore be extended to take account of an air concentration. The equivalent fluid will be reconstructed as a function of the volume fraction of the fluid in the mesh and the air concentration. We propose to use a methodology developed in the laboratory and based on a species diffusion potential that has been used to simulate dissolution/precipitation mechanisms [11]. This

diffusion potential, which is continuous across the interface, would include in this project, in addition to the classical concentration-dependent term, terms relating to gravity and pressure.

Candidate profile
The post-doctoral student we are looking for should have strong skills in physical and numerical modelling of two-phase flows. He/she should have experience both in the use of parallel CFD codes (MPI) and in the implementation of numerical methods (FORTRAN2008).

Application
Please send a CV, a covering letter detailing your interest in the subject, PhD. thesis reports (manuscript and defence), and contact details of referees to the contacts below.

Contacts
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Bibliography
[1] J.-P. Caltagirone, S. Vincent, C. Caruyer, A multiphase compressible model for the simulation of multiphase flows, J. Comput. Phys. 50 (201
[2] G. Huber, S. Tanguy, J.-C. Béra, B. Gilles, A time splitting projection scheme for compressible two-phase flows. Application to the interaction of bubbles with ultrasound waves, J. Comput. Phys. 302 (2015) 439–468.
[3] A Urbano, M Bibal, S Tanguy, A semi-implicit compressible solver for two-phase flows of real fluids, Journal of Computational Physics 456, 111034, 2022.
[4] A Toutant, General and exact pressure evolution equation - Physics Letters A, Volume 381, Issue 44, 29 November 2017.
[5] G.D. Weymouth and D.K.-P. Yue. Conservative Volume-of-Fluid method for free-surface simulations on Cartesian-grids. J. Comput. Phys., 229:2853-2865, 2010
[6] M Owkes, O Desjardins, A mesh-decoupled height function method for computing interface curvature, Journal of Computational Physics 281, 285-300, 2015.
[7] Krieger, I. M. (1972). Rheology of monodisperse latices. Advances in Colloid and Interface science, 3(2), 111-136.
[8] Phillips, R. J., Armstrong, R. C., Brown, R. A., Graham, A. L., & Abbott, J. R. (1992). A constitutive equation for concentrated suspensions that accounts for shear-induced particle migration. Physics of Fluids A: Fluid Dynamics, 4(1), 30-40.
[9] Maes, J. and Soulaine, C. (2020). A unified single-field volume-of-fluid-based formulation for multi-component interfacial transfer with local volume changes. Journal of Computational Physics, 402.
[10] Zanutto, C. P., Paladino, E. E., Evrard, F., van Wachem, B., and Denner, F. (2022b). Modeling of interfacial mass transfer based on a single-field formulation and an algebraic vof method considering non-isothermal systems and large volume changes. Chemical Engineering Science, 247.
[11] Bordère, S. and Glockner, S. (2021). Numerical modeling of diffusion-controlled phase transformation using the darken method: Application to the dissolution/precipitation processes in materials. Computational Materials Science, 186.