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MULTI-SCALE MODELLING AND HYBRID ATOMISTIC CONTINUUM SIMULATION FOR CONDENSATION OF GAS IN A MICROCHANNEL

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ABSTRACT

A hybrid atomistic-continuum method devoted to the study of multi-scale problems is presented. The simulation domain is decomposed into three regions: the bulk where the continuous Navier-Stokes and energy equations are solved, the neighborhood of the wall simulated by the Molecular Dynamics and the overlap region which connects the macroscopic variables (velocity and temperature) between the two former regions. For the simulation of long micro/nanochannels, we adopt multiple molecular blocks along the flow direction to capture accurately the velocity and temperature variations from the inlet to the outlet. The validity of the hybrid method is shown by comparisons with a simplified analytical model in the molecular region. The method is then applied successfully to the study the hydrodynamic and thermal development of a liquid flow in a long micro/nanochannel without and with condensation.

INTRODUCTION

The miniaturization of fluid systems induces an increase in the exchange surface for a given volume, for example, to improve the heat transfer through walls. Reducing the characteristic dimensions compared to molecular mean free path gives rise to many new physical phenomena related to the fluid/solid interface, i.e. velocity slip, temperature jump and thermal creep which are typically negligible at large-scale. In the literature, macroscopic models have been developed to account for these size effects. However, there is no unique way of writing boundary conditions which depend on many unknown parameters (velocity and energy accommodation coefficients TMAC, EAC, ...) and do not capture all the complexity of physics which occurs during the interaction between wall atoms and fluid molecules (for example in physisorption phenomena).

To enhance the description of the fluid flow in channels with a large aspect ratio, a hybrid numerical model coupling the Molecular Dynamics and the Finite Volume method has been recently developed to take into account the multi-scale character of transfer phenomena [7]. An atomistic approach is used in molecular blocks located along the fluid/solid interface in order to accurately describe the complex interactions at small scales while a description based on the continuum mechanics is adopted in the bulk to consider the large-scales relative to transfer phenomena in the axial direction of the channel.

The purpose of this paper is to extend the monophasic model of an incompressible fluid flow, based on our hybrid atomistic-continuum method recently proposed, to a model for which a gaseous phase condenses slightly at the vicinity of the walls.

MODELLING

We consider a channel of rectangular section of height $2H$ and depth $l \gg 2H$, and length $L \gg l$. The inner walls are made of platinum and argon fluid (in liquid or gaseous phase) is injected into the inlet section. The walls, located at $y = \pm l/2$ and $z = 0; 2H$, are thermally isolated and kept at the temperature T_w . Taking into account the aspect ratio $l/2H \gg 1$ and the adiabatic boundary conditions at $y = \pm l/2$, it is possible to adopt a two-dimensional geometry. Since the flow is symmetrical, the simulation domain can be halved by using a symmetry plane at $z = H$.

Domain decomposition: The rectangular geometry of the channel is divided into three sub-domains:

i) The continuum region (C) at the center of the channel is dominated by the bulk behavior, governed

by the continuous equations (domain above the dashed line in Figure 1).

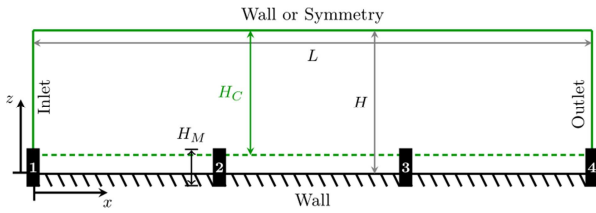


Figure 1

Sketch of simulation domain of height H and length L . The fluid region (height H_C) is governed by the Navier-Stokes and energy equations. An atomistic description is used to model the wall and the adjacent fluid (numbered rectangular blocks of heights H_M).

ii) The molecular/atomistic regions (M) where the particle approach is used to model fluid/solid interactions at the micro-/nanoscales (Figure 2)

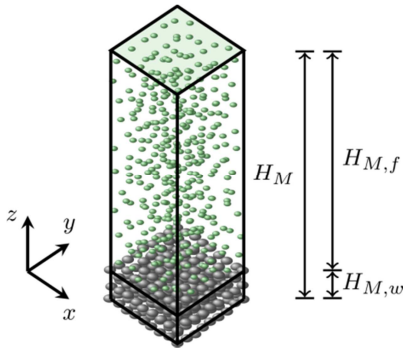


Figure 2

Example of a molecular simulation block of total height $H_M = H_{M,f} + H_{M,w}$, where $H_{M,f}$ is the fluid height and $H_{M,w}$ the wall thickness.

iii) The overlap region designed to enable the communications between both macro- and microscales (Figure 3).

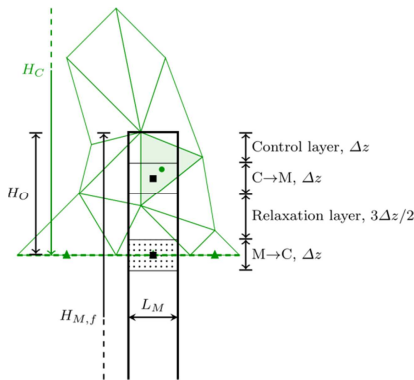


Figure 3

Example of the overlap zone ensuring the communication between the molecular region of dimensions $L_M \times H_M$, and the continuum region, here locally covered by a mesh of triangles. The sub-layer heights Δz of the overlap region are typically 10% of $H_{M,f}$.

The continuous region (C) communicates with each molecular domain (M) via an overlap region whose size H_O is typically 40% of $H_{M,f}$. This recovery area is divided into 4 sub-layers (Fig. 3): two of them guarantee exchanges between the continuous and molecular domains ($C \rightarrow M$ and $M \rightarrow C$), a relaxation layer decouples the dynamic between regions $C \rightarrow M$ and $M \rightarrow C$, and a control layer, which is used to control the number of particles in each molecular block and then the density.

Molecular model: In each molecular block, the Lennard-Jones potential is used to describe all pair interactions: argon/argon for fluid interactions and argon/platinum for solid ones. It reads:

$$V_{\alpha\beta}(r) = 4\varepsilon_{\alpha\beta} \left[\left(\frac{\sigma_{\alpha\beta}}{r} \right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r} \right)^6 \right]$$

where the subscript $\alpha\beta$ stands for ff (fluid/fluid) or fw (fluid/wall). The parameters $\varepsilon_{\alpha\beta}$ and $\sigma_{\alpha\beta}$ are respectively the potential well-depth and the “diameter”. Taking argon as the reference material, the potential parameters for the couple Ar/Pt and their atomic masses m_f and m_w can be expressed in the reduced Lennard-Jones units: $\varepsilon_{ff} = \varepsilon$, $\sigma_{ff} = \sigma$, $m_f = m$, $\varepsilon_{wf} = 0.535 \varepsilon$, $\sigma_{wf} = 0.906 \sigma$, $m_w = 4.8833 m$ with $\varepsilon = 1.656 \times 10^{-21}$ J, $\sigma = 3.405 \text{ \AA}$ and $m = 6.633 \times 10^{-26}$ kg. The reference scales for time, temperature and velocity are respectively: $\tau = \sqrt{m\sigma^2/\varepsilon} = 2.155 \times 10^{-12}$ s, $\varepsilon/k_B = 120$ K and $\sqrt{\varepsilon/m} = 158$ m/s.

The solid walls are modelled with three layers of platinum atoms arranged in a FCC(111) lattice with density $\rho_w = 12.76 m/\sigma^3$. Each solid atom is connected to its nearest neighbors with springs of stiffness $k = 3249.1 \varepsilon/\sigma^2$ which generates the harmonic potential $V_{ww}(r) = kr^2/2$. Two extra layers of “phantom atoms” are added below the three layers in order to keep the wall stationary and to impose the desired temperature T_w .

The potentials and the current positions $\mathbf{r}_1, \dots, \mathbf{r}_N$ of all the N fluid and solid atoms of the system being known, we are able to determine the force \mathbf{F}_i applied to any atom i and its acceleration $\dot{\mathbf{r}}_i$ according to Newton’s second law:

$$m_i \ddot{\mathbf{r}}_i(t) = \mathbf{F}_i(t) \stackrel{\text{def}}{=} -\frac{\partial}{\partial \mathbf{r}_i} V_{tot}(\mathbf{r}_1, \dots, \mathbf{r}_N)$$

where V_{tot} denotes all the possible interactions (i.e. fluid/fluid, solid/fluid or solid/solid):

$$\begin{aligned} V_{tot}(\mathbf{r}_1, \dots, \mathbf{r}_N) &= \frac{1}{2} \sum_{i,j \neq i} V_{ff}(\|\mathbf{r}_i - \mathbf{r}_j\|) \\ &+ \frac{1}{2} \sum_{i,j \neq i} V_{fw}(\|\mathbf{r}_i - \mathbf{r}_j\|) \\ &+ \frac{1}{2} \sum_{i,j \neq i} V_{ww}(\|\mathbf{r}_i - \mathbf{r}_j\|) \end{aligned}$$

A volumetric force \mathbf{F}_{ext} is also applied to the fluid particles to model the pressure contribution $\partial p / \partial x$. The temporal integration of the motion equations is performed with the Velocity-Verlet algorithm [1, 4]. The microscopic time step is $\delta t = 5 \times 10^{-3} \tau$. From a practical point of view, it is not necessary to treat all pair interactions: the Verlet list [1, 4] is adopted and the contributions of pairs in V_{tot} with distances higher than the cut-off radius $r_c = 2.5 \sigma$ are neglected in the force computation.

Periodic boundary conditions are applied in x - and y -directions leading to a zero mass flux in the vertical direction. In order to keep the wall at the desired temperature T_w , a force $\mathbf{F}_{i,w}$ is added to the equation of motion for the solid particles of the upper phantom layer. Using the Langevin thermostat, this force reads $\mathbf{F}_{i,w} = -\alpha_w \dot{\mathbf{r}}_w + \mathbf{R}_{i,w}$ with $\alpha_w = 168.3 \tau^{-1}$ and $\mathbf{R}_{i,w}$ a random force vector. Each independent component of $\mathbf{R}_{i,w}$ is sampled from a Gaussian distribution with a zero mean and a standard deviation dependent on the prescribed temperature: $\sqrt{2\alpha_w m_w k_B T_w / \delta t}$.

In the $C \rightarrow M$ layer, both dynamic and temperature must be controlled in a way that the mean velocity $\langle \dot{\mathbf{r}} \rangle(z)$ and the mean temperature $\langle m[\dot{\mathbf{r}}(z) - \langle \dot{\mathbf{r}} \rangle(z)]^2 \rangle / 3k_B$ coincide with the current linear macroscopic approximation of velocity $\mathbf{u}_{C \rightarrow M}(z)$ and temperature $T_{C \rightarrow M}(z)$ computed by the continuous equations [5, 6, 7]. To this purpose, Newton's equations are first solved with an additional constrain added by the following force for particles in the $C \rightarrow M$ layer:

$$\mathbf{F}_{i,f} = -\langle \mathbf{F}(t) \rangle + \xi \frac{m}{\delta t} (\mathbf{u}_{C \rightarrow M}(z) - \langle \dot{\mathbf{r}}(t) \rangle(z))$$

The computed intermediate acceleration $\ddot{\mathbf{r}}_i^*$ is then corrected via a Langevin thermostat:

$$m \ddot{\mathbf{r}}_i(t) = m \ddot{\mathbf{r}}_i^*(t) - m \alpha (\dot{\mathbf{r}}_i(t) - \langle \dot{\mathbf{r}}(t) \rangle(z)) + \mathbf{R}_{i,f}(T_{C \rightarrow M}(z)).$$

The used parameters are $\alpha = 1 \tau^{-1}$, $\xi = 2 \times 10^{-2}$ (resp. $\xi = 5 \times 10^{-3}$) for liquid (resp. gas). The upper

border of the molecular domain is modelled through a specular wall. In the case of a liquid simulation, an additional force is introduced in order to reduce the fluid stratification near to the wall [8]. When a condensation situation is studied, the density locally changes in the whole domain. The specular wall, combined with the USHER algorithm [3], allows the control of the density in the overlap region so that the densities of the molecular and continuum regions are the same.

Continuum approach: In the continuum region, the steady incompressible Navier-Stokes and energy equations are solved:

$$\begin{cases} \nabla \cdot \mathbf{u} = 0 \\ \rho \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot (\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) \\ \rho c \nabla \cdot (\mathbf{u} \otimes T) = \nabla \cdot (\lambda \nabla T) + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) : \nabla \mathbf{u} \end{cases}$$

where $\mathbf{u} = u \mathbf{e}_x + v \mathbf{e}_y$, p and T are the two dimensional velocity, the pressure and the temperature fields; ρ , μ , λ and c are the fluid density, the dynamic viscosity, the thermal conductivity and the specific heat. The boundary conditions for the continuum domain read:

$$\begin{cases} \text{at } x = 0: \begin{cases} \mathbf{u}(z) = u_{in}(z) \mathbf{e}_x \\ T(z) = T_{in}(z) \end{cases} \\ \text{at } x = L: \begin{cases} \partial_x u(z) = v(z) = 0 \\ \partial_x T(z) = 0 \end{cases} \\ \text{at } z = z_{M \rightarrow C}: \begin{cases} \mathbf{u}(x) = u_{M \rightarrow C}^{\text{macro}}(x) \mathbf{e}_x \\ T(x) = T_{M \rightarrow C}^{\text{macro}}(x) \end{cases} \\ \text{at } z = H: \begin{cases} \partial_z u(x) = v(x) = 0 \\ \partial_z T(x) = 0 \end{cases} \end{cases}$$

where $z_{M \rightarrow C}$ is the position of the lower bound of the continuum domain which coincides with the center of the $M \rightarrow C$ layer of the molecular region. Inlet velocity $u_{in}(z)$ and temperature $T_{in}(z)$ will be detailed for each problem in the corresponding sections. The two terms $u_{M \rightarrow C}^{\text{macro}}(x)$ and $T_{M \rightarrow C}^{\text{macro}}(x)$ from the lower boundary condition are piecewise linear functions. With $u_{M_i \rightarrow C}^{\text{macro}}$ the mean velocity of particles in the $M_i \rightarrow C$ layer of the i -th molecular block M_i , the macroscopic velocity reads:

$$u_{M \rightarrow C}^{\text{macro}}(x) = \sum_{i=1}^{n_b-1} \mathcal{H}(x, x_{M_i \rightarrow C}, x_{M_{i+1} \rightarrow C}) \left(u_{M_i \rightarrow C}^{\text{macro}} + \frac{u_{M_{i+1} \rightarrow C}^{\text{macro}} - u_{M_i \rightarrow C}^{\text{macro}}}{x_{M_{i+1} \rightarrow C} - x_{M_i \rightarrow C}} (x - x_{M_i \rightarrow C}) \right)$$

with $x_{M_i \rightarrow C}$ the center of the $M_i \rightarrow C$ layer of the i -th molecular block M_i , $\mathcal{H}(a, b, c) = H(a - x) \times H(x - b)$ where $H(x)$ is the Heaviside function, and n_b the number of molecular blocks. The same

process is used for the temperature profile $T_{M \rightarrow C}^{\text{macro}}(x)$. The discrete fields are approximated with a collocated Finite-Volume scheme suitable for some unstructured meshes [2]. The global algorithm is second order accurate in space. The resulting discrete non-linear system is solved with a Newton-Raphson algorithm.

RESULTS AND DISCUSSION

The hybrid approach has been validated for two one-dimensional transient cases: the Couette flow and the thermal conduction problem [7]. In the following sections, the validation for a one-phase flow in a long micro channel is briefly detailed; then a two-phase flow, with condensation near the wall is introduced.

One-phase flow: a liquid argon ($\rho = 0.81 \text{ m}/\sigma^3$) flow in a long microchannel is studied. The main parameters of the simulation are: $H_{M,f} = 99.44 \sigma$, $H_{M,f}/H_C = 1/25$, $H = 2545.6 \sigma$, $L = 4000 H$, $T_w = 1.1 \varepsilon/k_B$. The continuum region is discretized in $N_x \times N_z = 48000 \times 30$ rectangular volumes with refined cells near the inlet and close to the wall. The properties of argon, evaluated with tables or correlations at T_w , are $\mu = 2.073 \sqrt{m\varepsilon}/\sigma^2$, $\lambda = 6.832 k_B \sqrt{m\varepsilon}/\sigma^2$ and $c = 2.375 k_B/m$. The inlet velocity profile $u_{\text{in}}(z)$ must cancel at walls. A parabolic boundary layer profile is then chosen in the vicinity of the wall for $0 \leq z \leq 0.2 H$ and $u_{\text{in}}(z) = 1 \sqrt{\varepsilon/m}$ for $0.2 H \leq z \leq H$. The inlet temperature is $T_{\text{in}}(z) = T_w$.

A stochastic wall model is adopted to reduce as much as possible the velocity and temperature jumps, and then to perform comparisons with the solution achieved by the Finite Volume approximation. Every particle crossing the “wall” is reinserted at the same position with a velocity whose the tangential and normal components are sampled from a Gaussian and Rayleigh distributions respectively, with zero mean values and standard deviations corresponding to the wall temperature T_w .

With the multi-scale approach, the computational cost of the hybrid simulation is linked to the molecular dynamics: the computational cost of the steady state for the continuum region is few minutes while several cpu-days are needed for one block of the molecular region. Reducing the total cpu time is then a crucial issue. This is achieved using few hundreds of processors for each molecular block (MPI parallelization) and minimizing the number of blocks. Both the number and the position of the molecular blocks play an important role on the solution

accuracy. In order to parametrize the hybrid simulation, a one-dimensional analytical model is first developed: for the i -th molecular block M_i , the horizontal component of the analytical (subscript a) velocity reads:

$$u_a^i(z) = \frac{1}{2\mu} \frac{\partial p}{\partial x} \Big|_{C \rightarrow M_i} (z - z_{C \rightarrow M_i})z + u_{C \rightarrow M_i} \frac{z}{z_{C \rightarrow M_i}}$$

and the analytical temperature is:

$$T_a^i(z) = T_w + \frac{T_{C \rightarrow M_i} - T_w}{z_{C \rightarrow M_i}} z$$

where $z_{C \rightarrow M_i}$ is the center of the $C \rightarrow M_i$ layer of the block M_i . Note that the pressure gradient term allows a quadratic profile (Poiseuille) and the vertical velocity is set to zero. The main interests of this analytical model are to give a simple approximation of the mean fluid flow at the microscopic scale and to provide an initial condition for the velocity and the temperature fields in order to significantly reduce the number of the coupled iterations of the hybrid scheme (and then its computational cost). Once the analytical profiles are known, the relative difference in L_2 norm is computed between the solution obtained with N_x blocks (one for each face of the lower boundary in $z = 0$) and the solution with $n_b < N_x$ blocks arranged uniformly or with a geometric progression with a scale factor r_b according to:

$$x_i = \begin{cases} x_1 + \frac{(x_{n_b} - x_1)(1 - r_b^{i-1})}{1 - r_b^{n_b-1}} & \text{if } r_b \neq 1 \\ x_1 + \frac{(x_{n_b} - x_1)(i - 1)}{n_b - 1} & \text{if } r_b = 1 \end{cases}$$

The figure 4 shows that an optimal value $r_{b,opt}$ minimizes the relative difference on the velocity field and that it is preferable to overestimate r_b ($r_b > r_{b,opt}$) than underestimate its value.

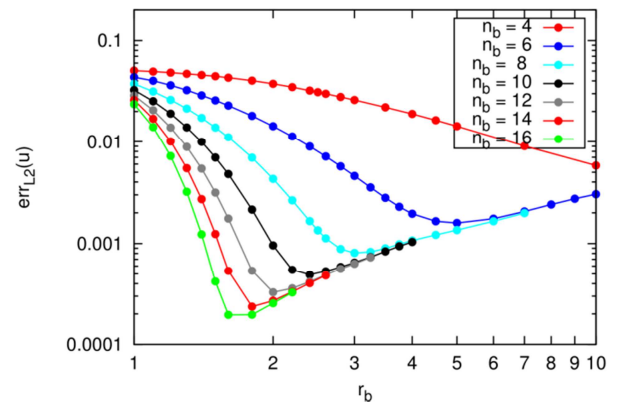


Figure 4

Relative difference on the velocity field for $x/H < 50$ (inlet section) between solutions with a number of blocks n_b arranged with the scale factor r_b and the reference ($n_b = N_x$).

The velocity profiles are shown in figure 5 in the different slices corresponding to the positions of the 8 molecular blocks. The velocity discrepancy, stemming from the simulations performed with the multi-scale approach and the continuum solution computed on the full domain (lines) appears to be very small. The same observation is done for the temperature field.

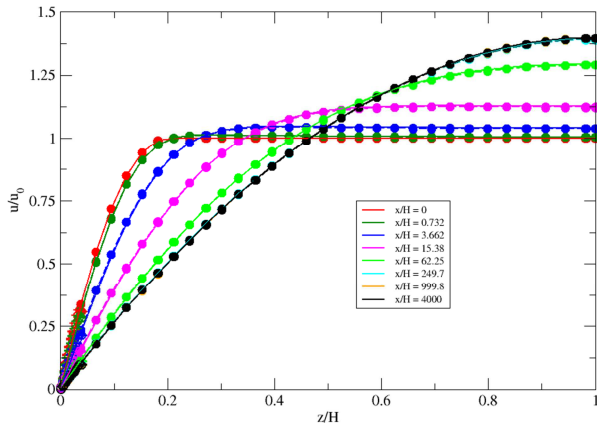


Figure 5

Comparison between hybrid solution for $n_b = 8$ and $r_b = 4$ (symbols and dashed lines) and the continuum solution computed on the full domain (lines).

This section has shown the usefulness and relevance of an analytical simple model to best position the blocks along the channel and has validated the hybrid multi-scale modeling that we developed. The next section aims to extend out hybrid method to a situation where the fluid in the channel is in gas phase and condenses on the walls.

Two-phase flow: The channel height and length are now respectively $H = 424.6 \sigma$ and $L = 500 H$. The walls temperature is $T = 0.925 \varepsilon/k_B$. Gaseous argon ($\rho = 0.05 m/\sigma^3$) enter the channel with the following established profiles: $u_{in}(z)/u_0 = (z/H)(2 - (z/H))$ and $T_{in} = T_{w,0} + \mu u_0^2 (1 - (1 - z/H)^4)/3\lambda$ with $u_0 = 2\sqrt{\varepsilon/m}$ and $T_{w,0} = 1.1 \varepsilon/k_B > T_w$. Argon properties, evaluated at the temperature $1.25 \varepsilon/k_B$ close to $T_{in}(z = H/2)$, are $\mu = 0.14 \sqrt{m\varepsilon}/\sigma^2$, $\lambda = 0.61 k_B \sqrt{m\varepsilon}/\sigma^2$ and $c = 1.76 k_B/m$. The other characteristics of the hybrid simulation are $H_{M,f} = 139.21 \sigma$ and $H_{M,f}/H_c = 1/2.45$.

Keeping in mind we are searching the best positions of the blocks, analytical profiles for the horizontal velocity and the temperature are established. The analytical model relies upon the following assumptions:

- i) The fluid properties are constants for each phase
- ii) Velocity profiles in both gas and liquid phases respectively read: $\mathbf{u}_{a,g} = u_{a,g}(z)\mathbf{e}_x$ and $\mathbf{u}_{a,l} = u_{a,l}(z)\mathbf{e}_x$
- iii) The pressure gradient in the x -direction is the same into the two phases and corresponds to $\nabla p \cdot \mathbf{e}_x(z = z_{C \rightarrow M})$ computed from the continuum region.
- iv) There is no dynamical slip at walls or between the phases
- v) The temperature field is continue between the gas and the liquid and is equal to the condensation temperature T_C at the interface.

Let δ_a the thickness of the condensation film, the Navier-Stokes and energy equations read:

$$\left\{ \begin{array}{l} \text{for } 0 \leq z \leq \delta_a : \left\{ \begin{array}{l} -\frac{dp}{dx}\Big|_{C \rightarrow M} + \mu_l \frac{d^2 u_{a,l}}{dz^2} = 0 \\ \lambda_l \frac{d^2 T_{a,l}}{dz^2} + \frac{\mu_l}{2} u_{a,l} \frac{du_{a,l}}{dz} = 0 \end{array} \right. \\ \text{for } \delta_a \leq z \leq z_{C \rightarrow M} : \left\{ \begin{array}{l} -\frac{dp}{dx}\Big|_{C \rightarrow M} + \mu_g \frac{d^2 u_{a,g}}{dz^2} = 0 \\ \lambda_g \frac{d^2 T_{a,g}}{dz^2} + \frac{\mu_g}{2} u_{a,g} \frac{du_{a,g}}{dz} = 0 \end{array} \right. \end{array} \right.$$

The set of boundary conditions reads:

$$\left\{ \begin{array}{l} \text{at } z = 0 : \left\{ \begin{array}{l} u_{a,l} = 0 \\ T_{a,l} - T_w = C \frac{dT_{a,l}}{dz} \end{array} \right. \\ \text{at } z = \delta_a : \left\{ \begin{array}{l} u_{a,l} = u_{a,g} \\ T_{a,l} = T_{a,g} = T_C \\ \mu_l \frac{du_l}{dz} = \mu_g \frac{du_g}{dz} \\ \lambda_l \frac{dT_l}{dz} = \lambda_g \frac{dT_g}{dz} \end{array} \right. \\ \text{at } z = z_{C \rightarrow M} : \left\{ \begin{array}{l} u_{a,g} = u_{C \rightarrow M} \\ T_{a,g} = T_{C \rightarrow M} \end{array} \right. \end{array} \right.$$

With this set of equations and boundary conditions, the condensation thickness δ_a is written as a function of the liquid and gaseous properties $\mu_l, \mu_g, \lambda_l, \lambda_g$, the velocity, temperature and pressure gradient from the continuum region $u_{C \rightarrow M}, T_{C \rightarrow M}$ and $\nabla p \cdot \mathbf{e}_x|_{C \rightarrow M}$, the condensation temperature T_C and the constant C from the temperature slip condition at the walls. These last two parameters T_C and C are evaluated with the hybrid simulation based on a single molecular block, for 4 values of the

pressure gradient $\nabla p \cdot \mathbf{e}_x|_{C \rightarrow M}$. The figure 6 presents profiles of density, horizontal velocity and temperature for $\nabla p \cdot \mathbf{e}_x|_{C \rightarrow M} = 3.11 \times 10^{-6} \varepsilon/\sigma^4$.

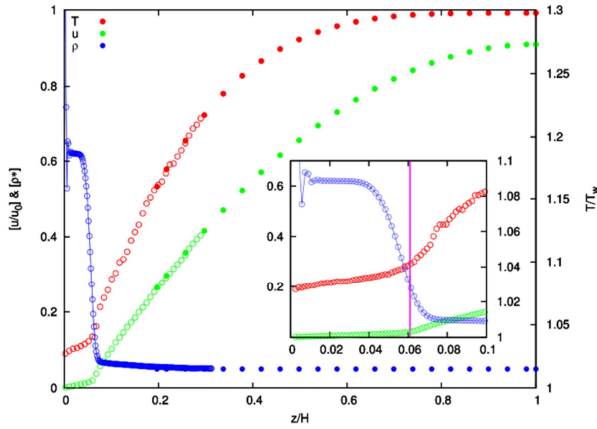


Figure 6

Profiles of density and horizontal velocity (left axe) and temperature (right axe) for and hybrid simulation on a single block with $\nabla p \cdot \mathbf{e}_x|_{C \rightarrow M} = 3.11 \times 10^{-6} \varepsilon/\sigma^4$.

In the molecular region (empty symbols), the variations of the transport coefficients μ and λ involve sudden changes in the velocity and temperature slopes. These discontinuities on the derivatives arise at $z/H \approx 0.06$. Unlike the analytical model, the interface in the hybrid simulation is rather diffuse: the density smooth variation from $\rho \approx 0.61 \text{ m}/\sigma^3$ to $\rho \approx 0.05 \text{ m}/\sigma^3$ is carried on a length of about 3% of z/H . If an arctangent function approximation of the density in the vicinity of the interface is assumed, the position of the interface δ/H , is slightly smaller, about 0.0552.

The condensation thickness and temperature are here $\delta_a = 0.06 H$ and $T(z = 0.06 H) \approx 1.04 T_w$. The constant C , defined by $C = (T(0) - T_w)/\partial_z T|_{z=0}$ is nearly independent of the pressure gradient. This is not the case for T_C , which is correlated with the velocity $u_{C \rightarrow M}$ and therefore with the temperature $T_{C \rightarrow M}$ through the viscous heating. The hybrid simulations performed in a single block provide the following results: $C = 55 \sigma$ and $T_C = 0.204 T_{C \rightarrow M} + 0.733 \varepsilon/k_B$. It is important to notice that the condensation thickness δ_a is very sensitive to the condensation temperature T_C : +0.1% variation on T_C increases δ_a by 6.5%. The analytical profiles being determined, the relative error on velocity and temperature fields can now be computed between a reference, built with the maximal number of blocks ($n_b = N_x$), and the hybrid simulation with $n_b \ll N_x$

and a scale factor r_b . Results are presented on the Figure 7.

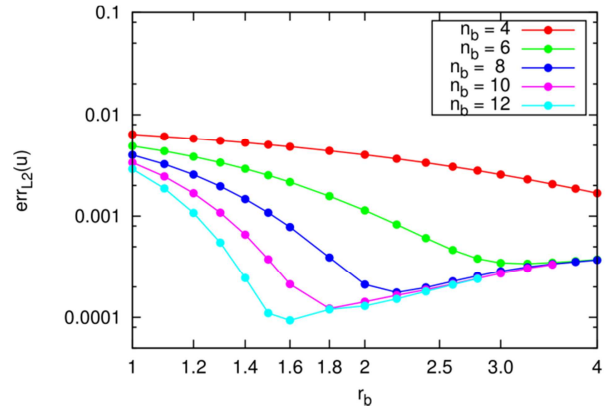


Figure 7

Relative difference between the velocity field in the inlet region ($x/H < 300$) for a number of blocks n_b positioned according to the scale factor r_b and the reference solution with $n_b = N_x$.

Choosing 10 molecular blocks and a scale factor $r_b = 2$, the relative difference on the velocity field (and the temperature as well) is lower than 0.1%. The figure 8 shows the temperature profiles for 7 slices corresponding to the positions of the molecular blocks. The hot gas enters the channel and is cooled at the walls whose temperature T_w is lower than the condensation temperature T_C . That leads to the phase change and the development of a liquid film of thickness δ nearly independent of the abscissae x/H (Fig. 9).

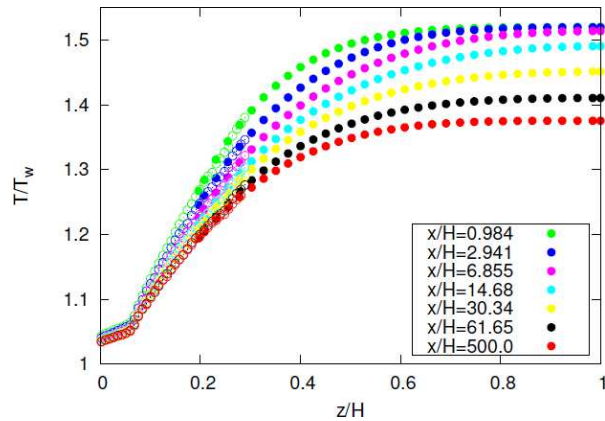


Figure 8

Temperature profiles in slices corresponding to the molecular blocks positions in the channel. Generally, the temperature in the overlap region and the continuum model are in good agreement.

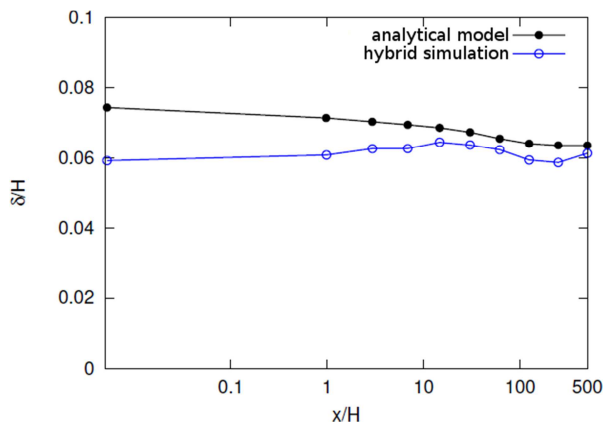


Figure 9

Thickness of the liquid film of condensation at molecular block positions. Comparison between the hybrid simulation and the analytical model with $\mu_l = 0.8\sqrt{m\varepsilon}/\sigma^2$ and $\lambda_l = 3.32 k_B\sqrt{m\varepsilon}/\sigma^2$.

CONCLUSION

The hybrid multi-scale model has been improved in order to account for gas condensation under the questionable assumption of an incompressible flow. The developed analytical model taking into account the condensation process is very sensitive to the condensation temperature and must be parametrized with independent molecular simulations. This preliminary work has to be improved to take into account compressible gas flow in the bulk.

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