

Lattice Boltzmann Modeling of Diesel Spray Formation and Break-Up

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ABSTRACT

Spray formation and break-up are crucial phenomena for mixture formation inside diesel engines, both for combustion control and pollutant formation. Since the emission restrictions have become more and more severe in the last years, many studies have been conducted in order to improve diesel injection. Numerical simulations have proven to be reliable in producing results in a faster and cheaper way than experimental measures. The recent great progresses in computer science, then, have allowed to reach great accuracy in the simulations.

In this work, a novel methodology based on Boltzmanns Kinetic Theory is applied to diesel injection. Lattice Boltzmann BGK (LBGK) provides an alternative method for solving fluid-dynamic problems and allows even superior accuracy as compared to conventional CFD.

The multiphase approach used in this paper to study spray formation and primary is based on the works by Shan and Chen and their successive modifications.

The results are compared to those predicted by means of the most accredited models in literature.

INTRODUCTION

The break-up of a liquid jet is governed by different mechanisms, depending on the relative velocity and other physical properties of the liquid and the surrounding gas, [1].

The different mechanisms are usually individuated according to the distance between the nozzle and the location in which the first droplet separates, the so-called *break-up length* and to the size of the separating droplets. According to Reitz and Bracco [2], four regimes can be distinguished, as reported in Fig. 1: the Rayleigh regime, the first and second wind-induced regimes and the atomization regime.

A quantitative description of the break-up process was performed by Ohnesorge [3], who performed measurements of the intact jet length and showed that the disintegration process can be described by means of two adimensional groups, the liquid Weber number and the Reynolds number:

$$We_l = \frac{u^2 D \rho_l}{\sigma} \quad (1)$$

<figure 1 here>

$$Re = \frac{u D \rho_l}{\mu_l} \quad (2)$$

in which the subscript *l* stands for the liquid phase.

By eliminating the jet velocity *u*, Ohnesorge derived his adimensional group,

$$Oh = \frac{\sqrt{We_l}}{Re} = \frac{\mu_l}{\sqrt{\sigma \rho_l D}} \quad (3)$$

The primary break-up process play a major role in the subsequent mixture formation inside the combustion chamber, thus the modeling of the transition from the nozzle to the dense spray is essential. Since the Lagrangian description of the liquid phase requires the existence of droplets, the spray simulations usually begin with such drops penetrating the combustion chamber: the task of a primary break-up model is to determin the starting of these drops and their physical properties.

There are very few detailed models in literature for the simulation of the primary break-up regime of high-pressure sprays, since the experimental setup is very difficult due to the small dimensions characterizing the phenomena and the high velocities related to the jet breaking-up. The different classes of break-up models are concerned with the mechanisms treated, such as aerodynamic-induced, turbulence-induced and cavitation-induced break-up, and all of such models have their special field of application [1].

The aim of this work is to apply a simulation technique based on the Boltzmann Kinetic Equation [17], different from the ordinary Navier-Stokes equations, to the study of primary break-up in diesel jets. It is the first time that a direct numerical simulation of the liquid jet break-up is conducted by means of the Lattice Boltzmann Method with the multiphase approach by Shan and Chen [19, 20] and its recent enhancements, [21, 22].

First of all, the description of the computational domain is presented, in which, for the first time for a multiphase application based on the Shan-Chen equation of state, a different level of grid spacing is used. Then, the evolution of liquid jet in time is followed with peculiar attention to the Rayleigh break-up regime and for different Weber numbers. The results are finally compared to those present in literature.

THEORETICAL BACKGROUND

BREAK-UP OF A LIQUID JET

Figure 2 shows the break-up curve as a function of the jet velocity u , [1, 2]. As shown in Fig. 2, at very low velocities, drip flow occurs and no jet forms. As the liquid velocity u increases, an unbroken jet forms, whose length increases with the velocity. This regime is called the Rayleigh break-up: the breaking-up of the jet occurs due to the growth of axisymmetric oscillations of the complete liquid volume, initiated by liquid inertia and surface tension forces [1]. The droplets are pinched off the jet and their diameter is larger than the nozzle one [26, 27, 28, 29].

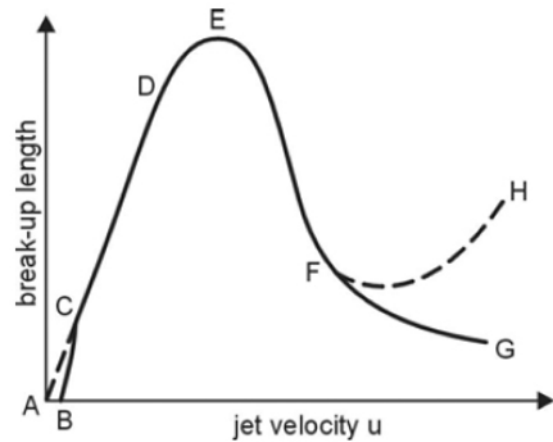


Figure 2. Jet break-up length as a function of the jet velocity u [1, 2]. ABC: drip flow; CD: Rayleigh break-up; EF: first wind-induced break-up; FG (FH): second wind-induced break-up; beyond G (H): atomization regime.

A further increase in the jet velocity results in a decrease of the break-up length, which still remains a multiple of the nozzle diameter. The average droplet size decreases to the range of the nozzle diameter: this is the first wind-induced regime [2]. In the second wind-induced regime, the flow inside the nozzle becomes turbulent and the jet break-up occurs due to the unstable growth of short wavelength surface waves, generated by jet turbulence and amplified by aerodynamic forces due to the relative velocity between liquid and gas [1]. The jet no longer breaks up as a whole and the resulting drops are smaller in diameter than the nozzle.

In the atomization regime, a conical spray develops, with the spray divergency beginning immediately after the jet leaves the nozzle.

Criteria for predicting the onset of break-up regimes have been reviewed by Chiegie and Reitz [30]. Ranz [31] found that dripping from the nozzle exit stops occurring if $We_l > 8$,

where $We_l = \frac{\rho_l u^2 2a}{\sigma}$, with a the nozzle radius. The Rayleigh break-up regime takes place when the We_g number is below a critical value, that is

$$We_g < 0.4 \text{ or } 1.2 + 3.41 Oh^{0.9} \quad (4)$$

with Oh the Ohnesorge number: the above threshold corresponds to the point where the inertia force of the surrounding gas reaches about 10% of the surface tension force [1, 32].

Ranz [31] argued that the gas inertia force is of the same order as the surface tension force when We_g approaches the

value of 13: this can be used as a definition of the end of the first wind-induced regime, which occurs when

$$1.2 + 3.41 Oh^{0.9} < We_g < 13 \quad (5)$$

The stability of the liquid jet surface to linear perturbations, which is of major concern for the rising of the break-up, was examined by Reitz and Bracco [2] and a dispersion equation was derived to relate the complex frequency ω of an initial perturbation of infinitesimal amplitude, to the wavelength Λ . The real part Ω of the complex frequency represents the growth rate. Reitz [24] generated curve-fits of numerical solutions to the dispersion equation for the maximum growth rate and for the corresponding wavelength [25]:

$$\frac{\Lambda}{a} = 9.02 \frac{(1 + 0.45 Oh^{0.5})(1 + 0.4 T^{0.7})}{(1 + 0.87 We_g^{1.67})^{0.6}} \quad (6)$$

$$\Omega \frac{\rho_l a^3}{\sigma} = \frac{0.34 + 0.38 We_g^{1.5}}{(1 + Oh)(1 + 1.4 T^{0.6})} \quad (7)$$

in which $T = Oh We_g^{0.5}$. As it is possible to see from eqs. 6 and 7, the maximum wave growth rate increases and the corresponding wavelength decreases rapidly as the value of the Weber number increases, while the increasing viscosity has a sensible effect in the opposite direction: an increase in the liquid viscosity, in fact, reduces the wave growth rate and increases the wave length.

LATTICE BOLTZMANN MODELS

It is well known that the LBGK method originates from lattice gas automata (LGA) method [4], a simplified fictitious molecular dynamics in which space, time and particle velocities are all discrete. Recently it has been shown that the LBGK method can also be viewed as a special discrete scheme for the continuum Boltzmann BGK equation for discrete velocities [6, 7, 8]

$$\frac{\partial f_i}{\partial t} + c \mathbf{e}_i \cdot \nabla f_i = -\frac{1}{\tau_0} (f_i - f_i^{eq}) \quad (8)$$

Where $f_i(\mathbf{x}, t)$ is a real number describing the particle distribution function (DF) at the site $\mathbf{x}$ and time t moving with speed c along the direction $\mathbf{e}_i$ (9 for 2D simulation and 15 or for 3D, [5]) associated with a uniform Cartesian lattice, τ_0 is the relaxation time and $f_i^{eq}(\mathbf{x}, t)$ is the equilibrium distribution function depending of the macroscopic variables of the flow. From the kinetic point of view, same new LBGK schemes has been proposed to extend the capability of the

method [9, 10, 11, 12, 13]. Actually any standard discrete scheme will serve the purpose of solving equation 8. This viewpoint also provides a way to understand the basis of the LBGK method, and an alternative approach to design LBGK models for complex system [14, 15]. In what follows, we will propose a scheme to solve eq. 8. We start from a time splitting of equation 8,

$$\frac{\partial f_i}{\partial t} = -\frac{1}{\tau_0} (f_i - f_i^{eq}) \quad (9)$$

$$\frac{\partial f_i}{\partial t} + c \mathbf{e}_i \cdot \nabla f_i = 0 \quad (10)$$

The advantage of this replacements is that the collision and propagation steps are treated with different numerical schemes respectively. In practical computation of equations 9 and 11 are solved sequentially, at each time step equation 9 is solved first and a new value of f_i is the used to solve equation 10. The solution of equation 9 is trivial since no spatial derivative is involved. We simply discretise it with an explicit Euler scheme:

$$f_i^+(\mathbf{x}, t + \Delta t) = f_i(\mathbf{x}, t) - \frac{1}{\tau} [f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)] \quad (11)$$

Where $\tau = \tau_0 / \Delta t$ is the dimensionless relaxation time and Δt is the time increment. The relaxation time is linked to the gas viscosity through the expressions:

$$\nu = \frac{(2\tau - 1)}{6} \frac{\Delta x^2}{\Delta t} \quad (12)$$

Clearly the collision (relaxation) process is the same as standard LBGK model; numerical stability requires that $\tau \geq 0.5$. There are many well know numerical scheme to solve the linear equation 10. Here will use an explicit two level three points scheme in general form:

$$\begin{aligned} f_i(\mathbf{x}, t + \Delta t) &= p_0 \cdot f_i(\mathbf{x}, t) + \\ &+ p_{-1} \cdot f_i(\mathbf{x} - \mathbf{e}_i \Delta t, t) + \\ &+ p_1 \cdot f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t) \end{aligned} \quad (13)$$

with $f_i(\mathbf{x}, t) = f_i^+(\mathbf{x}, t)$ and where p_0, p_1, p_{-1} are parameters that satisfy the following constrains:

$$p_0 + p_{-1} + p_1 = 1 \quad (14)$$

$$p_{-1} - p_1 = A \equiv c \frac{\Delta t}{\Delta x} \quad (15)$$

in which Δx is spacing uniform lattice, if let $p_1 = 0.5 \cdot (d - A)$, $p_{-1} = 0.5 \cdot (d + A)$ and $p_0 = 1 - d$, it is possible to rewrite equation 13 in the following form:

$$\begin{aligned} f_i(\mathbf{x}, t + \Delta t) = & f_i(\mathbf{x}, t) + \\ & + \frac{d}{2} [f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t) - 2f_i(\mathbf{x}, t) + f_i(\mathbf{x} - \mathbf{e}_i \Delta t, t)] - \\ & - \frac{A}{2} [f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t) - f_i(\mathbf{x} - \mathbf{e}_i \Delta t, t)] \end{aligned} \quad (16)$$

It can be shown that the truncated error of the scheme given by equation 16 for the numerical solution of equation 10 is

$$\begin{aligned} R(\mathbf{x}, t) = & \frac{1}{2} [A^2 - d^2] \Delta x^2 (\mathbf{e}_i \mathbf{e}_i : \nabla \nabla) f_i + \\ & + O(\Delta t^3) + O(\Delta x^3) \end{aligned} \quad (17)$$

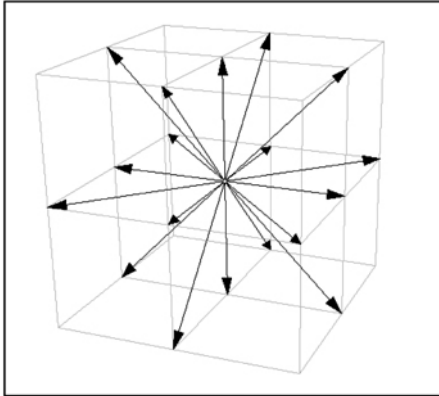


Figure 3. Sketch of a D3Q19 Lattice.

This means that this numerical technique presents a second approximation order both in time and space: a simple stability analysis results in the numerical stability condition

$$A^2 \leq d \leq 1 \quad (18)$$

Finally the combination of the collision scheme given by equation 11 and the propagation scheme given by equation 13 or 16 constitutes a lattice BGK model with general propagation. If the *EDF* is chosen appropriately correct hydrodynamic equations can be derived from equation 8 by means of a multi-scaling expansion [16]. In our simulation we use a lattice with 19 velocities as shown in Figure 3. The lattice velocity $\mathbf{e}_i$ is proportional to the sound velocity c_s , that

in the case of isothermal and incompressible fluid flow is linked to pressure and temperature through the equation of state (*EOS*) that, once written in lattice units, assumes the form:

$$\frac{p}{\rho} = c_s \quad (19)$$

While the link between the lattice velocity and the speed of sound for our model assume the form:

$$c_s = \frac{|\mathbf{e}_i|}{\sqrt{3}} \quad (20)$$

After the propagation and the collision phase it is possible to evaluate the macroscopic fluid properties by means of the following simple expressions:

$$\rho(\mathbf{x}, t) = \sum_{i=0}^{N-1} f_i(\mathbf{x}, t) \quad (21)$$

$$\rho \mathbf{u}(\mathbf{x}, t) = \sum_{i=0}^{N-1} \mathbf{e}_i f_i(\mathbf{x}, t) \quad (22)$$

Finally the equilibrium function assume the form:

$$\begin{aligned} f_0^{(eq)} &= \frac{1}{3} \rho \left(1 - \frac{3}{2} \mathbf{u}^2 \right) \\ f_i^{(eq)} &= \frac{1}{18} \rho \left[1 - \frac{3}{2} \mathbf{u}^2 + \mathbf{e}_i \mathbf{u} \cdot \left(3 + \frac{9}{2} \mathbf{e}_i \mathbf{u} \right) \right] \\ &\text{with } i = 1, 6, 11, 12, 13, 14; \\ f_i^{(eq)} &= \frac{1}{36} \rho \left[1 - \frac{3}{2} \mathbf{u}^2 + \mathbf{e}_i \mathbf{u} \cdot \left(3 + \frac{9}{2} \mathbf{e}_i \mathbf{u} \right) \right] \\ &\text{with } i = 2, 3, 4, 5, 7, 8, 9, 10, 15, 16, 17, 18, 19; \end{aligned} \quad (23)$$

MULTIPHASE FLOWS

Many applications in modern science and technology, however, need to investigate significantly more complicated problems, such as fast flows with substantial heat transfer, compressibility, chemical reactions and phase transition: to handle this much broader context a new generation of LBE's is called for. A very elegant way of generalizing LBE according to the above specifications is to convey the new physical effects into a generalized force term: