DETERMINATION OF SPINODAL POINTS IN EQUATION OF STATE USING NON LINEAR OPTIMIZATION SQP METHOD IN MULTIPHASE FLOW

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ABSTRACT

To solve multiphase flow among various models D2Q9 Lattice Boltzmann model is found to be very much effective. In order to apply this model the equation of state of fluid under consideration is to be known. In this EOS the proper detection of metastable region is a very important issue. This metastable region lies between two spinodal points having densities ρ_1 and ρ_2. Values of ρ_1 and ρ_2 can be obtained by solving the conditions of Mechanical and Chemical equilibrium. In the present study for the proper evaluation of these points Sequential Quadratic Programing (SQP)method is used, which gives better prediction of the values of ρ_1 and ρ_2 as compared to the same values calculated by other previous workers.

Keywords: Chemical Equilibrium, Equation of State, Mechanical Equilibrium, Multiphase Flow, Sequential Quadratic Programming

In oil and gas industry, it is important to meter the individual components of oil, water and gas stream. This will therefore focus on hydrocarbon multiphase flow measurement. Although multiphase flows also exist in other industries, the term multiphase flow is used to refer to any fluid flow consisting of more than one phase or component.

I. INTRODUCTION

In every processing technology multiphase flow exist starting from cavitating pumps and turbines to electrophotographic processes to papermaking to the pellet form of almost all raw plastics. The amount of granular material, coal, grain, ore, etc. that is transported every year is enormous and, at many stages, that material is required to flow. Clearly the ability to predict the fluid flow behavior of these processes is the effectiveness of those processes. Multiphase flows are also a ubiquitous feature of our environment whether one considers rain, snow, fog, avalanches, mud slides, sediment transport, debris flows, and countless other natural phenomena. Biological and medical flows like blood flow and semen are also multiphase. Two general topologies of multiphase flow can be usefully identified at the outset, namely disperse flows and separated flows. Disperse flows mean those consisting of finite particles, drops or bubbles (the disperse phase) distributed in a connected volume of the continuous phase. On the other hand separated flows consist of two or more continuous streams of different fluids separated by interfaces. A multiphase system can contain the same component with different phases such as liquid water and water vapor system. [1, 2]

II. D2Q9 LATTICE BOLTZMANN MODEL

The Lattice Boltzmann method was originated from Ludwig Boltzmann's kinetic theory of gases. The fundamental idea is that gases/Fluids can be imagined as consisting of a large number of small particles moving with random motions. The exchange of momentum and energy is achieved through particle streaming and billiard-like particle collision. This process can be modelled by the Boltzmann transport equation [3]. The LBM simplifies Boltzmann's original idea of gas dynamics by reducing the number of particles and connecting them to the nodes of a lattice. For a two dimensional model, a particle is restricted to stream in a possible of 9 directions, including the one staying at rest. These velocities are referred to as the microscopic velocities and denoted by e_i where i = 0…………...8.

This model is commonly known as the D2Q9 model as it is two dimensional and involves 9 velocity vectors. Figure1 shows a typical lattice node of D2Q9 model with 9 velocities and is defined by

$$e_i = \begin{cases} (0,0) & i = 0 \\ (1,0), (0,1), (-1,0), (0,-1) & i = 1,2,3,4 \\ (1,0), (0,1), (-1,0), (0,-1) & i = 1,2,3,4 \end{cases} \quad (1)$$

For each particle on the lattice, we associate a discrete probability distribution function $f_i(x, e_i, t)$ = which describes the probability of streaming in one particular direction.

The (D2Q9) Lattice Boltzmann model, i.e. two dimensional nine velocity LB model with a multiple relaxation time (MRT) collision operator is considered. The extensive details of D2Q9 model is given in next section. The MRT Lattice Boltzmann equation is given by [4]

$$f_{\acute{\alpha}}(x + e_{\acute{\alpha}}\delta_t, t + \delta_t) = f_{\acute{\alpha}}(x, t) - (\mathbf{M}^{-1}\Lambda\mathbf{M})_{\acute{\alpha}\beta}\left(f_\beta - f_\beta^{eq}\right) + \delta_t f_{\acute{\alpha}} \quad (2)$$

Where Λ = is the diagonal matrix,

$$\Lambda = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2+3|v|^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1-3|v|^2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & v_x & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -v_x & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & v_y & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -v_y & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & v_x^2 - v_y^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & v_x v_y \end{bmatrix} \quad (3)$$

M is the orthogonal transformation matrix, $F_{\acute{\alpha}}$ shows the forcing term in the space velocity. Taking the help of the transformation matrix, the R.H.S of Eq. (2) can be rewritten as

$$\mathbf{m}^* = \mathbf{m} - \Lambda(\mathbf{m} - \mathbf{m}^{eq}) + \delta_t \left(\mathbf{I} - \frac{\Lambda}{2}\right)\mathbf{S} \quad (4)$$

Where I is the unit tensor, S is the forcing term in the moment space with (I – 0.5 ʌ) S=MF, and the equilibrium m^{eq} is given by,

$$\mathbf{m}^{eq} = \begin{bmatrix} 0 \\ 6(v_x F_x + v_y F_y) + \frac{12\sigma |F|^2}{\psi^2 \delta_t(\tau_e - 0.5)} \\ -6(v_x F_x + v_y F_y) - \frac{12\sigma |F|^2}{\psi^2 \delta_t(\tau_\zeta - 0.5)} \\ F_x \\ -F_x \\ F_y \\ -F_y \\ 2(v_x F_x - v_y F_y) \\ (v_x F_y + v_y F_x) \end{bmatrix} \tag{5}$$

The streaming process of the MRT LB equation is given by

$$f_\alpha(x + e_\alpha \delta_t, t + \delta_t) = f_\alpha^*(x, t) \tag{6}$$

Where $\mathbf{f}^* = \mathbf{M}^{-1}\,\mathbf{m}^*$. The macroscopic velocity and the density can be computed by

$$\rho = \sum_\alpha f_\alpha, \quad \rho\mathbf{v} = \sum_\alpha e_\alpha f_\alpha + \frac{\delta_t}{2}\mathbf{F} \tag{7}$$

Here $\mathbf{F} = (F_x\, F_y)$ is the force of interaction

$$\mathbf{F} = -G\psi(x)\sum_{\alpha=1}^{8} w(|e_\alpha|^2)\psi(x + e_\alpha)e_\alpha \tag{8}$$

Where ψ is the pseudopotential, G is the interaction strength, and w $(|e_\alpha|^2)$ are the weights, which can be written as w (1) = 1/3 and w (2) = 1/12 for the nearest - Neighbor interactions on the D2Q9 lattice.

In the original psedopotential model of Shan-Chen, the pseudopotential ψ is expressed as $\psi = \psi_o \exp(-\rho_o/\rho)$, which is normally constrained to multiple flow of low density ratio. For obtaining high density ratios, the pseudopotential can be chosen as

$$\psi = \sqrt{2p(\rho) - \rho.c_s^2)Gc^2} \tag{9}$$

where $c_s = (c/\sqrt{3})$, the lattice sound speed and p (ρ) defines an expected equation of state such as the Carnahan-Starling equation of state. With such choice psedopotential model of LBM have to undergo the lack of thermal potential because of the non-reliable densities put up by the model after the solution that was given by the Maxwell construction. Again it was discovered that the thermal reliability can be maintained by slightly changing the mechanical stability conditions and that can be installed through the improved forcing scheme.

For the pseudopotential model of MRT, an updated forcing scheme is given as by

$$S = \begin{bmatrix} 0 \\ 6(v_x F_x + v_y F_y) + \frac{12\sigma |F|^2}{\psi^2 \delta_t(\tau_e - 0.5)} \\ -6(v_x F_x + v_y F_y) - \frac{12\sigma |F|^2}{\psi^2 \delta_t(\tau_\zeta - 0.5)} \\ F_x \\ -F_x \\ F_y \\ -F_y \\ 2(v_x F_x - v_y F_y) \\ (v_x F_y + v_y F_x) \end{bmatrix} \tag{10}$$

where $|\boldsymbol{F}|^2 = (F_x^2 + F_y^2)$ and σ can be used to update the mechanical stability conditions.

III. EQUATION OF STATE

Piecewise linear equations of state for the non-ideal fluids was proposed by Colosqui et al. [5]

$$p(\rho) = \begin{cases} \rho\theta_v \;\; if & \rho \le \rho_1 \\ \rho_1\theta_v + (\rho - \rho_1)\theta_M \; if & \rho_1 < \rho \le \rho_2, \\ \rho_1\theta_v + (\rho_2 - \rho_1)\theta_M + (\rho - \rho_2)\theta_L \; if \; \rho > \rho_2 & \end{cases} \tag{11}$$

The concerned equation of state graph is shown in figure 01 in which there exists a clear relationship between the pressure and the density of the droplet. It also explains the middle region or metastable region between the state 1 and state 2 by point M.

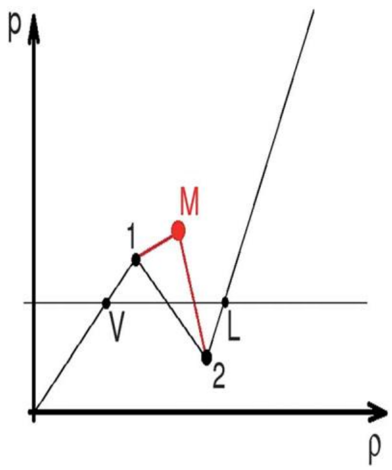

Figure 01: Graph Showing Relationship Between Pressure (P) and Density (ρ) in Equation of State

Where $\theta_V = (\partial P/\partial \rho)_V$, $\theta_L = (\partial P/\partial \rho)_L$, and $\theta_M = (\partial P/\partial \rho)_M$ are the slopes of p (ρ) in the region of vapor phase, liquid phase and the mechanically unstable area (θ_V>0 and θ_L>0, whereas θ_M < 0). Again, $\sqrt{\theta_v}$ and $\sqrt{\theta_L}$ are the respective speed of sound of the corresponding vapor and liquid phases. The two unknown variables ρ_1 and ρ_2 that express the spinodal points, are obtained by the solution of the following two simultaneous equations.

One is for the mechanical equilibrium

$$\int_{\rho_V^e}^{\rho_L^e} dp(\rho) = p(\rho_L^e) - p(\rho_V^e)$$
$$= (\rho_1 - \rho_V^e)\,\theta_V + (\rho_2 - \rho_1)\theta_M + (\rho_L^e - \rho_2)\theta_L = 0 \tag{12}$$

The second one for the chemical equilibrium

$$\int_{\rho_V^e}^{\rho_L^e} \frac{1}{\rho} dp(\rho) = \log\left(\frac{\rho_1}{\rho_V^e}\right)\theta_V + \log\left(\frac{\rho_2}{\rho_1}\right)\theta_M + \log\left(\frac{\rho_L^e}{\rho_2}\right)\theta_L = 0 \tag{13}$$

Where ρ_V^e and ρ_L^e are the density of the vapor and liquid respectively. It can be noted that for deriving the Maxwell construction the following condition is used.

$$\int_{\rho_V^e}^{\rho_L^e} \frac{1}{\rho^2}[p(\rho) - p(\rho_V^e)]d\rho = \int_{\rho_V}^{\rho_L}[p(\rho) - p(\rho_V^e)]\,d\left(\frac{-1}{\rho}\right) = \int_{\rho_V^e}^{\rho_L^e} \frac{1}{\rho} dp(\rho) = 0 \tag{14}$$

From reference [4], the parameters θ_V, θ_L, θ_M can be taken as

Table 1: Values of θ_V, θ_L, θ_M from Reference [4]

	θ_V	θ_L	θ_M
Case O	$0.04\ c_s^2$	c_s^2	$-0.36\ c_s^2$
Case A	$0.04\ c_s^2$	c_s^2	$-0.06c_s^2$
Case B	$0.49\ c_s^2$	c_s^2	$-0.06c_s^2$
Case C	$0.64\ c_s^2$	c_s^2	$-0.04\ c_s^2$

Table 2: Values of θ_V, θ_L, θ_M from reference [5]

	θ_V	θ_L	θ_M
Case D	$0.04\ c_s^2$	c_s^2	$-0.36\ c_s^2$
Case E	$0.04\ c_s^2$	c_s^2	$-0.36c_s^2$

Where ρ_V^e and ρ_L^e are given, and unknown parameters ρ_1 and ρ_2 can be calculated by the respective Eqs. (12, 13).

The speed of the sound in the liquid phase is fixed and can empirically be given as $(\theta_L)^{1/2} = c_s$.

IV. SQP METHODOLOGY

The second equation of chemical equilibrium i.e. Eq. (13) is highly non linear that contains logarithmic functions.

They can be written as,

$$F_1\ (\rho_1, \rho_1) = (\rho_1 - \rho_V^e)\ \theta_V + (\rho_2 - \rho_1)\theta_M + (\rho_L^e - \rho_2)\theta_L = 0 \qquad (15)$$

and

$$F_2\ (\rho_1, \rho_1) = \int_{\rho_V^e}^{\rho_L^e} \frac{1}{\rho}\, dp(\rho) = \log\left(\frac{\rho_1}{\rho_V^e}\right)\theta_V + \log\left(\frac{\rho_2}{\rho_1}\right)\theta_M + \log\left(\frac{\rho_L^e}{\rho_2}\right)\theta_L = 0 \qquad (16)$$

In the above equations, θ_V, θ_m, θ_L and ρ_L^e, ρ_V^e are known quantities equations. Now a non linear programming method is required to obtain the roots of above two equations.

According to Sequential Quadratic Programming (SQP) technique the roots of these equations (15) and (16) (i.e. values of ρ_1 and ρ_2) will be obtained if the function of equation (15) i.e. F_1 and the function of equation (16) i.e. F_2 satisfy the following conditions:

$$\mathrm{Min}\{F_1^2 + F_2^2\} = 0 \qquad (17)$$

In order to solve the above mentioned equations by using SQP technique a computer code has been developed using MATLAB [6].

This condition is implemented via the function 'fmincon' provided in the optimization toolbox in MATLAB.

V. RESULTS

A comparative study between the minimum value of the function coming from the conditions using 'fmincon' and the minimum value of the same function by placing the conditions given in reference [4] and [5] are compared in table 3.

Table3: Table Showing Values of ρ_1, ρ_2, min ($F_1^2+F_2^2$) for different values of ρ_l, in all these cases ρ_v = 1.These values are compared with the values reported in reference [8].

ρ_l	ρ_v	$\rho_{1,}$ (ref 5)	$\rho_{1,}$ This work	$\rho_{2,}$ (ref 5)	$\rho_{2,}$ This work	min ($F_1^2+F_2^2$), (ref 5)	min ($F_1^2+F_2^2$), This work
10	1	5.32	5.3181	8.88	8.8878	1.2689e-004	6.0627e-008
100	1	34.29	34.2841	83.59	83.5838	4.0981e-005	1.3279e-007
1000	1	240.82	238.8636	806.09	805.5182	3.1360e-005	5.9003e-006

VI. CONCLUSION

The SQP optimization technique proves to be a better solver for such non linear problems as the values suggested with the help of this method for the minimum of $F_1^2 + F_2^2$ predicts much lesser values as compare to the values of the same function calculated by previous workers for the values of ρ_1 and ρ_2 suggested by them.

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