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Modeling two-phase flow in a micro-model with local thermal non-equilibrium on the Darcy scale

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ABSTRACT

Loosening local equilibrium assumptions in two-phase flow in porous media gives rise to new, unknown variables. More specifically, when loosening the local thermal equilibrium assumption, one has to describe the heat transfer between multiple phases, present at the same mathematical point.

In this paper, we calibrate a macro-scale mathematical model which is free of local equilibrium assumptions to experimental observations. We emphasize the correct determination and upscaling of necessary input parameters from the experimental data achieved by image analysis. By choosing an appropriate scaling parameter, we are able to reproduce experimental measurements satisfactorily. This is a first step towards quantifying heat transfer in two-phase flow in porous media. Ultimately, our aim is to find the limits of the applicability of local equilibrium assumptions in two-phase flow in porous media.

1. Introduction

One of the most prominent assumptions in the field of two-phase flow in porous media is the assumption of local equilibrium. Basically, this means that energy and mass transfer between phases take place instantaneously [e.g. [9]]. In this work, we provide tools and conceptual as well as numerical models which allow us to describe and study two-phase flow in porous media without making local thermal equilibrium assumptions: We build on the concepts explained in Nuske et al. [17] and apply the macro-scale model developed in that work. In this work, we focus on the transfer of micro-scale measurements to macro-scale properties and application of those quantities in macro-scale models. The tools provided in that regard are explained in detail and made available as free software. Here, we make a proof of concept in order to show that principal characteristics of the micro-scale experiment can be captured by the macro-scale local thermal non-equilibrium model applying the measured input parameters. This is an important step in studying the applicability of the local thermal equilibrium assumption in two-phase flow in porous media.

Pure scientific curiosity is, of course, known to boost general progress, but there are also a number of practical applications which put the question of the applicability of local equilibrium assumptions on the agenda.

One effective technique for the cleanup of contaminated sites is the injection of hot steam into the subsurface [e.g. [18,7]]. This process involves temperature differences and flow velocities which are high compared with other flow processes in porous media. The correct prediction of contaminant behavior in this highly non-isothermal setting is crucial for solving environmental problems instead of creating new ones.

During in-situ combustion [19], heavy oil is partly oxidized in the reservoir in order to decrease its viscosity for mobilization, and ultimately production. If the temperatures of the individual phases are not correctly described, undesired reactions may take place. Or even worse: too much oil could be burnt instead of being produced.

After a severe nuclear accident, the core might collapse and can be treated as a porous medium [6,3]. It is of paramount importance to have a good understanding of the subsequent events in order to be able to orchestrate a fast cooling without causing any further (H_2) explosions.

At the interface between the subsurface and the atmosphere, two very different compartments share a boundary: the land surface. Here, evaporation takes place if the subsurface provides liquid water and the atmosphere can take up water vapor. However, flow velocities in the atmosphere can be very high and the exact

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interaction processes are not yet fully understood. Nonetheless, current models [20,15] assume local equilibrium.

What all these examples have in common is that they do not only involve temperature differences but also phase-change processes. In addition to that, there are to some extent sources present in the porous medium, which might prevent the system from reaching equilibrium.

The description of temperature effects by means of an energy balance equation is a standard approach in the modeling of miscible two-phase flow. However, to the best of our knowledge, there are only few approaches which allow to describe local thermal non-equilibrium in two-phase flow in porous media on the macro-scale and resolve phase-specific temperatures. Fichot et al. [6] describe local thermal non-equilibrium for the case of nuclear debris cooling, i.e. with a strong heat source present in the porous medium. However, they have to solve micro-scale closure problems in order to close the system.

Crone et al. [5] describe local thermal non-equilibrium, but only between the fluid phases and the solid phase. In other words: the fluid phases are still assumed to have locally the same temperature.

The macro-scale balance equations used in this work build on Ahrenholz et al. [2], extended in Nuske et al. [17]. In that work, local chemical and thermal non-equilibrium are allowed between the fluid phases and the solid and fluid phases respectively. To keep this work concise, we outline the main characteristics of that model briefly.

The main consequence of allowing different potentials in different phases is an increased number of primary variables. In the case of mass balance, not assuming local equilibrium leads to mole fractions in different phases not being connected via equilibrium relations. Therefore, individual balance equations are needed for each component in each phase. In the case of a two-phase two-component system, the number of mass balance equations is increased from two to four and mass transfer (i.e. the equilibration process) between the phases needs to be described. In this work, we focus on modeling experimental observations and refer to Appendix A and the literature for a discussion of the mathematical model.

In terms of energy balance, not assuming local thermal equilibrium leads to different temperatures present in the same control volume. Thus, individual energy balance equations for the respective (liquid as well as solid) phases need to be formulated. In the case of two-phase flow, the number of energy balance equations is increased from one to three and energy transfer (i.e. the equilibration process) between all phases needs to be captured. The exact structure of these balance equations is not the focus of this work. As mentioned above, the detailed discussion of the mathematical model is beyond the scope of this work. For the sake of brevity, we therefore refer to Appendix A and the literature.

In this work, we want to study the influence of heat transfer on reproducing experimental observations. The energy transfer processes between the phases are approximated by standard engineering approaches. However, no transfer relations for the case of two-phase flow in porous media could be found in the literature. Therefore, a scaling parameter, f_e, was introduced. It basically scales the heat and mass transfer relations between the respective phases, with $f_e = 0$ standing for an immiscible system and $f_e \to \infty$ representing the standard equilibrium case. A parameter study was conducted and it was found that variations in f_e lead to the expected and physically reasonable results. In this work, the macro-scale balance equations explained in Nuske et al. [17] are employed in order to simulate the experiment described in Karadimitriou et al. [11].

Karadimitriou et al. [11] presented an experimental setup for the measurement of phase specific temperatures, as well as phase distribution, during invasion and equilibration processes in a transparent micro-model, made of Polydimethylsiloxane (PDMS). The described setup is a continued development of a mature measurement setup engineered at Utrecht University, Netherlands. In that setup, a residing wetting phase (Fluorinert) was displaced by a hot, invading, non-wetting phase (water). Both phases were liquid. This invasion took place in a quasi two-dimensional micro-model, which allowed optical as well as infrared observation. The complete experimental procedure as well as relevant information about the production process were explained in detail. Subsequently, measurement and image processing techniques were demonstrated. Finally, qualitative results and findings showcasing the usability and versatility of the platform were presented.

In this paper, we build on the modeling and experimental foundation outlined above and take one further step towards the quantitative understanding and parameter estimation in the area of local thermal non-equilibrium in two-phase flow in porous media. To be more precise, we obtain an estimate of the proposed heat transfer scaling factor f_e by means of parameter calibration. In order to accomplish this, we simulate two experimental runs of the experiment explained in Karadimitriou et al. [11] with the macro-scale local thermal non-equilibrium model explained in Nuske et al. [17] and given for completeness in Appendices A and B. By comparing simulation and experiment, we obtain a first-order approximation of the up-to-now unknown scaling parameter f_e which was suggested in Nuske et al. [17]. However, it has to be clearly stated that the goal of this work is not the exact reproduction of all presented aspects of the experimental observations. We want to give a proof of concept, demonstrating that certain features of the phase-specific temperature measurements can be reproduced by a macro-scale model employing phase-specific energy balance equations.

Solving the system on the macro scale demands the determination of a number of non-standard relations. Most prominently, this is the interfacial area between the respective phases. Therefore, the micro-scale identification and measurement of volume specific interfacial area as well as its transfer to macro-scale relations is a special focus of this work. The employed image analysis pipeline is explained in detail and provided, along with the simulation source code, under a free license.

The structure of this work is the following: In Section 2, input parameters needed for the macro-scale model are presented. Fluid and material parameters are straight forward to obtain. However, matrix properties and two-phase properties require some more effort (Section 2.2). The determination of interfacial areas, which are inevitable input parameters to the macro-scale model, require the development of a new image analysis algorithm, explained in Section 3. Building on that information, macro-scale constitutive relations are fit to the obtained data in Section 4. Modeling choices and simulation setup are explained in Section 5. Employing these input parameters, the simulations of different experimental runs are presented in Section 6. We conclude in Section 7 and deduce future research goals.

2. Input parameters

A model can only be as good as its input. Therefore, the simulation of complex systems, like two-phase flow in porous media, requires the detailed understanding of the parameters which are input to the model.

This is even more so for a non-standard model, such as the local thermal non-equilibrium model employed here. In this case, in addition to the fluid (Section 2.1) and matrix (Section 2.2) properties (and their interaction), the interfacial area available to heat