FEASIBILITY STUDY ON MULTI-PHASE FLOW SIMULATION OF FUEL INJECTION USING LATTICE BOLTZMANN METHOD

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Keywords: *Lattice Boltzmann equations, atomization model, fuel spray nozzle, numerical method*

Abstract

General engineering challenge is the multi-phase flow simulation of the fuel injection system in the internal combustion engine such as aircraft engine. Although the dynamics of the phase interface, atomization and evaporation process of fuels are not well understood, it plays a vital role in the efficiency of burning process. Hence, in this paper, the emphasis has been laid on studying the feasibility of the Lattice Boltzmann Method (LBM) for modelling such a complex physical process as a column and surface break-up mechanism and vaporization, which are partially included and followed by fuel spray nozzle. Minimal forms of discrete Boltzmann equations prove capable of doing away with most computational complexities of the true Boltzmann equation, while still retaining a satisfactory degree of physical realism. The LBE method has been successfully applied to simulate droplet interactions, droplet deformation and break-up and spreading, free-surface phenomena. So we try to develop an appropriate robust finite difference LBM to achieve the enough stability for simulation of multi phase and multi component flow. Thus the Shan Chen intermolecular force is used and second order Strang time split algorithm applied for solving LBM. In addition implicit trapezoidal integral can handle the stiff Ordinary Differential Equation (ODE) appears in time splitting and the Total Variation Diminishing (TVD) is applied for advection part because of high density jump across the border of different phases. These well developed techniques could help us to reach enough stability for simulation of droplets dynamics.

1 Introduction

A gas turbine combustor is a complex combustion system, in which there are a wide ranges of coupled, interacting physical and chemical phenomena. The liquid fuel is used as the energy source must be atomized into smaller droplets in order to increase the surface of fuel exposed to the hot gases and to facilitate rapid gasification and mixing with the oxygen rich ambience. Spray dynamics and combustion studies are extremely important to determine flame stability behaviour at different operational condition to satisfy uniform combustion and oscillation free constant fuel flow rate to ensure safe and efficient utilization of energy. The atomization and initial droplet condition has the most significant effect on combustion performance and emission beside the motion and evaporation of the fuel droplets, which rather depend upon the proper integration of the fuel nozzle with the combustion system and fluid- and thermo-dynamical properties of the mixture. Moreover, the detailed analytical and numerical investigation of atomization process allows deeper insights, as well as the better understand the mechanisms of pollutants formation and destruction as a part of chemical process belongs to the combustion evolved together with certain noise level and durability. However, due to its complexity, the modelling of the atomization process is a very challenging problem and it is influenced by several factors as the aerodynamic liquid-gas interaction, the inner nozzle disturbances, the nozzle geometry, and the thermo-physical properties of fuel and air.

Nowadays, the fuel spray nozzles utilize the airspray principle, which employs high velocity air instead of high velocity fuel to cause atomization. This method allows atomization at low fuel flow rates thus providing an advantages over the so called "pressure jet atomization" by allowing fuel pumps of lighter construction to be used.

Generally, concerning the spatial location of the atomization process, it can be categorized into two break-up regimes. The first one is the inner-nozzle disturbances due to cavitations, which may lead to the liquid fragmentation within the injector. The second one is the ambient disintegration caused by the pressure waves and aerodynamic forces occur in the outside of the nozzle exit. Considering today's widely used fuel spray nozzles – which utilize the airspray principle – the focus is placed on the ambient disintegration in followings. The entire process of the combustion can be divided into four main segments as atomization (primary and secondary), transport (turbulent diffusion, dispersion and modulation), vaporization, and turbulent combustion. In the atomization region, the liquid column is disrupted into ligaments, fragments, clusters and droplets due to the hydrodynamic instabilities as a primary break-up. At this early stage of atomization two main mechanisms can be distinguished, which are known as surface break-up mechanism and the column break-up mechanism. The surface break-up mechanism is characterized by the gradual erosion of the jet, as droplets are stripped off from the sides of the liquid jet by the shearing action of the flow, leaving the core untouched. The column break-up mechanism is initiated by the growth of waves on the surface and in the inner part of the jet, which finally lead jet fracture across the wave, giving rise to the formation of ligaments and clusters of fragments. The dense spray region has significant liquid volume fraction and includes secondary break-up of drops and ligaments as well as drop-drop interactions, such as collisions and coalescence. In the dilute spray region, droplets are well formed and have strong interaction with turbulent airflow, by which heat, mass and momentum are exchanged intensively between components as a benefit of higher mixture rate coupled with intensive vaporization until the temperature reaches the ignition temperature.

There are numerous top-down mathematical approaches for modelling liquid break-up mechanism usually governed by continuum mechanics based macroscopic type empirical correlations. In several cases, the break-up of the liquids are caused by the aerodynamic forces as a result of hydrodynamic instabilities on the liquid-gas interface such as either Rayleigh-Taylor or Kelvin-Helmholtz instabilities. The Rayleigh-Taylor instability is due to inertia of the denser liquid opposing the system acceleration in a direction perpendicular to the interface of the denser fluid and the Kelvin-Helmholtz instability is caused by the viscous forces due to the relative motion of the fluids. Based on linear instability analyses of a 2D viscous incompressible flow moving thorough an inviscid incompressible gas, Reitz and Bracco [1] characterized the break-up regimes as follows: 1. Rayleigh break-up, 2. first wind-induced break-up, 3. second wind-induced break-up and 4. atomization, which are based on Reynolds and Weber numbers. In the first two regimes, the size of drops is greater than or equal to the nozzle diameter and the break-up occurs at distances far from the nozzle exit. In the last two regimes the drops sizes are the same order as the nozzle diameter and they are produced near to the nozzle exit. Intensive researches have been progressed to improve knowledge on the various kinds of instability [1-3], which are combined with some experimental observations to form the basis on the atomization and droplet break-up modelling of liquid sprays frequently used nowadays sorted by primary atomization models as Sheet Break-up, Air Blast, Blob Jet and BLS (Boundary-Layer Stripping) and secondary droplet break-up models as Rayleigh-Taylor, TAB (Taylor Analogy Break-up) and ETAB (Enhanced Taylor Analogy Break-up) [4]. In case of Sheet Break-up primary atomization model by Schmidt at al [5,6] for instance – which is preferable at pressure swirl atomizer – simple physical concepts has been utilized to determine the parameters of the spray and includes a limited number of empirical constants for the

calculation of injection velocity. The Air Blast atomization model is essentially based on the idea of pressure-swirl atomization model as the primary atomization of an air blast injector is based on the aerodynamic analysis involving the Kelvin-Helmholtz instability of a liquid jet in an incompressible gas. However, it differs from the pressure-swirl atomization model in the determination of the initial sheet velocity and thickness. The Blob Jet injection model is based upon the Hinze's assumption (1948), by which the dynamics of a liquid sheet break-up is indistinguishable from those of a train of globules with equal diameters. The atomization mechanism of the BLS model actually describes mass shedding due to aerodynamical shear. The origin of TAB type models have been proposed by O'Rourke and Amsden [7]. The approach is based on the Taylor analogy between an oscillating/distorting drop and a forced spring-mass system.

Over the mentioned statistical approaches, one of the most promising models, amongst the higher level approximations, is the Large Surface Structure (LSS) model based on level set/vortex sheet method initiated by Large Eddy Simulation (LES) [8]. The basic idea of the LSS model is to split the treatment of the primary break-up process into two parts. All phase interface dynamics occurring on scales larger than the local grid size are explicitly resolved and tracked by a level set approach, whereas interface dynamics occurring on subgrid scales are described by an appropriate subgrid model. The LSS subgrid model separates out all broken or subgrid scale liquid drops and transfer them to a secondary break-up model.

The different models in the presented review are still based on continuum mechanics, which has a limitation in Knudsen number point of view. There are wide ranges of massively developed disciplines introduced in aeronautical sciences as mechatronics or MEMS (Micro-Electro-Mechanical Systems) with applications of combustion chamber and afterburner technologies, which are out of the simulation scope based on Euler or Nevier-Stokes equations. Hence, more complex numerical approach has been proposed for modelling atomization process over the entire range of Knudsen number scale.

Although the bottleneck of the Lattice Boltzmann (LBM) method is the computational cost, due to the high evolution of computer science and technology, the LBM approach can come into prominence to solve complex problem of primary and secondary break-up mechanisms. The lattice Boltzmann method can be regarded as one of the simplest microscopic, or particle, approaches to modelling macroscopic dynamics. It is based on the Boltzmann transport equation for the time rate of change of the particle distribution function in a particular state. The Boltzmann equation simply state that the rate of change is the number of particles scattered into that state minus the number scattered out of that state. The molecular dynamics based LBM approach is more suitable compared to models of macroscopic dynamics – based on continuum mechanics – for understanding the fundamental interactions of different physics, implementing complex boundary conditions, schemes and parallelization techniques that underlie macroscopic phenomena.

2..Basic Formulations of Boltzmann Equation

The Boltzmann equation [9] is an equation for the time t evolution of the distribution (properly a density) function *f(x, p, t)* in one-particle phase space, where x and p are position and momentum, respectively.

$$\frac{\partial f}{\partial t} + v\nabla f + F\nabla_v f = \left(\frac{df}{dt}\right)_{collision} \qquad (1)$$

where the left hand side accounts for the changes in *f* due to motion of the particles and the external forces *F* acting on them, and the right hand side accounts for the changes in f due to collisions between the particles. The mass of particles of gas is considered unit as a fluid with density

$$\rho(r,t) = \int f(r,v,t)d^3v \qquad (2)$$

and average (macroscopic) velocity

$$u(r,t)=\frac{1}{\rho(r,t)}\int v\cdot fd^3v \qquad (3)$$

The average velocity is determined by the current or particle flux

$$j(x,t)=\int v\cdot fd^3v \qquad (4)$$

This is the first moment in the velocity of the distribution. The second moment determines the momentum flux tensor

$$\Pi_{ij}(r,t)=\int v_i v_j fd^3v \qquad (5)$$

3..Single Relaxation Time (BGK) Ansatz

If the system is not in equilibrium, it will relax towards equilibrium. In general, this relaxation can be very complicated. Relaxation is effected by the collision term in the Boltzmann equation, which can be written schematically

$$\left(\frac{df}{dt}\right)_{collision}=\int\int\left(f_1'f_2'-f_1f_2\right)v_{rel}\sigma d^3vd\Omega \qquad (6)$$

where σ is the differential scattering cross section for the two-particle collisions

$$v_1+v_2\rightarrow v_1'+v_2' \qquad (7)$$

and v_{rel} is the relative velocity and Ω is the scattering direction in the centre of mass system. Viscous effects arise from collisions between particles which transform the energy of fluid motion to internal particle motion in the fluid. A simple approximation for the collision term was introduced [10]

$$\left(\frac{df}{dt}\right)_{collision}=\frac{-\left(f-f^{eq}\right)}{\tau} \qquad (8)$$

where τ is a relaxation time constant. This approximation implies that the distribution relaxes exponentially to equilibrium with a time constant τ. Where the f^{eq} is the equilibrium distribution (Maxwell-Boltzmann):

$$f^{eq}=\rho\cdot\left(\frac{m}{2\pi kT}\right)^{3/2}\cdot\exp\left\{-\frac{m}{2\pi kT}\left[v-u\right]^2\right\} \qquad (9)$$

The forcing term of equation (1) can be calculated by the assumption of the system is close to the equilibrium state

$$\nabla_v f(r,v,t)\approx\nabla_v f^{eq}(r,v,t)$$
$$=\frac{-m}{kT}\left[v-u(r,t)\right]f^{eq}(r,v,t) \qquad (10)$$

4..Two-Phase Flow

In simulating multiphase flow, there are several traditional CFD methods, most of which can be fitted in two categories: the front-capturing method and front-tracking method.

In the Marker-and-Cell (MAC) method, the Lagrangian markers are used to represent the location of the liquid (one phase). The interface is then constructed based on the location of the markers. Physical properties, i.e. viscosity and density, for the fluid at each grid point are determined by the phase present. The MAC method is computationally very expensive.

The Volume-of-Fluid (VOF) method was introduced to reduce the heavy computational load of the MAC method. In the VOF method, instead of tracking a large number of markers, the volume fraction of fluid in each cell is used to track the movement of the liquid. Therefore, the computational cost is greatly reduced. However, the VOF method still has difficulties in determining the exact location of the interface. The level set method uses two sets of equations to model the two-phase flow system. The first set, like the other two methods, is comprised of the single fluid Navier-Stokes (N-S) equations, which are employed to determine the momentum. The second set is a transient scalar advection equation which tracks a level set function. The level set function equals zero at the interface, a negative value for locations inside one phase, and a positive value for locations inside another phase. The location of the interface is determined by interpolating between the level set function values. In the level set method, the interface is much easier to determine compared to the MAC and VOF methods. However, it has some problems with mass conservation, because the advection of the level set function is not based on a strictly conservative equation. Furthermore, the solution of front-capturing method is prone to numerical diffusion and dispersion problems.

Front-tracking methods directly 'track' the location of the two-phase interface. Therefore they allow more accurate calculation of the curvature of the interface. Most commonly used front-tracking methods are: the boundary-fitted grid method, Tryggvassons's hybrid method, and Boundary Element Method (BEM). In the boundary-fitted grid method, two sets of N-S equations are solved-one for each fluid. The grid of the computational domain is constructed in such a fashion that the interface between two phases is located along a grid line and the movement of the interface is determined by a force balance. In the hybrid method proposed by Tryggvasson, two sets of grids are used, i.e.: a stationary grid used to determine the fluid flow and a lower dimension grid used to track the interface. In the Boundary Element Method (BEM), a multitude of boundary nodes are employed to represent the two-phase interface. The movement of these boundary nodes is based on the potential function equations.

Although conceptually simple, it is more difficult to implement these traditional CFD methods in a two-phase flow simulation. The difficulties arise from the interface deformation and interaction. Computationally, one might be able to track a few, but hardly very many, interfaces in a system. Recently, simulating multiphase flow with the LBE method has attracted much attention. Microscopically, the phase segregation and surface tension in multiphase and multicomponent flow are because of the interparticle forces/interactions. Due to its kinetic nature, the LBE method is capable of incorporating these interparticle interactions, which are difficult to implement in traditional methods. Therefore, the key step in developing the LBE multiphase and multicomponent model is to correctly incorporate the particle interactions into the evolution of distribution function so that macroscopically correct multiphase and multicomponent flow behaviour can be obtained. [11]

5..Lattice Boltzmann Equation

The Boltzmann Equation (1) with the BGK approximation and including external force has a next formulation. [12, 13, 14]

$$\frac{\partial f}{\partial t} + v\nabla f = -\frac{f - f^{eq}}{\tau} + \frac{F}{kT}[v-u]f^{eq} \qquad (11)$$

This equation can be discredited in space through the following two dimensional D2Q9grid. (Fig. 1)

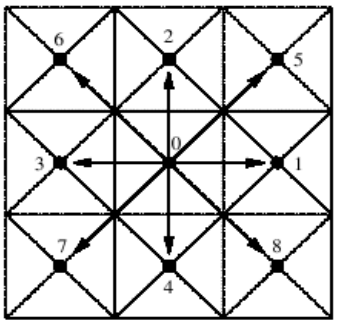

Fig 1. The D2Q9 two dimensional lattice.

The D2 means the two dimension and Q9 is the possible directions (e_i i=0..8) of particle move. If we suppose the constant speed of particle move c the e vector is

$$e_i = \begin{Bmatrix} 0 & i=0 \\ \left[\cos\pi\frac{(i-1)}{2}, \sin\pi\frac{(i-1)}{2}\right]c & i=1..4 \\ \left[\cos\left(\frac{\pi}{4}+\pi\frac{(i-5)}{2}\right), \sin\left(\frac{\pi}{4}+\pi\frac{(i-5)}{2}\right)\right]\sqrt{2}c & i=5..8 \end{Bmatrix} \qquad (12)$$

After the discretization by e_i and Taylor expansion of equilibrium distribution (9) we get

$$f^{eq_i} = \omega_i n\left[1 + \frac{e_i \cdot u}{\chi c^2} + \frac{(e_i \cdot u)^2}{2\chi^2 c^4} - \frac{u \cdot u}{2\chi c^2}\right] \qquad (13)$$

where χ= 1/3, $\omega_i(0)$ = 4/9, ω_i (1..4) = 1/9 and $\omega_i(5..8)$ = 1/36 and n is the numerical density. After the temporal discretization the finite difference Lattice Boltzmann equation is obtained [21, 22]

$$f_i(r,t+\delta t) = f_i(r,t) - \frac{\delta t}{\tau}\left[f_i(r,t) - f^{eq_i}\right] - \delta t e_i \cdot \nabla f_i(r,t) + \frac{\delta t}{kT} F(r,t)\left[e_i - u(r,t)\right] f^{eq_i} \quad (14)$$

The macroscopic variables density and speed can be extracted

$$n = \sum f_i(r,t) \quad and \quad u = \frac{1}{n}\sum e_i f_i \quad (15a,15b)$$

The viscosity after the Chapman-Enskog multiple times expansion [15] is derived

$$v = (\tau - 0.5)c^2 \delta t \quad (16)$$

6..Multi Component LBM

In case of multi component flow the Lattice Boltzmann equation (14) [16, 17, 18] should be wrote by components. For example in case of two components this means two sets of equations of (14) and two equations of equilibrium distribution (13) as well. In addition the barycentric velocity

$$u = \frac{\sum_\sigma m^\sigma n^\sigma u^\sigma}{\sum_\sigma m^\sigma n^\sigma} \quad (17)$$

can be used in the equation of (13). σ refers to the component and m is the molecular mass. The components speeds and densities are following formulas

$$u^\sigma = \frac{1}{n^\sigma}\sum e_i f_{i^\sigma} \qquad n^\sigma = \sum f_{i^\sigma} \quad (18a, 18b)$$

7..Molecular Force and Equation of State

The inter molecular force in the LBM can be introduced by Shan-Chen model [16, 17, 18]

$$F^\sigma = -G_{\bar\sigma\sigma}\nabla n^{\bar\sigma} \qquad \bar\sigma = 1 - \sigma \quad (19)$$

the G is symmetric matrix controls the force strength between components. In this case the mixture has ideal gas Equation of State (EOS). One can change the ∇n with arbitrary function of n as $\nabla\varphi_\sigma(n_\sigma)$. The φ function is called effective mass and can modify the EOS. By the Chapman-Enskog expansion and long time scale limit the EOS is

$$p = \frac{c^2}{D}\left(m_\sigma n_\sigma + \frac{b}{2} G_{\bar\sigma\sigma}\varphi_{\bar\sigma}\varphi_\sigma\right) \quad (20)$$

where D is the dimension and b is the next neighbouring number of nodes.

8..Salvation of Lattice Boltzmann Equation

Because of the high density and viscosity ratio between components quite robust salvation method should be chosen. Thus we apply Strang time splitting [19] with TVD (Total Variation Diminishing) scheme [20, 21, 22] and implicit trapezoidal integration [23, 24].
In the simplest case the splitting takes the form

$$U^{n+1} = S_\Psi(k) S_f(k) U^n \quad (21)$$

Here $S_f(k)$ represents the numerical solution operator for the system of conservation laws

$$u_t + f(u)_x = 0 \quad (22)$$

over a time step of length k, and $S_\psi(k)$ is the numerical solution operator for the Ordinary Differential Equation (ODE) system

$$u_t = \Psi(u) \quad (23)$$

To maintain second order accuracy, the Strang splitting can be used, in which the solution U^{n+1} is computed from U^n by

$$U^{n+1} = S_\Psi(k/2) S_f(k) S_\Psi(k/2) U^n \quad (24)$$

In case of Lattice Boltzmann equation (11) the equation (23) can be rewritten

$$\frac{\partial f_i}{\partial t} + e_i \nabla f_i = 0 \quad (25)$$

and

$$\frac{\partial f_i}{\partial t} = \Psi(f_i) = -\frac{f_i - f_i^{eq}}{\tau} + \frac{F}{kT}\left[e_i - u\right] f_i^{eq} \quad (26)$$

We use the implicit trapezoidal integration for solve the (23) equations

$$f_i^{n+1} = f_i^n + \frac{1}{4}\delta t[\psi(f_i^n) + \psi(f_i^{n+1})] \quad (27)$$

which need nonlinear equation solver. Thus Difference Newton-Raphson (DNR) method was applied.
The (27) expression can be regrouped

$$F(f_i^{n+1}) = f_i^{n+1} - f_i^n - \frac{\delta t}{4}[\psi(f_i^n) + \psi(f_i^{n+1})] = 0 \quad (28)$$

and then we can applie the DNR iteration.

$$f^{(n+1)_{k+1}} = f^{(n+1)_k} - J^{-1} \cdot F\left(f^{(n+1)_k}\right) \quad (29)$$

The J is the Jacobi matrix of F the analytical solution of the J is quite problematic in this case so the second order central difference scheme provides the approximation of Jacobi

$$J_{ij} \approx \frac{F_i(f_j + \delta) - F_i(f_j - \delta)}{2\delta} \quad (30)$$

and

$$\delta = \sqrt{(1 + \|f\|_2)\varepsilon_m} \quad (31)$$

here the ε_m is machine precision. In the initialization stage we use predictor-corrector step where the predictor is forward Euler.
The Riemann equation (25) solved by TVD because of high density drop at phase border. One dimensional TVD was applied in each possible speed direction (i=1..8).

$$f_i^{n+1} = f_i^n - CFL(F_{i+1/2} - F_{i-1/2}) \quad (32)$$

The F is numerically calculated flux and CFL is the Courant number $c\delta t/\delta x$

$$F_{i-1/2} = F_{i-I+1/2}$$
$$F_{i+1/2} = \frac{1}{2}\begin{pmatrix} ef_i + ef_{i+1} + L_i + L_{i+1} + g_i + g_{i+1} \\ -Q\left(e + v_{i+1/2}^{LM} + \gamma_{i+1/2}\right)\Delta_{i+1/2} \end{pmatrix} \quad (33)$$

$$\Delta_{i+1/2} = f_{i+1} - f_i \quad (34)$$

$$g_i = M(\breve{g}_{i-1/2}, \breve{g}_{i+1/2}) \quad (35)$$

$$\breve{g}_{i+1/2} = \frac{1}{2}\left(Q\left(e + v_{i+1/2}^{LM}\right) - CFL \cdot \left(e + v_{i+1/2}^{LM}\right)^2\right)\Delta_{i+1/2} \quad (36)$$

and M is the minmod function,

$$M(x_{1,..,}x_n) = \begin{Bmatrix} sign(x_1)min(|x_1|,...,|x_n|) & if\ \ all\ \ x_i\ \ have\ \ same\ \ sign \\ 0\ \ otherwise \end{Bmatrix} \quad (37)$$

$Q(x)$ is a function helpful to eliminate the so-called entropy violation,

$$Q(x) = \begin{Bmatrix} x^2/(4\varepsilon) + \varepsilon & |x| < 2\varepsilon \\ |x| & |x| \geq 2\varepsilon \end{Bmatrix} \quad (38)$$

where ε is a positive constant generally taken to be between 0.1 and 0.5. In the following numerical simulations, we choose e to be 0.2.
The definition of the rest functions are

$$\gamma_{i+1/2} = \begin{Bmatrix} (g_{i+1} - g_i)/\Delta_{i+1/2} & \Delta_{i+1/2} \neq 0 \\ 0 & \Delta_{i+1/2} = 0 \end{Bmatrix} \quad (39)$$

$$v^{LM}{}_{i+1/2} = \begin{Bmatrix} (L_{i+1} - L_i)/\Delta_{i+1/2} & ha & \Delta_{i+1/2} \neq 0 \\ 0 & ha & \Delta_{i+1/2} = 0 \end{Bmatrix} \quad (40)$$

$$L_i = S \cdot max(0, M(\eta L_{i-1/2}, L_{i+1/2}) \cdot S, M(L_{i-1/2}, \eta L_{i+1/2}) \cdot S) \quad (41)$$

$$\eta = 2\left|\frac{|\Delta_{i+1/2}|^\beta - |\Delta_{i-1/2}|^\beta}{|\Delta_{i+1/2}|^\beta + |\Delta_{i-1/2}|^\beta}\right| \quad (42)$$

$\beta = 2.5$
and $S = sign(L_{i+1/2})$.

9..Algorithm Validation

The first validation is the proving of Laplace law (43). (Fig. 2) For a droplet in equilibrium with its vapour, the tension surface increases the internal pressure of the droplet, according to Young-Laplace law:

$$\Delta P = (D-1)\frac{\sigma}{R} \quad (43)$$

where ΔP is pressure difference between inside and outside of the droplet and σ is the surface tension D is the dimension and R is the droplet radius. In the Shan Chen model the G controls surface tension as well.

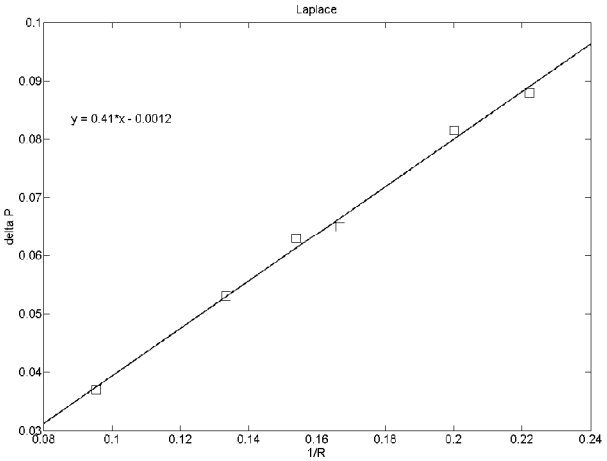

Fig 2. Shows the Laplace law $\Delta P = 0.41/R$

The next pictures show the evolution of drops in time (Fig 3-5)

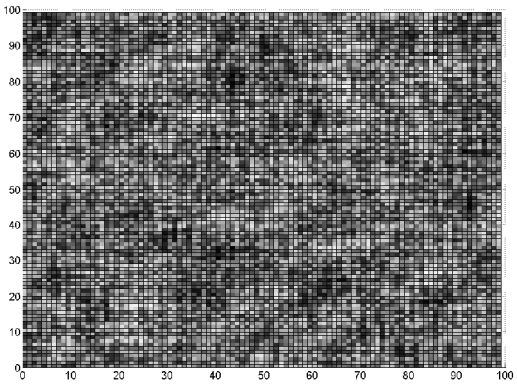

Fig 3. Time step = 10

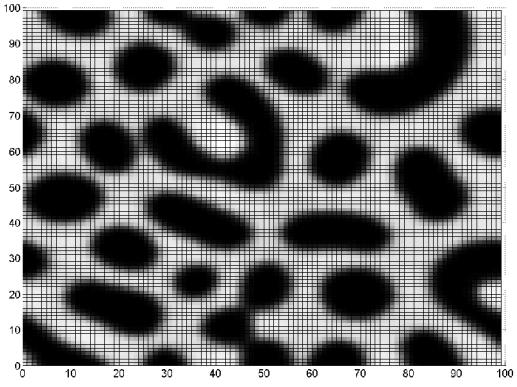

Fig 4. Time step = 2500

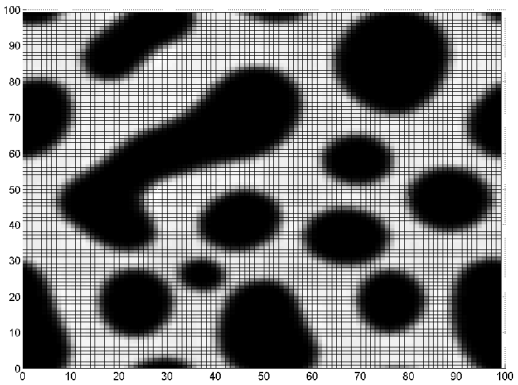

Fig 5. Time step = 5000

10..Conclusion and Next Step of the Project

During this project we try to develop highly robust LBM algorithm to simulate such a complex flow like vaporization using well developed and enough stable techniques as Strang time splitting, TVD and Stiff ODE solver. This code can pass trough the first test proving the Laplace law which is one of the basic phenomena of multi phase and multi component flow.
This simulation is considered only ideal gas mixtures which is not sufficient in our purpose. Thus we will try to introduce Carnahan Starling EOS (44) [11, 25] which is more precocious than Van der Waals EOS.

$$p = \rho RT\left(\frac{1+b\rho/4+(b\rho/4)^2-(b\rho/4)^3}{(1-b\rho/4)^3}\right)-a\rho^2$$

(44)
After the insertion of (44) in (20) the G can be obtained. This equation of state can describe phase transition of liquid and it's vapour helping the development of liquid and gas phase decomposition. The application of appropriate EOS is mandatory for our project because it plays important rule in two phase flow.

[1] Reitz R D and Bracco F V. Mechanism of Atomization of a Liquid Jet. *Physics of Fluids*, Vol. 25, ch. 10, Oct., 1982.

[2] Reitz R D and Diwakar R. Structure of High-Pressure Fuel Sprays, *SAE paper 870598*, 1987.

[3] Reitz R D. Modelling Atomization Processes in High-Pressure vaporizing Sprays. *Atomization and Spray Technology*, Vol. 3, pp. 309-337, 1987.

[4] Raju M. S. Numerical Investigation of Various Atomization Models in the Modeling of a Spray Flame. *NASA/CR—2005-214033, AIAA–2006–0176 Report*, 2006.

[5] Schmidt D, Nouar I, Senecal P, Rutland C, Martin J, Reitz R. Pressure-Swirl Atomization in the Near Field., *SAE Technical Paper Series* 1999-01-0496.

[6] Senecal P, Schmidt D, Nouar I, Rutland C, Reitz R, Corradini M. Modeling High-speed Viscous Liquid Sheet Atomization., *Int. J. of Multiphase Flow*, 25, pp. 1073-1097, 1999.

[7] Peter J. O'Rourke and Anthony A. Amsden The Tab Method for Numerical Calculation of Spray Droplet Break-up, *SAE paper 872089*, 1987.

[8] Hermann M. Modeling primary break-up: A three-dimensional Eulerian level set/vortex sheet method for two-phase interface dynamics. Center for Turbulence Research Annual Research Briefs, 2003.

[9] Landau L.D. Lifsic E.M. Elméleti Fizika V. Statisztikus Fizika, Tankönyvkiadó Budapest, 1981

[10] Bhatnagar, Gross and Krook in Phys. Rev. 94, 511 1954

[11] Peng Yuan, Thermal Lattice Boltzmann Two-Phase Flow Model for Fluid Dynamics, PhD Thesis 2005

[12] S. Chen and G. D. Doolen, Lattice Boltzmann method for fluid flows, Ann. Rev. Fluid Mech. 30, pp. 329-364, 1998.

[13] L.-S. Luo, The lattice-gas and lattice Boltzmann methods: Past, Present, and Future, Proceedings of the International Conference on Applied Computational Fluid Dynamics, Beijing, China, pp. 52-83, 2000.

[14] R.R. Nourgaliev, T.N. Dinh, T.G. Theofanous and D. Joseph: The lattice Boltzmann equation method: theoretical interpretation, numerics and implications, International Journal of Multiphase Flow, Vol. 29, pp. 117-169. 2003

[15] S. Chapman and T. G. Cowling, The Mathematical Theory of Non-Uniform Gases, 3rd ed. Cambridge University Press, London, 1970.

[16] Shan, X. & Chen, H. Lattice Boltzmann model for simulating flows with multiple phases and components. Phys. Rev. E47, 1815-1819. 1993

[17] Shan, X. & Chen, H. Simulation of nonideal gases and liquid-gas phase transitions by the Lattice Boltzmann equation. Phys. Rev. E 49, 2941-2948. 1994

[18] Xiaowen Shan and Gary Doolen. Journal of Statistical Physics 81, 1995

[19] J. LeVeque and H. C. Yee, A study of numerical methods for hyperbolic conservation laws with stiff source terms, J. Comput. Phys., 86, 1990

[20] Shulong Teng, Yu Chen, Hirotada Ohashi, Lattice Boltzmann simulation of multiphase fluid flows through the total variation diminishing with artificial compression scheme. International Journal of Heat and Fluid Flow 21 112-121, 2000

[21] Artur Cristea, Victor Sofonea, Two component lattice Boltzmann model with flux limiters, Central European Journal of Physics, 382–396, 2004

[22] V. Sofonea, A. Lamura, G. Gonnella and A. Cristea, Finite-difference lattice Boltzmann model with flux limiters for liquid-vapor systems Phys. Rev. E 70, 2004

[23] D.A. Knoll, D.E. Keyes, Jacobian-free Newton–Krylov methods: a survey of approaches and applications, Journal of Computational Physics 193, 357–397, 2004

[24] Gill, P.E., Murry W., Wright M.H., Practical Optimization. Academic Press, New York. 1981

[25] Xiaoyi He, Shiyi Chen, and Raoyang Zhang, A Lattice Boltzmann Scheme for Incompressible Multiphase Flow and Its Application in Simulation of Rayleigh–Taylor Instability Journal of Computational Physics 152, 642–663 (1999)

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