

Modeling liquid break-up through a kinetic approach

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ABSTRACT

Liquid atomisation is an important technical field for a wide range of engineering and industrial applications, particularly in the field of internal combustion engines. In these engines, in fact, the amount of pollutants at the engine-out interface is directly related to the quality of the combustion process, which is in turn determined by the quality of the air-fuel mixture preparation in Direct Injection (DI) engines. As a consequence numerical-experimental research is crucial to their development. Despite the significant amount of research that has been carried out on DI engines simulation, breakup modelling is still a challenge.

In this paper we present a new numerical model for multiphase flows that could be particularly suited for liquid jet and droplet breakup simulation. The model is based on a Lattice Boltzmann (LB) solver coupled to a higher order finite difference treatment of the kinetic forces arising from non-ideal interactions (potential energy). Direct comparisons with literature data for Rayleigh Taylor instability on a liquid jet and single droplet breakup are presented.

The analysis on the single droplet allows highlighting different regimes of secondary break-up of a liquid drop immersed in a continuous medium under the influence of a gravitational force.

INTRODUCTION

The growing concern with the environmental issues together with the customer desire of reduced specific fuel consumption and increased specific power output

have been pushing the development of automotive engines in the last two decades. In this scenario, the automotive industry has already significantly improved passenger car engine performances through the introduction of new technologies. Diesel fuel injection pressures have been increased up to 1800 bar and beyond and stratified charge DI gasoline engines are now close to the commercial stage, as the fully electronic controlled direct injection systems allow an accurate control of injection parameters. However, the new emission limits for the next years appear very severe targets to be reached. Together with the further development of after treatment strategies, that seem crucial for small passenger cars, a very accurate control of the combustion process is therefore needed to improve engine performances.

In DI engines liquid atomisation and the in-cylinder mixing between fuel and the surrounding gas are the processes that govern the entire combustion event. The atomisation phenomena are related to liquid surface instabilities due to several elements such as turbulence, cavitation, liquid-gas interaction etc. An accurate experimental characterisation of the atomisation phenomena is very difficult and onerous, particularly for the ligaments and droplets that form after the atomisation of the liquid column. Therefore, it is necessary to support the research with adequate numerical models that allow simulating the evolution of a two phase flow and the occurrence and the growth of surface instabilities. Moreover, as the dimensions of the post-breakup structures (ligaments and droplets) play a fundamental role in the following mixture formation process (coalescence, secondary breakup, vaporization, spray-wall interaction), their prediction is particularly

important for the design of the combustion chamber of modern internal combustion engines.

However, the task of simulating the behaviour of multiphase flows is very challenging, due to the inherent complexity of the involved phenomena (emergence of moving interfaces with complex topology, droplet collision and break-up), and represents one of the leading edges of computational physics [1,2]. As a matter of fact, a general computational approach encompassing the full spectrum of complexity exposed by multiphase flows is still not available.

The numerical methods based on the traditional continuum approach (i.e. Navier-Stokes with closure relationships) are usually based on rather complex correlations and often require transient solution algorithms with very small time steps.

Our research group is working on a new class of mesoscopic methods, based on minimal lattice formulation of the Boltzmann kinetic equation with the ambitious objective of performing the direct numerical simulation of the atomisation process, of the droplets breakup and of the coalescence process, thus limiting or avoiding the utilisation of turbulence models (i.e. LES models), as it is for traditional numerical techniques.

LBMs have gained significant interest as an efficient alternative to continuum methods based on the discretization of the NS equations for non ideal fluids [3]. The main philosophy of the LBM is to compute the physical reality of a flow field through a kinetic approach that preserves the hydrodynamic conservation laws, by taking into account groups of representative particles. It is important to underline that this approach is not purely microscopic-lagrangian, with the application of the molecular dynamics laws, but is more a statistical method with particle distribution functions f as the unknowns. The particle distribution functions (also called populations) represent the probability of finding a certain number of particles at a certain site, at a certain time and with a certain velocity. Summarising, the LBM is usually indicated as a mesoscopic method since it is something in the middle between microscopic and macroscopic.

The multiphase simulations presented here are performed by implementing in the LBM environment the model proposed by Lee et al. [4-7] and further developed by Chiappini et al. [8]. This method is based on a higher order finite difference treatment of the kinetic forces arising from non-ideal interactions (potential energy). This method allows tracking and maintain diffuse interfaces with no need of any special treatment of the interface (as in the well-known Volume Of Fluid - VOF technique) and without the presence of unphysical features (i.e. spurious velocities), typically encountered with other LB multiphase models [9].

The model is first tested for a gravity-driven Rayleigh-Taylor (RT) instability of a liquid jet and validated with literature data. Then we propose a detailed analysis of a

liquid droplet break-up in a continuous gas system. The aim of this test is to investigate the behaviour of the liquid drop by varying the Eotvos number and to compare results with literature data available. The relative velocity between two phases and the surface tension are the fundamental parameters for this study.

THE PARAMETRIC REGIMES

The dynamics of multiphase flows is characterized by a number of dimensionless parameters which measure the relative strength of the various competing mechanisms. Among others, the most important ones are the Weber

number, $We = \frac{\rho D U^2}{\sigma}$, measuring the competition

between inertia and surface tension, the Reynolds number, $Re = \frac{DU}{\nu}$, measuring the ratio of inertia and

dissipation, and the Eotvos number defined below, expressing the relative strength of external drive (e.g. gravity) versus surface tension effects. In the above ρ

is the liquid density, U the typical speed, D the typical droplet diameter, σ the surface tension, ν the liquid kinematic viscosity. In practical applications involving the motion of small liquid droplets moving across a continuum gaseous phase, the Weber and Reynolds numbers can reach up to several thousands. It is therefore of interest to provide a semi-quantitative assessment of the capability of the present method to reach up these parametric regimes. To this purpose, we remind the main limitations inherent to the LB models in general. These read as follows:

- $U_{LB} < 0.1$ (finite-compressibility constraint);
- $\nu_{LB} \sim 0.01$ (dissipative stability constraint);
- $\sigma_{LB} < 1.0e^{-3}$ (surface tension stability constraint).

The first constraint stems from the fact that LB is a weakly-compressible scheme, based on a small-Mach number perturbation of the local Maxwellian equilibria. As a result, if the local flow speed gets in the proximity of the sound speed $c_s = 1/\sqrt{3}$, the LB local equilibria may become negative, thereby ruining the stability of the scheme. The second constraint is related to the fact that if the viscosity becomes too low, typically 0.01 in lattice units, local gradients of the flow field can develop, which may undermine the very basis of the hydrodynamic limit, namely a weak departure from local equilibria. Both constraints are well known from the single phase LB literature [15]. The third constraint is inherent to the present LB-FD formulation of non-ideal fluids. Indeed, our direct numerical experience shows that it is very hard to bring the surface tension above $\sigma_{LB} \sim 1.0e^{-3}$ without experiencing numerical instabilities. It is of interest to observe that this value is about the same as the

smaller than the typical surface tensions with the (standard) Shan-Chen model. This is most likely due to the different expression of the discrete forcing term, which in the Lee's case involves second-neighbors, while the standard Shan-Chen scheme only involves first-order neighbors (more precisely, the first Brillouin zone, including the diagonal neighbors). In this respect, it would be of interest to compare the Lee method with recent multi-range formulations of the Shan-Chen model. Based on the above constraints, a resolution of 1000x1000 grid points permits to explore approximately the following range:

- $Re = \frac{D_{LB} U_{LB}}{\nu_{LB}} \leq 1000$
- $We = \frac{\rho_{LB} D_{LB} U_{LB}^2}{\sigma_{LB}} \leq 1000$

These appear reasonably close to the one encountered in many applications.

THE DIMENSIONLESS APPROACH

When a liquid is injected into a gas, disturbances on the jet surface appear because of the aerodynamic interactions between the jet and the surrounding ambient. The disturbances on the surface of the jet grow and become large scale coherent structures that interact with the gas-phase and break up into smaller scale droplets. Then the non-homogeneous pressure distribution on the surface of the droplet leads to shape deformation and then to atomization into smaller droplets. These processes are referred to as primary and secondary break-up. Various models have already been developed for the secondary breakup process, as the front tracking method [2,10] or the statistical representation of fluid particles [11-13]. Moreover there are a large number of hybrid empirical/numerical methods which are based on the definition of characteristic lengths and sizes and allow studying the behaviour of group of identical and non interacting droplets that exchanges mass momentum and energy with the surrounding air.

In order to facilitate the comparison with other models and to extend the analysis to any liquid and gaseous media, the present study is performed using a dimensionless approach [1,2] based on the following parameters:

- Density Ratio - R
- Viscosity Ratio - M
- Ohnesorge Number - Oh
- Eotvos Number - Eo

The density ratio is defined as follows:

$$(1) \quad R = \frac{\rho_d}{\rho_0}$$

where ρ_d represents the liquid density and ρ_0 the continuous medium density. This parameter rules the magnitude of the interaction forces, as when R is large the effect of the surrounding fluid is weaker and the heavy fluid element travels a longer distance before breaking up. The density ratio is characteristic of the interacting media and it implicitly depends on the operating conditions, as the continuous medium is treated as a compressible gas.

In the following, the subscripts d and 0 will refer to the liquid phase, and the continuous medium, respectively.

The viscosity ratio, defined as:

$$(2) \quad M = \frac{\mu_d}{\mu_0}$$

allows establishing the interaction between the two phases while the interface is modifying its shape. The viscous stresses have, in fact, a deep influence on the interface deformation.

The viscosity ratio is sometimes replaced by the Ohnesorge number, which is a dimensionless group that combines the Reynolds and Weber numbers as follows:

$$(3) \quad Oh_d = \frac{\mu_d}{\sqrt{\rho_d D \sigma}} = We_d^{1/2} Re_d^{-1}$$

$$(4) \quad Oh_0 = \frac{\mu_0}{\sqrt{\rho_0 D \sigma}} = We_0^{1/2} Re_0^{-1}$$

where D represents the diameter of the drop and σ the surface tension between two phases. The Oh is one of the most fundamental dimensionless parameter to classify jet disintegration in fluid mechanics.

Fixing the density ratio and the Ohnesorge number for both the liquid and the continuous medium, the viscosity ratio is automatically determined.

The last dimensionless parameter crucial for the present analysis is the Eotvos number (sometimes called also Bond number) expressing the ratio of body forces (often gravitational) to surface tension forces:

$$(5) \quad Eo = \frac{a \Delta \rho D^2}{\sigma}$$

The Eo is commonly used to classify the breakup regime of a liquid droplet under a constant acceleration (a) [1, 14]. It is important to highlight that the Eo expression contains the term $\Delta \rho$ (i.e. the difference between densities) and not the density ratio previously defined, as