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HIGHER ORDER DISCRETIZATION OF PSEUDO-POTENTIAL MODEL

Ricardo Leite Martins Bazarin
ricardobazarin@alunos.utfpr.edu.br
Research Center for Rheology and Non-Newtonian Fluids (CERNN), Curitiba, Brazil
Christian Naaktgeboren
naaktgeborenC@utfpr.edu.br
Research Center for Thermal Sciences, Guarapuava, Brazil
Silvio Luiz de Mello Junqueira
silvio@utfpr.edu.br
Research Center for Rheology and Non-Newtonian Fluids (CERNN), Curitiba, Brazil

Abstract. In this paper several discretization schemes that result in a improved multicomponent pseudo-potential model of the Lattice-Boltzmann method are investigated. The discretization scheme here proposed, when compared to the model original of Shan and Chen [1], considers the explicitness of the force term, the second order discretization of the stream term, the regularization model and also higher orders of discretization of derivative terms. To verify the accuracy of the proposed model, the effect of the viscosity ratio and the spurious currents obtained for the static bubble problem is investigated. The resulting algorithm maintains the simplicity of the pseudo-potential model while allowing an easy implementation for multicomponent problems. The results show that the current model, besides showing a higher viscosity ratio range than the literature results, show a significant improvement in the spurious currents range.

Keywords: Discretization, pseudo-potential, multicomponent, Lattice-Boltzmann mehtod.

1 Introduction

Over the past decades the Lattice Boltzmann method (LBM) has become a promising alternative tool to simulate the fluid dynamics of multi-component flows. Originated from evolution of the Lattice-Gas Automaton method, the LBM consists of a discrete form of the Boltzmann equation that has gained popularity by allowing simple implementation even for complex geometries, as in the case of porous media and airfoils. In addition, the method can be designed to provide high computational efficiency by parallelizing numeric codes.

Regarding the modeling of fluid-fluid and fluid-solid interfaces, the LB models found in the literature are classified as force method (color gradient and pseudo-potential) and pressure method (free-energy and interface tracking) [2]. As expected, despite their use bring advantages and disadvantages, all of of these approaches seek stability for high viscosity and density ratios, low spurious currents, as well as a low computational cost [3].

The present work focuses on the study of the pseudo-potential model, developed by Shan and Chen [1].This model incorporates the interaction of different phases and components by repulsive and/or attractive forces. However, regardless its advantages, the model also presents some limitations such as high spurious currents and instability for both low density and viscosity ratios.

In the study of multicomponent problems, particularly of immiscible fluids, Porter et al. [4] demonstrates that with the explicitness of the force term, second-order discretization of stream term, high order discretization of derivative terms in the force calculation and the collision model of multi-relaxation time - MRT, one verifies the occurrence of stability in high viscosity ratios and max value of spurious currents in the order of, 10^3 and 10^{-3} $l.u/t.s$ (lattice units/ time steps), respectively. In the most recent work, Otomo et al. [5] applies the regularization method proposed by Latt and Chopard [6], using a first order discretization of the stream term with explicitness of the force term, obtaining stability in high viscosity ratios and max value of spurious currents, both in the same orders of magnitude found by Porter et al. [4].

Remarkably, the works mentioned above contribute with specific aspects of the pseudo-potential model for multicomponent problems of immiscible fluids, but none of them are dedicated to combine such improvements. Therefore, the pseudo-potential model for multicomponents presented here combines the regularization model with the second order discretizations of the stream term, the explicitness of the force term and also higher orders of discretization of derivative terms. For that, the static bubble problem is investigated and the stability for the parameters of viscosity ratio and low spurious currents are analyzed.

2 Lattice-Boltzmann Method

The Lattice-Boltzmann method consists of a discretized form of the Boltzmann equation:

$$\frac{df}{dt} = \partial_t f + \vec{\xi} \cdot \nabla_{\vec{x}} f + \vec{g} \cdot \nabla_{\vec{\xi}} f = \Omega, \tag{1}$$

in space velocity and stream term (space-time), representing the evolution of the distribution function f which describes the probability of a particles set are in a certain position at a certain speed at a specific time. The Boltzmann discretized equation represented in the present work, called the Lattice-Boltzmann equation, using the model proposed by Bhatnagar et al. [7] for simplification of the collision operator, is written for the first order discretization of stream term in the form

$$f_i(\vec{x} + \vec{e}_i\delta_t, t + \delta_t) = f_i(\vec{x}, t) - \frac{1}{\tau}(f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)) + \delta_t F_i. \tag{2}$$

where f^{eq} is the equilibrium distribution function, F is the force term, i represents the index of space velocity discretization, $\vec{e}$ is the vector direction of velocity space discretization, δ_t is the discrete time increment and τ represents the non-dimensional relaxation time given by

$$\tau = \frac{\nu}{c_s^2} + \frac{1}{2}, \tag{3}$$

where ν and c_s are the kinematic viscosity and sound speed, respectively.

The equilibrium distribution function is given by the Maxwell-Boltzmann distribution function, which represents the probability of the particle set, like f, at a steady state. Using a second order discretization of velocity space, the equilibrium distribution function is written in its discretized form truncated in the second order term [2]:

$$f_i^{eq}(\rho, \vec{u}) = \rho w_i \Big(1 + \frac{\vec{e}_i \cdot \vec{u}}{c_s^2} + \frac{1}{2c_s^4}\vec{u}\vec{u}\colon (\vec{e}_i\vec{e}_i - c_s^2 I)\Big), \tag{4}$$

where w_i are the weight factors for the corresponding index of space velocity discretization.

The macroscopic properties of the problem are recovered from the moments of the distribution functions, i.e.,

$$\rho = \sum_i f_i, \quad \rho\vec{u} = \sum_i \vec{e}_i f_i, \quad \Pi^{neq} = \sum_i (f_i^{eq} - f_i)\vec{e}_i\vec{e}_i, \tag{5}$$

Π^{neq} is the viscous stress tensor.

The discretization of the velocity space is done using a second-order approximation for nine points, obtaining the two-dimensional lattice D2Q9, where

$$\vec{e}_{i=0} = (0,0),$$

$$\vec{e}_{i=1,2,3,4} = \left(\cos\frac{i-1}{2}\pi, \sin\frac{i-1}{2}\pi\right), \tag{6}$$

$$\vec{e}_{i=5,6,7,8} = \sqrt{2}\left(\cos\frac{i-5}{2}\pi + \frac{\pi}{4}, \sin\frac{i-5}{2}\pi + \frac{\pi}{4}\right).$$

The D2Q9 lattice weight factors are given by $w_0 = 4/9$, $w_i = 1/9$ for $i = 1,2,3,4$; and $w_i = 1/36$ for $i = 5,6,7,8$; and the sound speed by $c_s = 1/\sqrt{3}$.

2.1 Multicomponent Pseudo-Potential Model

The pseudo-potential model proposed by Shan and Chen [1] is one of the first and most widely used in the literature for describing phase transitions and immiscible flows. This model was initially constructed based on the pseudo interaction of potential mass forces between the particles of each component, so that each component σ has its own distribution function, i.e.,

$$f_{i,\sigma}(\vec{x} + \vec{e}_i\delta_t, t + \delta_t) = f_{i,\sigma}(\vec{x}, t) + \frac{1}{\tau_\sigma}(f_{i,\sigma}^{eq}(\rho_\sigma, \vec{u}_\sigma^M) - f_{i,\sigma}), \tag{7}$$

where the macroscopic properties of each component and the adjusted velocity $\vec{u}_\sigma^M$ are obtained by

$$\rho_\sigma = \sum_i f_{i,\sigma}, \quad \rho_\sigma\vec{u}_\sigma = \sum_i \vec{e}_i f_{i,\sigma}, \quad \Pi_\sigma^{neq} = \sum_i (f_{i,\sigma}^{eq} - f_{i,\sigma})\vec{e}_i\vec{e}_i, \quad \vec{u}_\sigma^M = \frac{\sum_\sigma \frac{\rho_\sigma \vec{u}_\sigma}{\tau_\sigma}}{\sum_\sigma \frac{\rho_\sigma}{\tau_\sigma}} + \tau_\sigma \vec{g}_\sigma. \tag{8}$$

The vector force per unit mass $\vec{g}$ which describes the potential mass forces between the components, characterizing the pseudo-potential model, is given by

$$\vec{g}_\sigma = \vec{g}^{ex} + \frac{\psi_\sigma}{\rho_\sigma}\sum_{\overline{\sigma}} G_{\sigma\overline{\sigma}} \sum_i w_i(\vec{e}_i)\psi_{\overline{\sigma}}(\vec{x} + \vec{e}_i\delta_t, t)\vec{e}_i \tag{9}$$

where $\vec{g}^{ex}$ represent forces resulting from external sources, ψ is the virtual mass, $\overline{\sigma}$ indicates a other component than σ and $G_{\sigma\overline{\sigma}}$, called of interaction strength, is the molecular parameter only dependent on the $\sigma - \overline{\sigma}$ intermolecular interaction. In the present work the virtual mass parameter (ψ) is represented by the density (ρ) and $G_{\overline{\sigma}\sigma} = G_{\sigma\overline{\sigma}}$.

Explicit Force Term

The velocity $\vec{u}_\sigma^M$ in the equilibrium distribution function, which incorporates the force per unit of mass $\vec{g}_\sigma$, proposed by Shan and Chen [1] results in an discretization form of the force term that introducing errors in the problem. In this way, the explicitness of the term force becomes essential for a reduction of errors introduced in the model. Rewriting the Equation (7) with the force term in the explicit form:

$$f_{i,\sigma}(\vec{x} + \vec{e}_i\delta_t, t + \delta_t) = f_{i,\sigma}(\vec{x}, t) + \frac{1}{\tau_\sigma}(f_{i,\sigma}^{eq}(\rho_\sigma, \vec{u}_\sigma) - f_{i,\sigma}) + \delta_t F_{i,\sigma}(\vec{g}_\sigma). \quad (10)$$

With the explicitness of the force term, different schemes can be used in their representation, for more details see Huang et al. [8]. The present work uses the scheme proposed by He et al. [9], which consists of the distribution function approximation by the equilibrium distribution function, given by

$$F_{i,\sigma}(\vec{g}_\sigma) = \vec{g}_\sigma \cdot \nabla_{\vec{e}_i} f_{i,\sigma} \approx \vec{g}_\sigma \cdot \nabla_{\vec{e}_i} f_{i,\sigma}^{eq} = \vec{g}_\sigma \cdot \frac{\vec{e}_i - \vec{u}}{c_s^2} f_{i,\sigma}^{eq}. \quad (11)$$

Secon Order Discretization of the Stream Term

The Discretization of the Equation (1) in the stream term (space-time) is represented initially by an expansion in Taylor series of the forward term to a first-order forward difference of the $\frac{df}{dt}$ term, algebraically write in the simplified form by

$$\begin{aligned} f_i(\vec{x} + \vec{e}_i\delta_t, t + \delta_t) &= f_i(\vec{x}, t) + \delta D_t f_i + \frac{\delta^2}{2} D_t^2 f_i + \frac{\delta^3}{6} D_t^3 f_i + ... \\ &= f_i(\vec{x}, t) + \sum_{j=1}^{\infty} \frac{\delta^j}{j!} D_t^j f_i. \end{aligned} \quad (12)$$

where D_t is the advective derivative term given by

$$D_t() = \partial_t() + \vec{e}_i \cdot \nabla_{\vec{x}}(). \quad (13)$$

From this point the truncation orders on the right-hand side of the Equation (12) represent the discretization orders of the time-space. By truncating in terms of the third order, i.e.,

$$f_i(\vec{x} + \vec{e}_i\delta_t, t + \delta_t) = f_i(\vec{x}, t) + \delta D_t f_i + \frac{\delta^2}{2} D_t^2 f_i + \mathcal{O}(\delta^3), \quad (14)$$

replacing the derivative term of $D_t f_i = \Omega_i + F_i$ and applying first order forward difference in the term $D_t\Omega_i$, we have

$$f_i(\vec{x}+\vec{e}_i\delta_t, t+\delta_t) = f_i(\vec{x}, t) + \frac{\delta}{2}[\Omega_i(\vec{x}+\vec{e}_i\delta_t, t+\delta_t) + \Omega_i(\vec{x}, t)] + \frac{\delta}{2}[F_i(\vec{x}+\vec{e}_i\delta_t, t+\delta_t) + F_i(\vec{x}, t)]. \quad (15)$$

Since $f(\vec{x}+\vec{e}_i\delta_t, t+\delta_t)$ is an unknown value and depends on $\Omega_i(\vec{x}+\vec{e}_i\delta_t, t+\delta_t)$ which is another unknown value in time t. In this way, the explicit numerical scheme is applied considering $\hat{f}_i = f_i - \frac{1}{2}(\Omega_i + F_i)$, obtaining the final form of LBE in the second order

$$\hat{f}_i(\vec{x} + \vec{e}_i\delta_t, t + \delta_t) = \hat{f}_i(\vec{x}, t) + \frac{f_i^{eq} - \hat{f}_i}{\hat{\tau}} + \left(1 - \frac{1}{2\hat{\tau}}\right) F_i\delta. \quad (16)$$

where $\hat{\tau} = \frac{\tau}{\delta} + \frac{1}{2}$.

Regularization

Historically, the regularization scheme was initially applied by Ladd [10] and later defined by Latt and Chopard [6], showing improvements in stability and accuracy of the simulations. Such a scheme has some variations in the application process according to the discretization schemes applied in the stream term. However, the method is based on the idea of representing the non-equilibrium distribution function (f_i^{neq}), eliminating high order ghost moments that cannot be controlled.

In regularized form the Equation (16) is written by

$$\hat{f}_i(\vec{x} + \vec{e}_i\delta_t, t + \delta_t) = f_i^{eq}(\vec{x}, t) + \left(1 - \frac{1}{\hat{\tau}}\right)\hat{f}_i^{neq} + \left(1 - \frac{1}{2\hat{\tau}}\right)F_i\delta. \tag{17}$$

where

$$\hat{f}_i^{neq} = w_i\left(-\frac{\vec{e}_i}{c_s^2}\frac{\delta_t}{2}\cdot\vec{g} + \frac{(\vec{e}_i\vec{e}_i - c_s^2 I)}{2c_s^4}:\Pi^{neq}\right). \tag{18}$$

For more details of the regularization process considering a second-order discretization of the stream term with forces, see Latt and Chopard [6] and Silva and Semiao [11].

High Order Discretization of the Derivative Terms

In the correct representation of surface forces present in non-ideal fluid mixtures, in this case in immiscible multicomponent fluids, appear derivative terms that are represented in the proposed force model by Shan and Chen [1].

Applying a Taylor series expansion on the term $\psi_{\overline{\sigma}}$ present in Equation (9)

$$\psi_{\overline{\sigma}}(\vec{x} + \vec{e}_i\delta_t, t) = \sum_{n=0}^{\infty}\frac{1}{n!}\left[\nabla^{(n)}\psi_{\overline{\sigma}}\right]\cdot\underbrace{\vec{e}_i\vec{e}_i...\vec{e}_i}_{n\text{ terms}}, \tag{19}$$

and substituting in the Equation (9) without external forces has

$$\begin{aligned}\vec{g}_\sigma &= \frac{\psi_\sigma}{\rho_\sigma}\sum_{\overline{\sigma}}G_{\sigma\overline{\sigma}}\sum_i^d w_i|(\vec{e}_i)|^2\psi_{\overline{\sigma}}(\vec{x} + \vec{e}_i\delta_t, t)\vec{e}_i \\ &= \frac{\psi_\sigma}{\rho_\sigma}\sum_{\overline{\sigma}}G_{\sigma\overline{\sigma}}(E^{(2)}\cdot\nabla\psi + \frac{1}{3!}E^{(4)}\cdot\nabla^{(3)}\psi + \frac{1}{5!}E^{(6)}\cdot\nabla^{(5)}\psi + ...)\end{aligned} \tag{20}$$

where d represents the different distances considered in the interaction of ψ and $E^{(n)}$ is the tensor of (n) order described by

$$E^{(n)} = E^{(n)}_{\alpha_1,\alpha_2,...,\alpha_n} = \sum_i^d w_i|(\vec{e}_i)|^2\vec{e}_{i,\alpha_1}\vec{e}_{i,\alpha_2}...\vec{e}_{i,\alpha_n}, \tag{21}$$

the values of $E^{(n)}$ are directly related to the velocity space discretization, so that the odd orders of the tensor are null, i.e., $E^{(n*2+1)} = 0$. Truncating the Equation (20) gives different interaction distances for each order, in the Figure 1 the respective distances up to the sixteenth order are illustrated. For more details of the discretization processes and the respective weights $w_i|(\vec{e}_i)|$ for each order, see Shan [12] and Sbragaglia et al. [13]. In the present simulations the tenth order discretization in derivative terms is used.

3 Results and Discussion

In order to examine the feasability of the improvements resulting from the specifications applied to the pseudo-potential model, two-dimensional static bubble problem are simulated and compared to the results of Porter et al. [4] and Otomo et al. [5].

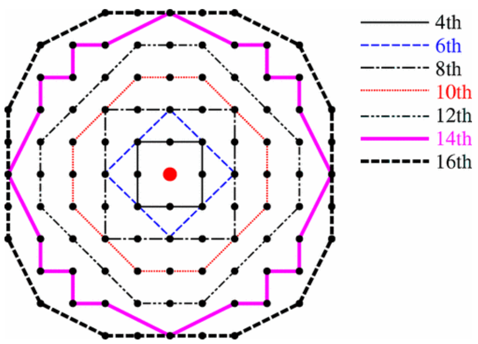

Figure 1. Immiscibility.

Aiming to verify the surface tension, spurious currents and its viscosity dependencies, simulations of the static bubble problem are performed using different viscosity, viscosity ratio and interaction strength. The problem geometry consists of a circular bubble of ratio r_b (fluid 2) located at the center of a square domain with length $H = 120\ l.u$ (lattice units) containing another suspending (fluid 1), where periodic conditions are applied on all boundaries (see Figure 2 **b)**). The considerations problem is assumed to be in steady regime, constant temperature, null gravitational force, being both fluids incompressible and Newtonian. The simulation is performed until the equilibrium point is reached.

Before any specific analysis, a components immiscibility test is required. For that, the influence of the $G_{\sigma\overline{\sigma}}$ coefficient, which controls the intensity of the cohesive force between components, is performed to estimate the miscibility and immiscibility ranges. In this test, densities of fluid 2 ($\rho_2 = 1$) and fluid 1 ($\rho_2 = 1$) are monitored at the center of the volume with $r_b = 37.5 l.u.$, for three different viscosity ratios ($M = \frac{\nu_2}{\nu_1}$), $M = 10^0$, $M = 10^3$ and $M = 10^6$.The results obtained for the range of $G_{\sigma\overline{\sigma}}$, verified in Figure 2 **a)**, show that values of $G_{\sigma\overline{\sigma}} \leq 2$ occurs the diffusion of one fluid over the other, while the range $2 < G_{\sigma\overline{\sigma}} \leq 2.5$ perceives a transition region of the fluid interaction. Furthermore, the interval $2.5 \leq G_{\sigma\overline{\sigma}}$ can be considered, with a certain tolerance, the immiscibility condition. Notably, for a certain tolerance, the behavior of the components with the variation of $G_{\sigma\overline{\sigma}}$ is independent of M. In Figure 2 **b)**, one can see the representation of the density field of fluid 2 for the immiscibility range of $G_{\sigma\overline{\sigma}}$ mentioned.

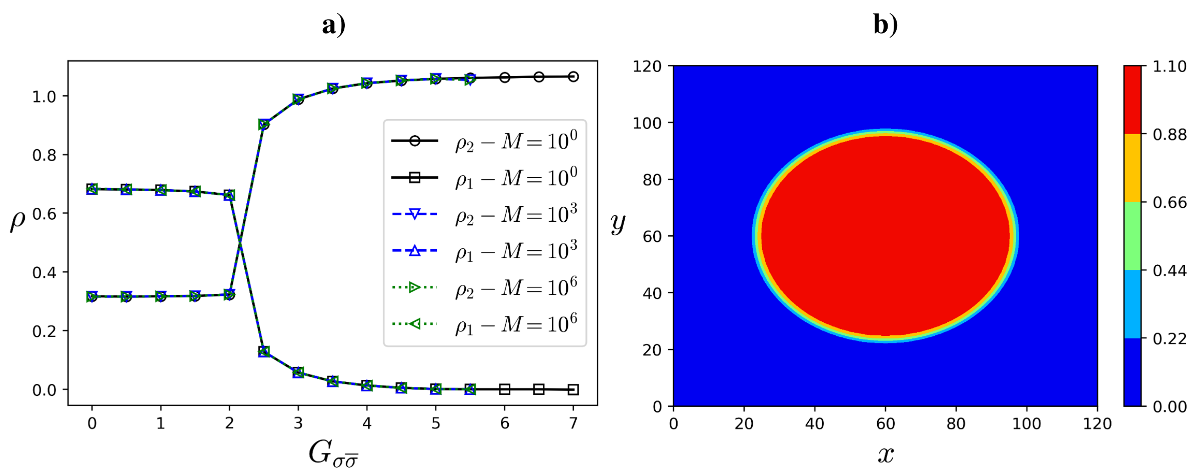

Figure 2. Immiscibility test: **a)** variation of the density ρ_1 and ρ_2, in the center of the volume for different values of $G_{\sigma\overline{\sigma}}$ ($M = 10^0$; $M = 10^3$; $M = 10^6$); **b)** density field in the immiscible range.

Once the immiscibility range is defined, the superficial tension analysis between immiscible fluids 1 and 2 is based on the Laplace equation, varying r_b as a function of Δp:

$$\Delta p = p_2 - p_1 = \frac{\gamma}{r_b}. \tag{22}$$

That way, the physical representation of superficial tension (γ) is verified by the modified pseudo-potential model for three different viscosity ratios $M = 10^0$, $M = 10^3$ and $M = 10^6$, considering $G_{\sigma\overline{\sigma}} = 3.0$, $G_{\sigma\overline{\sigma}} = 3.5$ and $G_{\sigma\overline{\sigma}} = 4.0$. The results obtained in Figure 3 **a)** demonstrate a correct linear behavior of Δp as a function of $1/r_b$, as well as an independence of γ to M and a proportionality for the increase of γ with the increase of $G_{\sigma\overline{\sigma}}$.

Investigating the influence of spurious currents on the model in terms of ν_1 and M for the static bubble using $r_b = 37.5$, the results obtained can be seen in Figure 3 **b)** compared to Porter et al. [4] and Otomo et al. [5]. Varying ν_1 to $M = 1$ generally has $|u|_{max}$ in the order 10^{-4}, i.e, one order less than the other results compared. In the variation of M keeping constant $\nu_1 = 0.0067$, as well as in the variation of ν_1, was observed in general $|u|_{max}$ in the order 10^{-4}, while the other works compared show results in the order of 10^{-3}.

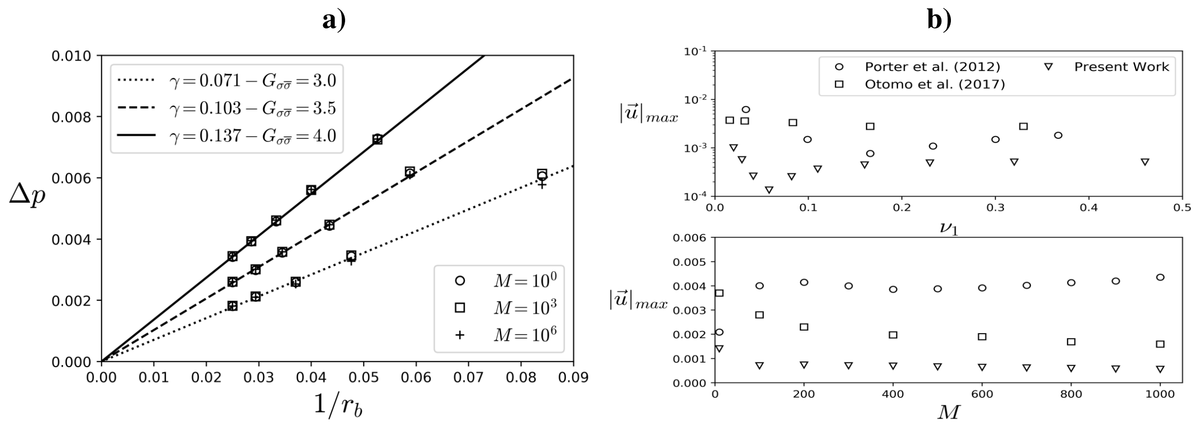

Figure 3. Superficial tension and spurious currents: **a)** Laplace equation verification for different values of M and $G_{\sigma\overline{\sigma}}$; **b)** Comparison of the max value of spurious currents in function of ν_1 and M.

4 Conclusions

The present pseudo-potential multicomponent model based on discretization enhancements in relation to the original proposed by Shan and Chen [1], was used to simulate the static bubble problem in order to observe the influence of the force term explicitness, second order discretization of stream term, regularization and tenth order discretization of the derivative terms, both combined.

The obtained results demonstrate a correct representation of the static bubble problem, identifying the miscibility, transition and immiscibility ranges, as well as the verification of the Laplace equation (Eq. 22). Compared to other works in the literature, especially Porter et al. [4] and Otomo et al. [5], the present model demonstrates three more order in the variation of viscosity ratio (M) and one less order in the influence of spurious currents. Consequently, the present model allows a relation of viscosity ratios of up to 10^6, enabling multicomponent interactions between fluids such as gases and highly viscous fluids, with spurious currents in the order of 10^{-4}.

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