MULTIPLE-RELAXATION-TIME LATTICE-BOLTZMANN MODEL FOR IMMISCIBLE FLUIDS

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Abstract. *Classical (macroscopic) modelling of immiscible fluid flow at steady state is treated performing a momentum balance around the transition layer, plus mass and momentum equations and coupling conditions just right at interface. We propose a lattice-Boltzmann based model where the fluid/fluid interface appears from mesoscopic interaction between the fluids themselves through a long-range strength field which intensity is transferred using pseudo-particles called field mediators. These null-mass particles transfer information of the concentration of each fluid to the neighborhood at each time step, allowing the use of this information to create interfacial tension. This lattice Boltzmann model has Galilean invariance and a larger range of viscosities than other models in the lattice Boltzmann framework . Moreover, we use in this model a procedure based on Moment's Method, with a splitted collision operator for mutual and cross collisions, which increases the number of free-paramenters from three to thirteen in two dimensions, which possibly will improve the numerical stability of the model. Quantitative and qualitative numerical simulations are carried out to demonstrate the efficiency of the model.*

Keywords*: immiscible fluids, lattice-Boltzmann methods, moment's method.*

1. Introduction

The Lattice Boltzmann Method (LBM) has been used, in the last decade, in the simulation of the Navier-Stokes equations in the low Mach number limit. Since the pioneer work of Frisch et al. (1986), at that time using lattice gas methods, these models had attracted much attention and were applied in a great variety of problems, including complex flow, such as the modeling of viscoelastic and biologic fluids.

Such kinds of systems describe the dynamics of particles in a regular lattice through a particle distribution function. Each evolution time step δ_t is divided in two main ones: streaming and collision. In the streaming process, at a site $\vec{x}$ and time *t*, the number of particles at direction *i*, $K_i(\vec{x},t)$, hop to the site $\vec{x}+\vec{c}_i\delta_t$, according to the velocity set $\vec{c}_i$, $i=0,1,\ldots,b$. During the collision process, the particles at the same site are stirred towards a prescribed equilibrium distribution function, in a way that quantities such as mass, momentum, chemical species and energy are preserved.

In this work is presented an athermal, bidimensional model for immiscible fluids, in which the collision process is performed in the moment space (d'Humières, 1992), instead in velocity space. Furthermore, we also use the idea of field mediators, proposed by Santos & Philippi (2002), and introduced in the lattice Boltzmann framework by the same authors (Santos et al., 2003).

Gustensen et al. (1991, 1992) are attributed to be the first who introduced immiscible fluids color based models in the frame of the LBM. A more popular two-phase flow model, based on a pseudopotential function, was derived by Shan and Chen (1993). The first tentative to a two-phase thermodynamically consistent model was performed by Swift et al. (1995), but the model that they proposed cannot lead to correct energy transport and it is not Galilean invariant. A detailed comparison between all these models has yet to be done.

This paper is divided as follows. In the next section, the model is explained. Section 3 is used to provide a collection of equilibrium moments in order to correctly retrieve the Navier-Stokes equations. In section 4, results from simulations are compared with theoretical predictions for the model. Section 5 concludes the paper.

2. Model

This LBM is defined in a 2D square lattice, unit length and nine directions for the velocity, called D2Q9. Assuming $\delta_t = 1$, one can define the velocity set as $\vec{c}_0$=(0,0), $\vec{c}_1$=(1,0), $\vec{c}_2$=(0,1), $\vec{c}_3$=(-1,0), $\vec{c}_4$=(0,-1), $\vec{c}_5$=(1,1), $\vec{c}_6$=(-1,1), $\vec{c}_7$=(-1,-1), $\vec{c}_8$=(1,-1), where $\vec{c}_\alpha = (c_{\alpha,x}, c_{\alpha,y})$.

Considering two immiscible fluids *r* and *b*, the long range attraction between the particles is represented through the use of the concept of field mediators at each lattice site. Defining $R_i(\vec{x},t)$ as the *r*-particle distribution function, and in a similar manner $B_i(\vec{x},t)$ for *b*-particles, field mediators for the *k*-phase are created in the following manner

$$M_i^k(\vec{x},t) = \frac{\sum_i K_i}{\sum_i R_i + B_i}, \tag{1}$$

and they are streamed as

$$M_i^k(\vec{x}+\vec{c}_i, t+1) = M_i^k(\vec{x},t). \tag{2}$$

The interference of field mediators in the particle distribution function is described in the following. The evolution of the system of particles is described by the lattice-Boltzmann equation,

$$K_i^{'}(\vec{x},t) - K_i(\vec{x},t) = \sum_j \left[\Lambda_{ij}^k (R_0,\ldots,R_b,B_0,\ldots,B_b)\right], \tag{3}$$

$$K_i(\vec{x}+\vec{c}_i, t+1) = K_i^{'}(\vec{x},t), \tag{4}$$

$K = R, B$, and Λ^k is the collision operator.

The splitted collision operator is proposed in the following manner

$$\sum_j \left[\Lambda_{ij}^k (R_0,\ldots,R_b,B_0,\ldots,B_b)\right] = \sum_j \left[\omega^k \Lambda_{ij}^{kk}(K_0,\ldots,K_b) + \omega^{\bar{k}} \Lambda_{ij}^{rb}(R_0,\ldots,R_b,B_0,\ldots,B_b)\right], \tag{5}$$

where $\omega^k = \rho^k/(\rho^k + \rho^{\bar{k}})$ is the *k*-phase concentration and $\omega^{\bar{k}}$ is the $\bar{k} = b, r$-phase concentration. The first term of the right-hand side of Eq. (5) refers to collisions between particles of same species (e. g., *r*-*r* collisions), while the second term of the r.h.s. refers to cross collisions. This last term is responsible for the phase segregation.

Considering K_i distributions near the equilibrium K_i^{eq}, the collision operator can be linearized, $\Omega : \Re^{b+1} \to \Re^{b+1}$, in the following way

$$\sum_j \left[\omega^k \Lambda_{ij}^{kk}(K_0,\ldots,K_b) + \omega^{\bar{k}} \Lambda_{ij}^{k\bar{k}}(K_0,\ldots,K_b,\bar{K}_0,\ldots,\bar{K}_b)\right] = \sum_j \left[\omega^k \Lambda_{ij}^{kk} K_j^{(neq),kk} + \omega^{\bar{k}} \Lambda_{ij}^{k\bar{k}} K_j^{(neq),k\bar{k}}\right], \tag{6}$$

where $K_j^{(neq),pq} = K_j - K_j^{(eq)}(\rho^p, \vec{u}^q)$, $\bar{k}$ is the other phase of the $k - \bar{k}$ system, and Λ^{pq} is the linearized collision operator.

In this way, the full lattice-Boltzmann equation for this model is

$$K_i(\vec{x}+\vec{c}_i, t+1) = K_i(\vec{x},t) + \sum_j \left[\omega^k \Lambda_{ij}^{kk} K_j^{(neq),kk} + \omega^{\bar{k}} \Lambda_{ij}^{k\bar{k}} K_j^{(neq),k\bar{k}}\right]. \tag{7}$$

The collision process has to preserve the individual mass of species,

$$\sum_i K_i = \sum_i K_i^{(eq)} = \rho^k, \tag{8}$$

and has also to preserve *total* momentum,

$$\sum_i \left(R_i + B_i\right)\vec{c}_i = \sum_i \left(R_i^{(eq)} + B_i^{(eq)}\right)\vec{c}_i = \rho^r \vec{u}^r + \rho^b \vec{u}^b = \rho\vec{u} \cdot \tag{9}$$

The collision operator is defined in such a way that the eigenvalues associated to the eigenvectors of the conserved quantities are set to be zero, and that its eigenvectors form an orthogonal basis for $\Re^{b+1}$. This basis is obtained through a Gram-Schmidt orthogonalization process of the polynomials of $\vec{c}_i$, leading to the D2Q9 result

$$\Psi_{0,i} = \left\|\vec{c}_i\right\|^0, \vec{\Psi}_0 = \left(1,1,1,1,1,1,1,1,1\right), \tag{10}$$

$$\Psi_{1,i} = c_{i,x}, \vec{\Psi}_1 = \left(0,1,0,1,-1,1,-1,-1,1\right), \tag{11}$$

$$\Psi_{2,i} = c_{i,y}, \vec{\Psi}_2 = \left(0,0,1,0,-1,1,1,-1,-1\right), \tag{12}$$

$$\Psi_{3,i} = 3\left\|\vec{c}_i^2\right\| - 4\left\|\vec{c}_i\right\|^0, \vec{\Psi}_3 = \left(-4,-1,-1,-1,-1,2,2,2,2\right), \tag{13}$$

$$\Psi_{4,i} = c_{i,x}^2 - c_{i,y}^2, \vec{\Psi}_4 = \left(0,1,-1,1,-1,0,0,0,0\right), \tag{14}$$

$$\Psi_{5,i} = c_{i,x}c_{i,y}, \vec{\Psi}_5 = \left(0,0,0,0,0,1,-1,-1,1\right), \tag{15}$$

$$\Psi_{6,i} = c_{i,x}\left(3\left\|\vec{c}_i\right\|^2 - 5\left\|\vec{c}_i\right\|^0\right), \vec{\Psi}_6 = \left(0,-2,0,2,0,1,-1,-1,1\right), \tag{16}$$

$$\Psi_{7,i} = c_{i,y}\left(3\left\|\vec{c}_i\right\|^2 - 5\left\|\vec{c}_i\right\|^0\right), \vec{\Psi}_7 = \left(0,0,-2,0,2,1,1,-1,-1\right), \tag{17}$$

$$\Psi_{8,i} = \left(9\left\|\vec{c}_i\right\|^4 - 21\left\|\vec{c}_i\right\|^2 + 8\left\|\vec{c}_i\right\|^0\right)/2, \vec{\Psi}_8 = \left(4,-2,-2,-2,-2,1,1,1,1\right) \cdot \tag{18}$$

Due to the orthogonality of the basis, an expansion of K_i reads

$$K_i = \frac{a_0^k \Psi_{0,i}}{\Psi_0^{\,2}} + \frac{a_1^k \Psi_{1,i}}{\Psi_1^{\,2}} + \ldots + \frac{a_b^k \Psi_{b,i}}{\Psi_b^{\,2}} = \sum_{\theta=0}^{b} \frac{a_\theta^k \Psi_{\theta,i}}{\Psi_\theta^{\,2}} \cdot \tag{19}$$

Applying this formulation to the evolution equation, Eq. (7), it turns out to be an evolution equation for the moments of the equilibrium distribution function. Hence,

$$a_\theta^{k'} - a_\theta^k = \omega_k \lambda_\theta^{kk} a_\theta^{(neq),kk} + \omega_{\bar{k}} \lambda_\theta^{k\bar{k}} a_\theta^{(neq),k\bar{k}}, \tag{20}$$

where λ_θ^{pq} is the eigenvalue from Λ^{pq} associated to Ψ_θ; $a_\theta^{(neq),kk} = a_\theta^{(neq),kk}\left(\rho^k, \vec{u}^k\right)$ and $a_\theta^{(neq),k\bar{k}} = a_\theta^{(neq),k\bar{k}}\left(\rho^k, \vec{\vartheta}^{\bar{k}}\right)$. The first term of the r.h.s. of Eq. (20) is related to the relaxation of the moment a_θ^k towards a prescribed equilibrium, given density and velocity of the component k. The second term considers $r-b$ (i.e. $k-\bar{k}$) collisions, and is related to the relaxation of the moment a_θ^k towards a prescribed equilibrium dependent of density ρ^k and velocity

$$\vec{\vartheta}^{\bar{k}} = \vec{u}^{\bar{k}} \mp A\hat{u}^m, \tag{21}$$

$\bar{k} = r, b$, where A is a free parameter of the model and is related to the interfacial tension. If $A = 0$ the model reduces to a miscible model (Facin et al., 2003). Otherwise, the model mimics two immiscible fluids, where k-particles are taken away from $\bar{k}$-particles by a long-range field. In Eq. (21),

$$\hat{u}^m = \begin{cases} \dfrac{\vec{u}^m}{\left|u^m\right|}, & \text{se } u_m \neq 0\,, \\ 0, & \text{se } u_m = 0\,, \end{cases} \tag{22}$$

where the mediators velocity is given by

$$\vec{u}_m = \sum_i \left(M_i^r - M_i^b\right)\vec{c}_i\,. \tag{23}$$

In this way, the collision process is performed in moment space, and in order to execute the streaming step, one has to find again the new *r* and *b* particle distributions. To do that, one applies Eq. (19).

It is interesting to see that the proposed model reduces to the model of Santos et al. (2003) if $\lambda_3^{kk} = \lambda_4^{kk} = \ldots = \lambda_8^{kk}$, $\lambda_3^{\bar{k}\bar{k}} = \lambda_4^{\bar{k}\bar{k}} = \ldots = \lambda_8^{\bar{k}\bar{k}}$ and $\lambda_3^{k\bar{k}} = \lambda_4^{k\bar{k}} = \ldots = \lambda_8^{k\bar{k}}$, where $\lambda_\theta^{kk} = 1/\tau^k$, $\lambda_\theta^{\bar{k}\bar{k}} = 1/\tau^{\bar{k}}$ and $\lambda_\theta^{k\bar{k}} = 1/\tau^m$.

3. Macroscopic Equations

In order to retrieve the Navier-Stokes equations for incompressible athermal fluids, the equilibrium moments must be chosen as

$$a_0^{(eq),pq} = \rho^p\,, \tag{24}$$

$$a_1^{(eq),pq} = \rho^p u_x^q\,, \tag{25}$$

$$a_2^{(eq),pq} = \rho^p u_y^q\,, \tag{26}$$

$$a_3^{(eq),pq} = -2\rho^p + 3\rho^p u^{q^2}\,, \tag{27}$$

$$a_4^{(eq),pq} = \rho^p (u_x^{q^2} - u_y^{q^2})\,, \tag{28}$$

$$a_5^{(eq),pq} = \rho^p u_x^q u_y^q\,, \tag{29}$$

$$a_6^{(eq),pq} = -\rho^p u_x^q \tag{30}$$

$$a_7^{(eq),pq} = -\rho^p u_y^q \tag{31}$$

$$a_8^{(eq),pq} = \rho^p - 3\rho^p u^{q^2} \tag{32}$$

The macroscopic equations of the LBM are retrieved applying the Chapman-Enskog expansion. Far from the interface for the pure *k*-phase these equations are the continuity equation and the Navier-Stokes equations,

$$\partial_t \rho^k + \partial_\alpha(\rho u_\alpha^k) = 0\,, \tag{33}$$

$$\partial_t \rho^k u_\alpha^k + \partial_\beta(\rho^k u_\alpha^k u_\beta^k) = -\partial_\alpha p^k + \nu^k \partial_\beta\left[\rho(\partial_\alpha u_\beta^k + \partial_\beta u_\alpha^k)\right] + \zeta^k \partial_\alpha(\rho^k \partial_\gamma u_\gamma^k)\,, \tag{34}$$

which first and second viscosity coefficients are related with the collision operator eigenvalues in the following manner:

$$\nu^k = \zeta^k = \frac{1}{3}\left(\frac{1}{\lambda_4^{kk}} - \frac{1}{2}\right) = \frac{1}{3}\left(\frac{1}{\lambda_5^{kk}} - \frac{1}{2}\right). \tag{35}$$

For isotropy reasons, one does $\lambda_4^{kk} = \lambda_5^{kk}$ e $\lambda_6^{kk} = \lambda_7^{kk}$. Far from the interface, pressure p_k is proportional to density, $p_k = {c_s}^2 \rho_k$, where ${c_s}^2 = 1/3$ is the square of the sound speed. In order to conserve momentum, $\lambda_1^{k\bar{k}} = \lambda_2^{k\bar{k}}$.

4. Results

4.1 Interfacial Tension

Santos et al. (2003) used the mechanical definition of interfacial tension in order to deduce an analytical expression, function of the parameters of the model, and in this work the same method will be used to measure interfacial tension. The final expression, after some algebra, reduces to

$$\sigma^{rb} = \frac{{c_s}^2 \rho_0 A}{2\left(2\tau^m - 1\right)} \left\{ \begin{array}{l} \dfrac{1}{\left(\tau^m - \tau^b\right)\left(\tau^m - \tau^r\right)} \left[\left({\tau^m}^2 - \tau^m(\tau^r + \tau^b) + \tau^r \tau^b \right) + 4\tau^m \left(\tau^m \tau^b - 2\tau^r \tau^b + \tau^m \tau^r \right) \right] + \\ 4{\tau^m}^2 \left[\dfrac{\tau^r}{\left(\tau^m - \tau^r\right)^2} \left(1 + \tau^m - \tau^r\right) \ln \dfrac{\tau^r}{\tau^m} + \dfrac{\tau^b}{\left(\tau^m - \tau^b\right)^2} \left(1 + \tau^m - \tau^b\right) \ln \dfrac{\tau^b}{\tau^m} \right] \end{array} \right\}. \tag{36}$$

In this simulation one uses the fact that the present model reduces to the model of Santos et al. (2003) to allow a comparison of the results.

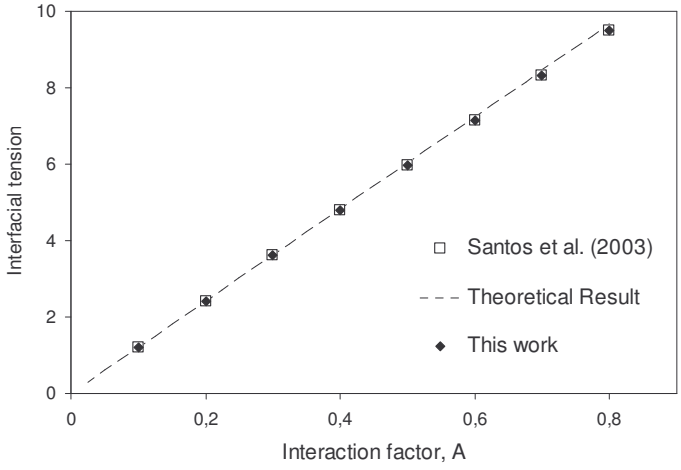

Figure 1 – Interaction factor versus interfacial tension

For this simulation, a unidimensional lattice with 2000 sites was used, where the two phases are initially segregated and periodic boundary conditions were used. The values for the parameters are the following $\tau^r = 1/\lambda_\theta^{rr} = 1.0$, $\tau^b = 1/\lambda_\theta^{bb} = 3.0$, $\theta = 3,\ldots,8$ e $\tau^m = 1/\lambda_\theta^{rb} = 1.0$, $\theta = 1,\ldots,8$. Results are shown in Fig. 1, and are in excellent agreement with theoretical prediction.

4.2 Laplace's Law

Immiscible fluid models must obey Laplace's Law, which predicts a linear dependence between pressure drop and droplet radius, at equilibrium, through interfacial tension σ^{rb}, in such a way that

$$\Delta p = \frac{\sigma^{rb}}{R}. \tag{37}$$

The initial condition for the simulation is a 2D *r*-phase droplet with radius *R*, placed in a 10*R* x 10*R* lattice domain, in order to avoid boundary influence in the simulation results.

Figure 2 shows the pressure difference against $1/R$ in seven runs. Initial density is $\rho_r = \rho_b = 1.0$, interaction factor *A=0.*4 and relaxation times $\lambda_3^{rr} = 0.65$, $\lambda_4^{rr} = 0.75$, $\lambda_6^{rr} = 0.7$, $\lambda_8^{rr} = 0.8$, $\lambda_3^{bb} = 0.75$, $\lambda_4^{bb} = 0.7$, $\lambda_6^{bb} = 0.65$, $\lambda_8^{bb} = 0.8$, $\lambda_1^{rb} = 1.0$, $\lambda_3^{rb} = 0.95$, $\lambda_4^{rb} = 0.9$, $\lambda_6^{rb} = 0.95$ e $\lambda_8^{rb} = 1.1$.

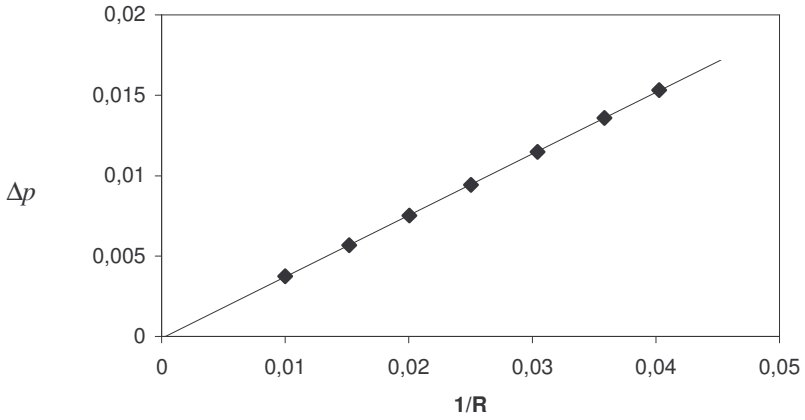

Figure 2 – Laplace's Law

In this way, the interfacial tension, which is precisely the slope of the curve, could be determined by a simple linear curve fitting. By this method, interfacial tension is 0.3827 net units, very near to the value given by the method in the former section, which gives 0.3744 n.u.

4.3 Capillary Waves

The dispersion of capillary waves is a problem commonly used to test LBM for immiscible fluids.The initial condition for this problem can be seen in Fig. 3, where a L×2L (y=2L) domain is filled with *r*-fluid if y<L and filled with *b*-fluid otherwise. A sinusoidal wave is imposed as initial condition to the interface. For this problem, an analytical formulation is described in Landau & Lifschitz (1987) which gives the relation

$$\omega^2 = \frac{\sigma^{rb} k^3}{2\rho}, \tag{38}$$

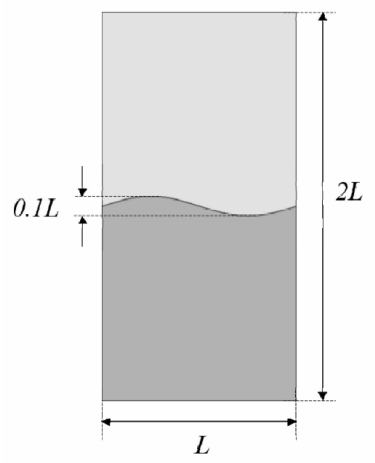

Figure 3 – Initial condition for the capillary waves problem

where k is the wave number and ω is related to the damping. The following parameters were used in the simulation: $\tau^r = \tau^b = 0.52$, $\tau^m = 1.0$, interaction factor $A = 0.4$ and $\rho = 1.0$. The results are shown in Fig. 4, and agree well with the theoretical prediction.

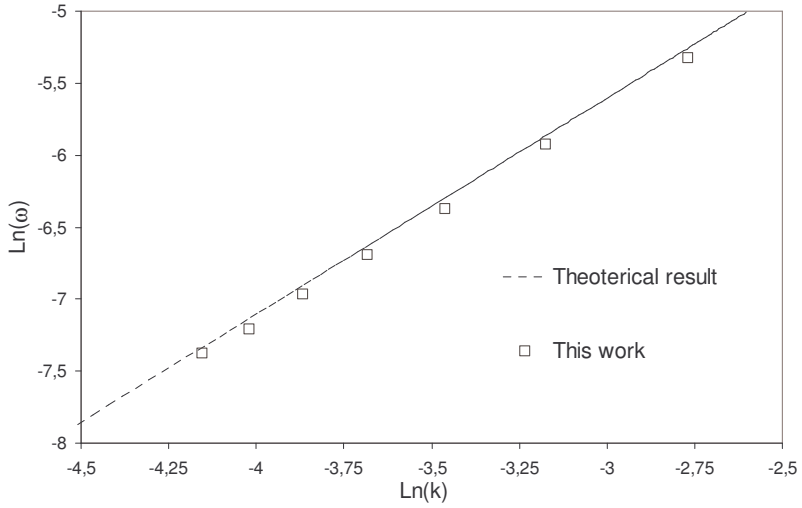

Figure 4 – Comparison between theoretical and simulated results for the cappilary waves problem

5. Conclusions

In the present paper, a model for immiscible fluids with multiple relaxation times based in the lattice Boltzmann equation was proposed. The collision term was splitted, considering cross and mutual collisions between the two species of fluids in moment space. Long range field forces were simulated taken into account long range interaction. Usual simulations for immiscible fluids models were carried out numerical results are in agreement with theoretical ones. For future works, one should perform the Von Neumann stability analysis, and also the Chapman-Enskog expansion for the transition layer. A point that should be emphasized is the easy extensibility of this model to the 3D case, using for that the corresponding lattice and equilibrium distribution function.

6. Acknowledgements

Authors are greatly indebted to ANP (Agência Nacional de Petróleo), CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico), FINEP (Financiadora de Estudos e Projetos) and Petrobras S.A. for the financial support.

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8. Responsibility notice

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