A Multi-Scale Strategy for Computationally Simulating Turbulent Two-Phase Processes

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Summary

A strategy for computationally simulating processes involving turbulent two-phase flow is proposed that combines a coarse-grain Euler-Euler simulation for the whole-flow domain with local Direct Numerical Simulations (DNS). These DNS are carried out in periodic boxes while a forcing technique imposes the turbulent-flow conditions pertinent to specific positions in the whole-flow domain. The most difficult step of this strategy – feeding the results of the local DNS back into the Euler-Euler simulations - has not yet been realized however. This paper reviews a number of relevant computational results which may serve as stepping stones for such an approach.

Keywords

Multi-scale analysis; multiphase and particulate reactors

Introduction

Often, dilute two-phase flows are computationally simulated by means of an Euler-Lagrange (E-L) method: first, the flow of the continuous or carrier phase is calculated in an Eulerian framework (RANS - Reynolds Averaged Navier-Stokes, LES - Large Eddy Simulation, or DNS - Direct Numerical Simulation), after which the path of point particles is tracked in a Lagrangian way. This can be done one-way (the particles feel the flow of the carrier phase, while the latter does not feel the particles) [1] or two-way and iteratively [2]. At the same time, the moving, usually solid, particles may be subjected to physical [3] or chemical processes [4]. This strategy, however, may be limited to dilute flows in which the volume fraction of the particulate phase amounts to a few percent only.

For more dense flows, tracking all individual particles becomes computationally too intensive, although particles may be clustered to mimic mass loading effects [2]. The best alternative might be to pursue Euler-Euler (E-E), or two-fluid, simulations in which the two phases are conceived as two interpenetrating continua. Usually, this type of simulation is of the RANS type, although recently also results of an E-E LES have been reported [5]. Drastic assumptions as to how to model the turbulent character of the two-phase flow are not uncommon. In addition, in two-fluid models particle size is just a parameter in the phase interaction force for which an empirical expression is used – usually restricted to the steady-state drag force for a single particle in an unbounded uniform 1-D flow. Some papers (*e.g.*, [6]) present results from combining E-E with Population Balance Models taking into account varying particle size distributions, but this combination is still quite cumber-some and very time consuming.

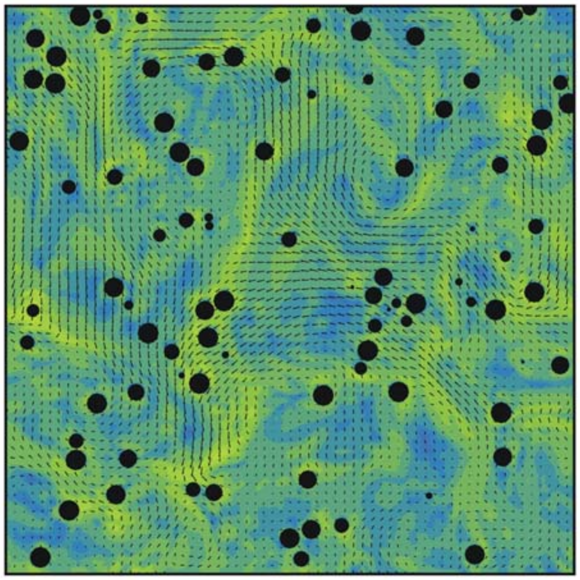

Figure 1 - Cross-sectional area through a periodic box showing the results of a DNS of an assembly of colliding particles subjected to forced turbulence

The Idea in a Nutshell

The strategy proposed in this paper is very different. The idea is to rely on a DNS in a small periodic box for mimicking the detailed two-way interaction between the turbulent carrier phase and the particles as well as the particle-particle interactions. This idea is best illustrated by the Figure 1 that shows how, thanks to a specific forcing technique [7], the flow field between colliding mono-sized spherical particles was completely resolved. Ten Cate *et al.* [8] present and analyze data as to the turbulence modulation in the carrier phase that is the result from the presence, the motion and the collisions of the particles. In this way, it is possible - by feeding different turbulence conditions (as prevailing at different positions in a vessel or reactor) to the periodic box via the forcing technique – to assess the response of the dense particle system to the spatially varying flow conditions in a vessel or reactor.

Pursuing on Ten Cate's approach, several more steps have to be made. First of all, the method has to be extended to (solid) particles of different sizes. More importantly, the method should be made applicable to fluid particles and allow for bubble/droplet coalescence and break-up in response to the local in-box turbulence level. Lattice-Boltzmann techniques seem to be very attractive to this purpose. An example of such an approach can be found in a paper due to Derksen and Van den Akker [9]. A novel result obtained by an in-house implementation of a Shan-Chen Multi-Component Multi-Phase Lattice-Boltzmann technique, is presented in Figure 2.

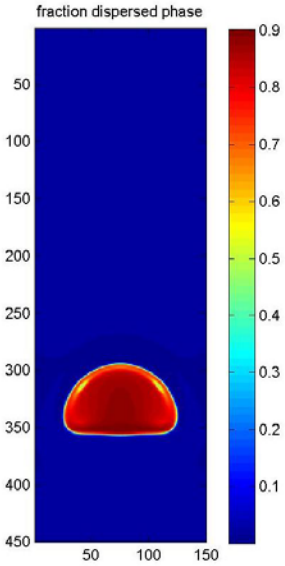

Figure 2 – A single gas bubble rising through a liquid.

The most challenging aspect of the strategy proposed in this paper, however, is about how to feed the results of the local DNS results back into a coarse-grained (RANS or LES) simulation of the whole vessel or reactor. One option would be to allow spatial variations of the bubble or drop size (distribution) resulting from spatial variations in turbulence level as found by means of local periodic-box DNS. Of course, important issues are then the (necessarily limited) number of periodic boxes which have to be carried out, and the spatial interpolation between the drop or bubble sizes found this way. *In situ* tabulation techniques such as those exploited in simulating turbulent flames could be useful here as well.

Combining RANS (or LES) for the vessel or reactor domain with several (tens?) periodic-box DNS in an iterative procedure really requires massive computer power. These days, however, computers have turned so fast and cheap that massive computations have become quite affordable – recently, Gillissen and Van den Akker [10] used more than 4 billion grid points distributed over 128 computers for a DNS of a stirred vessel operating under (just) turbulent conditions.

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