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# EQUATIONS OF STATE IN A FINITE DIFFERENCE LATTICE BOLTZMANN MODEL

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The objective of this work is the investigation of the stability and the miscibility gap recovered in finite difference lattice Boltzmann models for two phase liquid – vapour systems. Various equations of state were considered as well as various finite difference schemes. Second order numerical schemes were used to minimize the numerical effects and the spurious velocity in the interface region

*Key words*: Numerical schemes; Two phase fluids; Fluid interfaces.

## 1. INTRODUCTION

Finite difference Lattice Boltzmann (FDLB) models provide an alternative to current methods in computational fluid dynamics. LB models are based on the physics at the mesoscopic scale, so that the macroscopic phenomena are recovered without solving the equations of continuum media mechanics. The starting point of any LB model is the Boltzmann equation [1]:

$$\left[\frac{\partial}{\partial t}+v\cdot\nabla+\frac{F(r,t)}{m}\cdot\nabla_v\right]f(r,v,t)=\left(\frac{\partial f}{\partial t}\right)_{colisions}, \tag{1}$$

where $f(r,v,t)$ is the distribution function, v is the velocity and *F(r, t)* is the force acting on a particle of mass *m*. The collision term in the Boltzmann equation (1) is usually linearized using the Bhatnagar-Gross-Krook (BGK) approximation [2] after introducing a relaxation time τ. After convenient discretization of the phase space [3–5] the velocities are reduced to a discrete set $\{e_i\}$, $i=0,1,...,N$ and the corresponding distribution functions $f_i=f_i(r,v,t)$ are defined only in the nodes of a discrete lattice. When using the forward finite difference scheme [3–5] with time step *δt*, the distribution functions evolve in each lattice node according to the following evolution equations:

$$\begin{aligned} f_i(r,t+\delta t)&=f_i(r,t)-\frac{\delta t}{\tau}\left[f_i(r,t)-f_i^{eq}(r,t)\right]-\\ &-\delta t\cdot e_i\nabla f_i(r,t)+\frac{\delta t}{k_BT}F(r,t)\cdot\left[e_i-u(r,t)\right]f_i^{eq}(r,t). \end{aligned} \tag{2}$$

The equilibrium distribution functions $f_i^{eq}=f_i^{eq}(r,t)$ in the equation above are expressed as a series expansion with respect to local velocity *u* [3–6]. For a liquid-vapour system, the expression of the force term in Eq.(2) is [7]:

$$F=-\frac{1}{\rho}\nabla\left[-p_{EOS}+p_i\right]+3k\nabla\left(\nabla^2\rho\right), \tag{3}$$

where $p_{EOS}$ is the nonideal gas pressure in the equation of state (EOS), $p_i$ is the ideal gas pressure and $\kappa$ is a parameter which controls the surface tension $\sigma$ [8].

The aims of this paper are to investigate the effects introduced by the various non-dimensionalized equations of state [10], as well as by the finite difference schemes in the isothermal lattice Boltzmann model. The parallel computer code developed during this project uses the MPI protocol and the parallel computing techniques incorporated in the PETSc library developed at Argonne National Laboratory, Argonne, Illinois [11]. The ACAD parallel computing cluster has four dual processor Apple Mac workstations running the MAC OS X version 10.5 Leopard and is located at the Center for Fundamental and Advanced Technical Research, Romanian Academy – Timişoara Division.

Reference quantities for temperature, speed, mass, density and pressure [7]: $T_R$, $c_R$, $m_R$, $\rho_R$, $p_R$ are used to express the dimensionless form of various equations of state. The pressure $p_{EOS}$ in Eq.(3) should be correlated with the quantities used to get the dimensionless form of the evolution equations (2). Since the LB model discussed in this paper refers to a nonideal fluid, a natural choice for the reference temperature $T_R$ is the critical temperature $T_c$ of the fluid [7]. The reference speed $c_R$ is correlated to the reference temperature $T_R$, in order to satisfy the definition of the lattice speed $c$ [6]. The reference pressure is $p_R=c^2R\rho_R$ which leads to the non-dimensionalized expression of the ideal gas pressure ($\chi$ = 1/3 is a characteristic of the D2Q9 LB model)

$p_i=\chi\, c^2\rho$ [7]. However, other authors [12, 13] choose the reference temperature equal to the physical value ($T_R=T$). The dimensionless equations of state are [9, 10]:

● Van der Waals EOS :

$$p_{vdW}=\frac{3\rho T}{3-\rho}-\frac{9}{8}\rho^2; \tag{4}$$

● Redlich-Kwong EOS:

$$p_{RK}=\frac{\rho T}{3-\rho}-\frac{9}{8}\frac{\rho^2}{\sqrt{T}\left(3+\rho\right)}. \tag{5}$$

## 2. FINITE DIFFERENCE SCHEMES

The first order upwind scheme is widely used to compute the term $e_i\cdot\nabla f_i$ in Eq.(2) [14, 15]. According to the general approach to high order flux limiters [15–17], the updating rule Eq.(2) is rewritten in a conservative form using the two fluxes as mentioned in [15]:

$$\begin{aligned} f_{i,j}^{n+1}&=f_{i,j}^{n}-\mathrm{CFL}\left[F_{i,j+1/2}^{n}-F_{i,j-1/2}^{n}\right]+\\ &+\frac{\delta t}{k_BT}F\left(r,t\right)\cdot\left[e_i-u\left(r,t\right)\right]f_i^{eq}\left(r,t\right)-\frac{\delta t}{\tau}\left[f_i\left(r,t\right)-f_i^{eq}\left(r,t\right)\right], \end{aligned} \tag{6}$$

where CFL = $c\delta t/\delta s$ ($\delta s$ – lattice spacing) is the Courant-Friedrichs-Levy number.
The flux limiter $\psi\left(\theta_{i,j}^{n}\right)$ [15–17] is expressed as a function of the smoothness:

$$\theta_{i,j}^{n}=\frac{f_{i,j}^{n}-f_{i,j-1}^{n}}{f_{i,j+1}^{n}-f_{i,j}^{n}}. \tag{7}$$

The first order upwind scheme is recovered as a particular case when $\psi\left(\theta_{i,j}^{n}\right)=0$. In this paper we will use the MCD (Monitorized Central Difference) flux limiter [17], since other flux limiter schemes provide similar results:

$$\psi\left(\theta_{i,j}^{n}\right)=\begin{cases}0 & , \quad \theta_{i,j}^{n}\le 0\\ 2\theta_{i,j}^{n} & , \quad 0\le\theta_{i,j}^{n}\le\dfrac{1}{3}\\ \dfrac{1+\theta_{i,j}^{n}}{2} & , \quad \dfrac{1}{3}\le\theta_{i,j}^{n}\le 3\\ 2 & , \quad 3\le\theta_{i,j}^{n}.\end{cases} \tag{8}$$

## 3. PHASE SEPARATION

The main characteristic of liquid-vapour systems is the phase separation which occurs when the temperature of the system is lowered below the critical value. We always started our LB simulations from an homogenous system with small fluctuations (0.1%). We used periodic boundary conditions on a square lattice with $N^2 = 128 \times 128$ nodes and set the lattice spacing $\delta s = 1/128$, relaxation time $\tau = 10^{-3}$ and the time step $\delta t = 10^{-5}$.

Figure 1 shows the coexistence curves recovered from the simulations using various equations of state, as well as upwind vs. MCD finite difference schemes. The coexistence diagrams for these EOS were evaluated by comparing the simulations with the theoretical curves predicted by Maxwell equal-area construction. Simulations were done using both upwind and MCD flux limiter numerical schemes. One can see that the simulations performed using the MCD scheme have smaller deviations from the theoretical curves than in the case of using the upwind scheme. Although, even when the surface tension parameter is not vanishing (Fig. 2), the MCD flux limiter scheme proves to be more efficient than the upwind scheme in simulating the liquid-vapour phase separation.

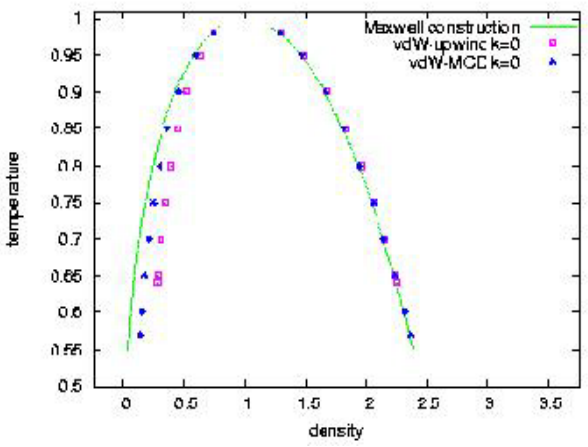


Fig. 1a – Phase separation diagrams for the van der Waals EOS without surface tension (upwind / MCD).

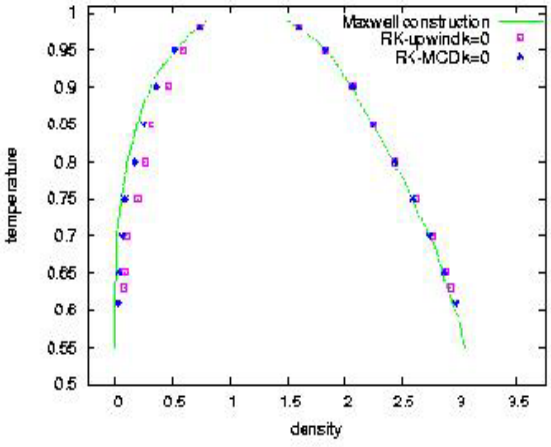


Fig. 1b – Phase separation diagrams for the Redlich-Kwong EOS without surface tension (upwind / MCD).

The van der Waals EOS is the simplest and most famous equation of state. However, by replacing the Van der Waals EOS with a more realistic equation like the Redlich-Kwong EOS, better performance is achieved. In particular, the highest density ratio $\rho_{liquid} / \rho_{vapours}$ is recovered with the Redlich-Kwong EOS (≈120) which is significantly larger than the one obtained with the Van der Waals EOS (≈30), when using the same numerical scheme (e.g. MCD scheme) and unvanishing surface tension parameter ($\kappa = 0.0001$) at the lowerest possible temperature, as seen in Table 1.

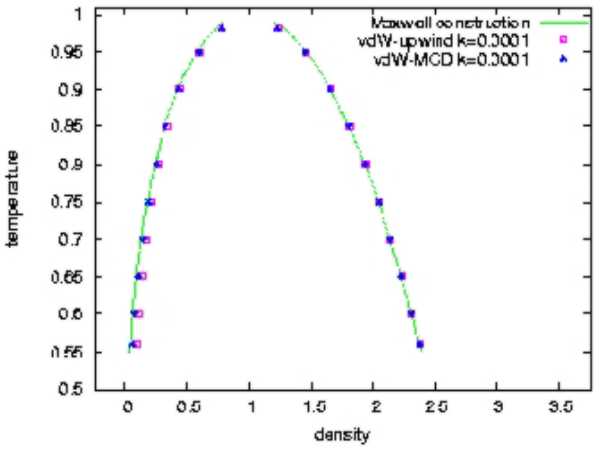


Fig. 2a – Phase separation diagrams for the van der Waals EOS with surface tension (upwind / MCD).

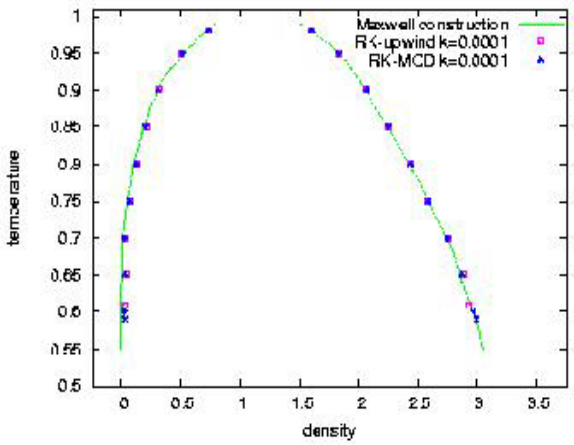


Fig. 2b – Phase separation diagrams for the Redlich-Kwong EOS with surface tension (upwind / MCD).

*Table 1*

Density ratio $\rho_{liquid} / \rho_{vapours}$ for different EOS

| Temperature | vdW EOS | RK EOS |
|---|---|---|
| 0.95 | 2.44 | 3.59 |
| 0.90 | 3.82 | 6.65 |
| 0.85 | 5.49 | 11.24 |
| 0.80 | 7.71 | 19.49 |
| 0.75 | 10.77 | 37.25 |
| 0.70 | 15.11 | 90.81 |
| 0.65 | 21.41 | 98.99 |
| 0.60 | 30.61 | 117.34 |

The lattice Boltzmann simulation of a liquid-vapour system cannot be operated at temperatures below the threshold because negative values of the distribution functions are achieved and the computer code switches off. This conclusion is in accordance with other authors [10,12,13], who also observed the existence of a threshold temperature. The value of the threshold temperature is strongly dependent on the numerical scheme.

## 4. THE ORIGIN OF THE SPURIOUS VELOCITIES

At equilibrium, the fluid velocity in the interface region should be zero when the fluid is at rest [18]. Solving the real LB equations (up to second order with respect to the lattice spacing $\delta s$) as done in [7, 14] we get:

$$u_\beta = \frac{\psi}{\rho}\partial_\gamma\left[\chi c^2 \rho \delta_{\beta\delta} + \rho u_\beta u_\gamma\right] \approx \frac{\psi\chi c^2}{\rho}\partial_\beta \rho \,. \tag{9}$$

The spurious velocity appears in the interface region because of the density gradient, being also strongly related to the numerical errors introduced by the numerical schemes. The width of the interfaces can be controlled by the surface tension tuned by $\kappa$. The spurious velocity is always smaller when using higher order numerical scheme (MCD) as seen in Fig. 3 and Fig. 4 for both EOS: van der Waals and Redlich-Kwong.

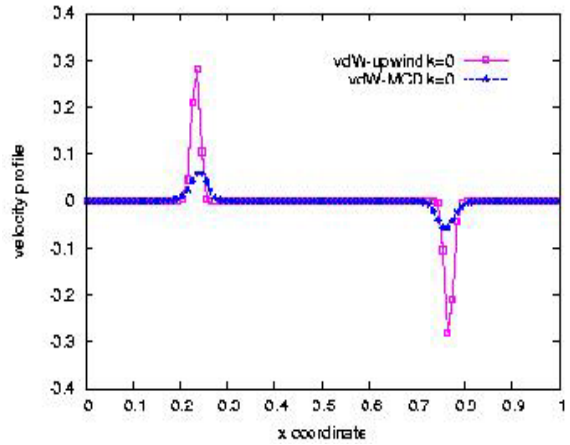


Fig. 3a – Local velocity profile for the van der Waals EOS without surface tension (upwind / MCD).

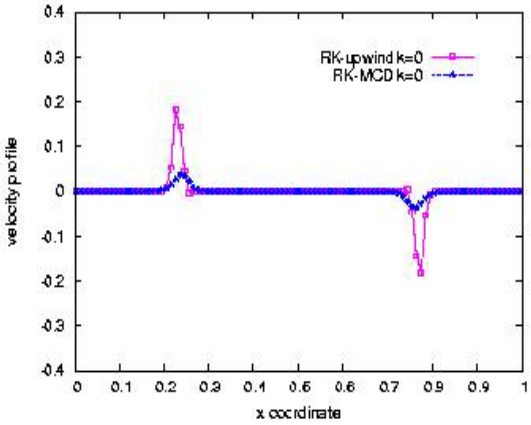


Fig. 3b – Local velocity profile for the Redlich-Kwong EOS without surface tension (upwind / MCD).

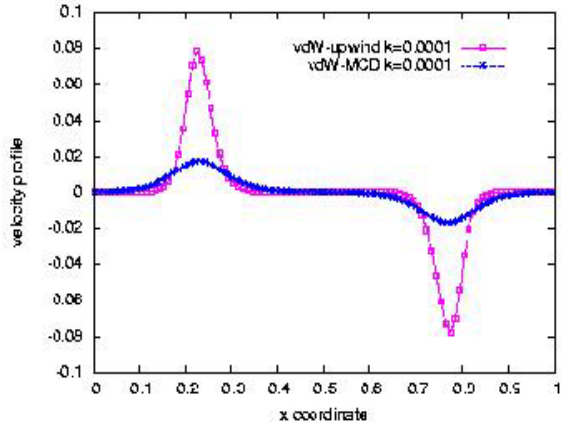


Fig. 4a – Local velocity profile for the van der Waals EOS with surface tension (upwind / MCD).

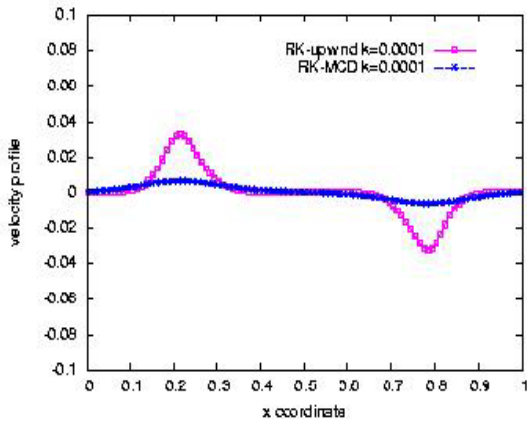


Fig. 4b – Local velocity profile for the Redlich-Kwong EOS with surface tension (upwind / MCD).

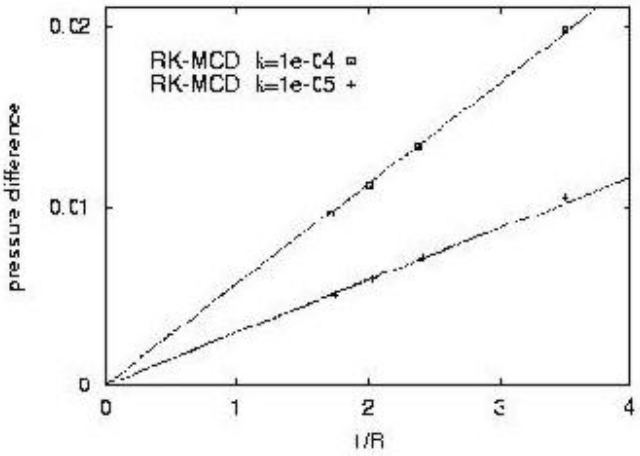


Fig. 5 – Laplace law ($T$=0.60).

## 5. LAPLACE LAW

For a gas bubble immersed in liquid, the Laplace law reads $p_{ext} - p_{int} = \frac{\sigma}{R}$,

where $p_{int}$ is the value of pressure inside the bubble (of radius $R$), $p_{ext}$ is the outside pressure value (the value of pressure in the liquid) and $\sigma$ is the surface tension. The dependence $\Delta p = f\left(\frac{1}{R}\right)$ is shown in Fig. 5 for two values of the surface tension. The dimensionless temperature was set here to 0.60 in order to be closer to the threshold value of the temperature. The linear dependence is clearly observed.

## 6. CONCLUSIONS

In this paper we compared the simulations results recovered using various equations of state: (the van der Waals and the Redlich-Kwong) in a finite difference lattice Boltzmann model. Replacing the van der Waals equation of state with a more realistic one like the Redlich – Kwong equation of state, one can get a better performance related to the higher density ratio. Significant differences between the magnitude of the spurious velocities in the interface region were recovered when various equations of stare are used.

Second order flux limiter schemes significantly reduce the spurious velocity and should be preferred to the first order upwind finite difference schemes in order to reduce the numerical effects during numerical simulations.

The presence of the surface tension stretches the interface width and therefore the numerical stability is improved because the density gradient becomes smaller.

The Laplace law is very well verified with our finite difference lattice Boltzmann model.

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