Numerical Computation of Two-Phase Flow in Porous Media

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Abstract: In this study we investigate the heat and mass transfer in a porous media with phase change. The liquid fluid is injected from one side and heated from the other side, where it leaves the porous material in a gaseous state. Dominant forces are capillary interactions and two-phase heat conduction.

To model the process we use a two-phase mixture model on a macroscopic scale. This model is presented in two versions. The first version is a one-equation model for energy conservation, while the second is a two-equation model. The versions are implemented in COMSOL and then compared with other results in the literature. A parameter study is done for the second model.

Keywords: Two-phase flow, porous media, heat transfer, boiling

1. Introduction

In many technical applications two-phase flow with phase change is of importance. In burner with small thermal output the fuel is injected in a liquid state. For an optimal combustion the fuel should leave the porous material in a gaseous state. In other cases such as transpiration cooling, we consider a phase change for cooling processes in porous media. We have to simulate the process of the evaporation to predict the critical heat flux at the surface, at which the fluid is only in a gaseous state. This state known as dryout is an important characteristic for technical design aspects.

To simulate these processes, we implement a two-phase mixture model (TPMM), first mentioned by Wang und Beckermann [1], in COMSOL. This model uses the simplification of a local thermal equilibrium (LTE) between the solid matrix and the fluid. Since this one-equation model uses strong assumptions, we also implement an advanced version, which was presented by Shi et al. [2]. This version drops the assumption of the local thermal equilibrium. A qualitative comparison between the two versions is presented.

In the first part of this paper, we present the governing equations. The numerical

implementation and the treated problem are described in the following part. The results of the computations and the comparison with results from the literature are done in the next section. In the last part of the paper we give a future prospect.

2. Theory and Governing Equations

In this study we consider a homogenous and isotropic porous medium. The one-equation two-Phase Mixture Model is based on the assumption of a local thermal equilibrium (LTE), i.e. the temperature of the solid and fluid phases is the same. The expansion of this version is a two-equation model, which is called the local thermal non-equilibrium model (LTNE). The two versions are only different in the number of energy equations.

These models use mixture variables to reduce the number of PDEs. Mixture variables such as mixture density ρ and mixture velocity vector \mathbf{u} , are denoted without index. With the help of a diffusive mass flux we can obtain the flow characteristics of the individual phases.

2.1 Conservation of Mass

With introduction of the mixture quantities (see [1],[2]) the conservation of mass is defined, with the porosity ε , as

$$\varepsilon \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0. \tag{1}$$

2.2 Momentum Conservation

In this model we use Darcy's Law

$$u = -\frac{K}{\mu} \left(\nabla p - \rho_k \boldsymbol{g} \right) \tag{2}$$

for the momentum conservation. The dynamic viscosity μ and the pressure p are also mixture quantities.

2.3 Diffusive Mass Flux

The diffusive mass flux j connects the mixture mean velocity with the velocity of the individual phases.

$$\rho_l \mathbf{u}_l = \lambda_l \rho \mathbf{u} + \mathbf{j} \tag{3}$$

$$\rho_{\nu} \boldsymbol{u}_{\nu} = \lambda_{\nu} \rho \boldsymbol{u} - \boldsymbol{j} \tag{4}$$

 $\rho_{\nu} u_{\nu} = \lambda_{\nu} \rho u - j$ Wang and Beckermann introduced the diffusive flux as

$$\mathbf{j} = D(s)\nabla s + f(s)\frac{K\Delta\rho}{\nu_{\nu}}\mathbf{g}.$$
 (5)

In this definition f is the hindrance function for phase migration and separation and D(s) is the capillary diffusion coefficient as a function of liquid saturation.

2.4 Energy Conservation

As we mentioned above, the energy equations are different for the two versions. For the numerical handling, Wang presented a pseudo-mixture enthalpy H. For further details the reader is referred to ref. [3].

First, we present the local thermal equilibrium version. The energy conservation is defined as

$$\nabla \cdot (\gamma_h \mathbf{u} H) = \nabla \cdot (\Gamma_h \nabla H) +$$

$$\nabla \cdot \left(f \frac{K \Delta \rho h_{fg}}{\nu_v} \mathbf{g} \right),$$
(6)

where h_{fg} is the enthalpy of evaporation, Γ_h is the effective diffusion coefficient and γ_h is a corrector coefficient. For detailed information we refer to ref. [3].

Second, the local thermal non-equilibrium version consists of two energy equations. The first equation is similar to equation (6). It is the energy equation of the fluid:

$$\nabla \cdot (\gamma_h \mathbf{u} H) = \nabla \cdot (\Gamma_h \nabla H) +$$

$$\nabla \cdot \left(f \frac{K \Delta \rho h_{fg}}{\nu_v} \mathbf{g} \right) + \dot{q}_{sf},$$
(7)

The equation for the solid matrix is the classic conduction of heat equation

$$\nabla \cdot \left(k_{s_{\text{eff}}} \nabla T_s \right) = \dot{q}_{sf}, \tag{8}$$

where $k_{s_{\text{eff}}}$ is the effective heat conductance. The source term \dot{q}_{sf} describes the heat transfer between fluid and solid matrix and varies for each domain (liquid, two-phase-domain and gas).

3. Implementation in COMSOL

The purpose of this work is to present a useful tool in COMSOL to simulate arbitrary two-phase flows with heat transfer. The introduced model can be implemented in different ways. We used the Darcy's Law Module and the coefficient form of the PDE Interfaces to implement the rest of the equations.

To validate the implemented model we compare the results with ref. [2] and the analytical temperature at the outlet. This validation is done for the one-dimensional findings.

3.1 Boundary Conditions

The principal set-up is shown in figure 1. A continuous mass flux flows against the gravitation from the bottom to the top of the domain. The velocity at the inlet is defined by:

$$u_{in} = \frac{\dot{m}_{in}}{\rho_l}. (9)$$

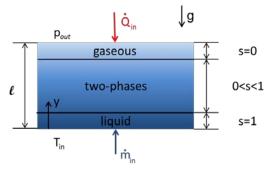


Figure 1. Sketch of the one-dimensional problem

The pseudo-mixture enthalpy at the inlet is defined by the inlet-temperature

$$H(y=0) = \rho_l (c_l T_{in} - 2h_{v_{\rm sat}}).$$
 (10) For the local thermal non-equilibrium version the solid temperature at the inlet corresponds to T_{in} .

During the crossing the fluid is heated from the top by a heat source \dot{Q}_{in} and starts to boil. The Neumann boundary condition for the enthalpy at exit is given by

$$\Gamma_h \frac{\mathrm{d}H}{\mathrm{d}y}(y=l) = \dot{Q}_{in} - f \frac{K\Delta\rho h_{fg}}{\nu_v} g. \tag{11}$$

In case of the local thermal non-equilibrium version the heat is delivered in the solid material, i.e. $\dot{Q}_{in} = 0$ in equation (11). The boundary condition for the solid energy equation is then defined as

$$k_{s_{\text{eff}}} \frac{dT_s}{dy} (y = l) = \dot{Q}_{in}. \tag{12}$$

If the heat source is large enough, dryout will be reached. The pressure has the constant value p_{out} at the outlet.

3.2 Challenges of the Implementation

The main challenge of simulating problems with phase change is the jump in the fluid characteristics at the phase transition. Because of the changing characteristics the model is numerical unstable. The effective diffusion coefficient Γ_h , shown in figure 8, degenerates at the phase boundaries, denoted by s=0 (condensation front) and s=1 (evaporation front).

To avoid this problem we smoothed the function with the smoothing function of COMSOL. By using a small relative smoothing length, the effect on the result was very slightly (see figure 9).

4. Simulation and results

This section is separated in three parts. First, we present the results of the local thermal equilibrium and the local thermal non-equilibrium model and compare the outcomes with each other. Second, we compare the solutions of the local thermal equilibrium model with the results of Shi et al. [2]. Finally, we check the influence of different parameters on the result for the second model.

The coolant respectively fuel in our cases is water. The solid material is steel.

4.1 LTE and LTNE

The results of the simulations are presented in figure 2, where the temperatures are displayed. The simulation was done for a heating source of $\dot{Q}_{in}=1.5e6\frac{W}{m^2}$ and a mass flux of $\dot{m}_{in}=0.5\frac{kg}{m^2s}$.

The temperature at the outlet is for each version roughly the same. This is to be expected, because both versions are based on the same theoretical background. We can compute an analytic temperature with the following equation:

$$T_{\text{analytic}}$$

$$= \begin{cases} T_{\text{in}} + \frac{\dot{Q}_{in}}{\dot{m}_{in}c_{l}} & \text{if } \dot{Q}_{in} \leq \dot{Q}_{\text{Boil}} \\ T_{\text{sat}} & \text{if } \dot{Q}_{\text{Boil}} < \dot{Q}_{in} \leq \dot{Q}_{\text{Dryout}} \\ T_{\text{sat}} + \frac{\dot{Q}_{in} - \dot{Q}_{\text{Dryout}}}{\dot{m}_{in}c_{v}} & \text{if } \dot{Q}_{\text{Dry}} \leq \dot{Q}_{\text{in}} \end{cases}$$

The heat constants are defined by

$$\dot{Q}_{\text{Boil}} = \dot{m}_{in}c_l(T_{\text{sat}} - T_{\text{in}})$$
 and

$$\dot{Q}_{\text{Dryout}} = \dot{Q}_{\text{Boil}} + h_{fg}.$$
 (14)

However, the distributions are different. The two-phase domain of the local thermal equilibrium is just one third of that from the local thermal non equilibrium version. The reason for this observation is because of the assumption of a thermal equilibrium. This leads to the constant temperature $T_{\rm sat}$ of the solid and fluid within the two-phase domain, i.e. the heat transfer in the solid matrix is zero. We have an artificial thermal insulation.

The local thermal non-equilibrium avoids this problem, by using a second energy equation for the solid material. Thus, temperature gradient for the solid is unequal zero and heat can be conducted in the two-phase region.

4.2 Comparison with Shi

Shi et al. [2] use also water as the coolant and steel as the solid matrix. In figure 3 the results of Shi and the results achieved of COMSOL are displayed. These results are computed for different mass fluxes and a heat flux of $\dot{Q}_{in} = 1e6 \frac{W}{m^2}$.

Our input temperature differs from the input temperature of Shi et al. This difference has no big influence on the results, which we checked for a test case (see figure 10). The results are comparable.

The temperature at the outlet is almost the same. And also the qualitative shift of regimes is for both results the same. If we increase the mass influx the temperature at the outlet will decrease and the location of the two-phase domain will be pushed upstream.

The main difference in the outcomes is the length of the two-phase domain. The results, computed by Shi, own a longer two-phase region. COMSOL uses the finite element

method, while Shi et al. computes the results with a finite volume method.

The results of the COMSOL solver are confirmed by another self-written solver. A finite volume method, implemented in Matlab, delivered the same results in terms of temperature distribution. The discrepancy is not caused by the different solvers.

As we mentioned above the different inlet temperature is not the source for the discrepancy.

To estimate the quality of the solvers, we compare the temperature at the outlet with the analytical temperature $T_{\rm analytic}$

$$r = \frac{T_{\rm analytic}}{T_{\rm out}}. \tag{15}$$
 The Matlab and COMSOL solver provide the

better performance (see table 1).

	Shi [2]	Matlab	COMSOL
BC 1	0,94	0,99	0,99
BC 2	0,98	1	1

Table 1. Coefficient r (eq. (15))

4.3 Parameter Variation

In this section we present two interesting outcomes. First, we show the influence of the coolant on the result and second, the dependence of the relative permeability on the saturation.

In figure 4 the results for water respectively ethanol are displayed. Because of the smaller enthalpy of evaporation for ethanol the twophase domain is shorter and the temperature at the exit is much higher.

There is a strong connection between the relative permeability k_{rl} and the length of the two-phase domain, which we can see in figure 5. Power-law is used for $k_{rl}(s)$. The higher the power of the saturation is, the smaller is the twophase domain. A small power pushes the twophase domain upstream.

5. Discussion and future prospect

In the previous section we presented the results and saw, that the different models give qualitative the same outcomes. The local thermal equilibrium version delivers roughly the same temperature at the outlet as the local thermal non-equilibrium version. Because of the lower computational cost, this version is good for qualitative analyses. For more realistic

temperature distributions, the local thermal nonequilibrium is the better choice.

In this work we revealed the possibility to implement the two-phase mixture model in COMSOL.

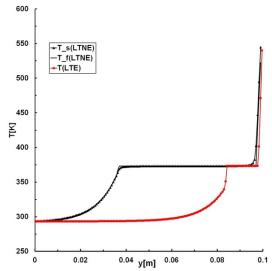


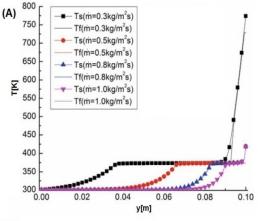
Figure 2. Results of the local thermal equilibrium (LTE) and the local thermal non-equilibrium (LTNE)

5.1 Future Research Points

The future work at this topic will concentrate on three points. First, a two-dimensional model will be implemented. In figures 6 and 7 the result of a computation for two dimensions is presented. For this computation, we used large relative smoothing length and gravitational aspects were neglected.

The second research point has the aim to drop the assumption of a constant fluid temperature in the two-phase domain. A good approach provides the model of Wei et al. [4]. This model is based on the Gibbs free energy. This energy has to be equal for the liquid and gaseous state within the two-phase domain.

Last but not least, we need to verify the model with experimental results.



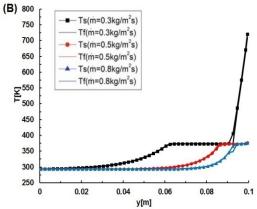


Figure 3. Comparison between Shi et al. [2] (A) and the COMSOL solver (B)

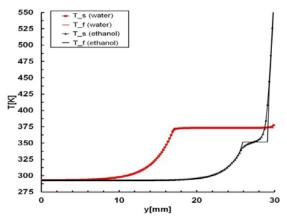


Figure 4. Comparison between water and ethanol as coolant

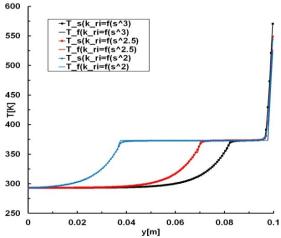


Figure 5. Results for different relative permeabilities

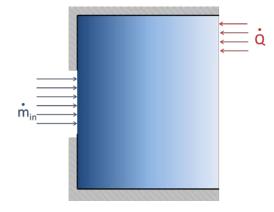


Figure 6. Two-dimensional setting of the problem

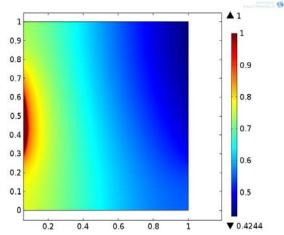


Figure 7. Saturation distribution

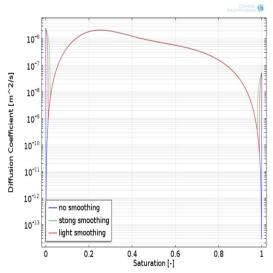


Figure 8. Diffusion Coefficient with different smoothing degrees

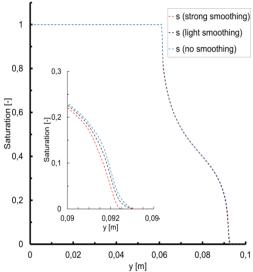


Figure 9. Saturation distribution for different smoothing degrees

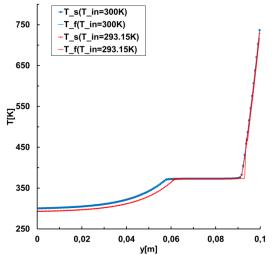


Figure 10. Different inlet temperatures

6. References

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