Evaluation of the PhD-Thesis of
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Modeling Multiphase Flow in Porous Media With an Application to Permafrost Soil

This thesis is the first dissertation within the contract of the Charles University, Prague, and the University of Heidelberg. It started from a problem originating from questions in environmental physics: What are the proper mathematical models for the dynamical processes in permafrost soil, evolving in time and space under the influence of the daily and the seasonal rhythms?

These processes lead to a many component system and to phase transitions in a porous media causing many problems to mathematical modelling, analysis and numerical simulation. Heida persues in his thesis the aim to tread a large class of multi-scale, multi-component and multiphase systems, considering the permafrost system as a test case.

Already systems consisting of two components, e.g. water and air, without phase transitions in porous media are demanding mathematical modelling reducing the complexity, but still representing the real situation well enough. Modelling the processes in full detail, if at all possible, does not make sense since the arising complex systems cannot be handled neither analytically nor numerically and also the data situation can not justify a fine granular modelling.

Heida´s investigations are based on the assumption that the components and the phases can be described by fields in space and time. That means, he is starting his modelling already on a higher scale level. In order to derive model equations, consistent with thermodynamics, from first principles, it is necessary to associate to the processes a proper energy density and an entropy. Heida persues an ansatz based on assumptions on a conjecture of Rajagopal and Srinivasa on the entropy production rate. This rate is a function of the thermodynamical fluxes and the thermodynamical affinities. It is assumed that this nonnegative rate function is maximal with respect to the thermodynamical fluxes. Starting from just two constitutive laws for an energy density and an entropy production rate, the desired constitutive equations for the underlying processes are derived with help of an associated Lagrange functional .

Using this concept Heida succeeded in deriving model systems for several fluids and phases in porous media. Since the media consist of a solid matrix and a pore part, the approach had to include the processes on the interfaces. Proper boundary or transmission conditions have to be derived for the solutions to the various equations modelling the dynamics of the components and the phases. An essential contributions of this thesis is the extension of the method to the interfaces of the underlying domains. Whereas in the interior of the domains the method has been used in other, but less complex situations, including the pore boundaries was necessary to handle porous media.

The next step is to perform the scaling limit with respect to proper scales in the considered system. Haida is introducing in addition to the usual approach by traditional non-dimensionalization and homogenization (e.g. with respect to underlying periodic structures) a new concept of scaling, based on the assumption of a maximal entropy production rate. He is introducing a thermodynamical consistent scaling with respect to energy and entropy production rate. As soon as the scaling is fixed, an asymptotic expansion with respect to the scale parameter ε can be performed, which is leading to a reduced approximating system. This can be used to compute appoximations to the solutions for small ε. It is important that consistency with thermodynamics is observed in this approach. Heida keeps in his approximations some ε dependent terms in order to controle the remainder terms at least in a formal expansion. This proceedure seems to be necessary as examples in the well known asymptotic laws for fluids, derived with error estimates, are suggesting.

In this thesis so far only formal expansions are presented, that means the problem of deriving error estimates is not included. A decision had to be made between the followig alternative:

- treading a general system and being content with formal expansions at this stage of investigation or
- reducing the model systems essentially and to give an error estimate.

Heida followed our advice to choose the first of the alternatives and is presenting more general results, which are very useful for future research. As he has shown in other investigations, published already, he is able to master approximations with error estimates. In the rather general situation considered here, error estimates would have gone beyond the scope of this thesis.

The approach presented here is allowing to derive model equations for complex processes from first physical principles in a rational way and thus providing a very useful tool for modelling multi-component and multi-phase flows in complex media. Examples for model systems are derived, e.g. the Cahn-Hilliard-Navier-Stokes system and the Stephan problem with an Allen- Cahn phase field .

Heida finally is treading as test case also the permafrost problem he had started from in his investigations, including phase transitions like condensation, evaporation, freezing and melting. Also the phenomena of hysteresis effects discussed as developed before in the theory.

It is especially important that in the approach that information about the micro-scale can be preserved at least partially and integrated into a macroscopic description, similar to the usual approach in proper homogenization. Using phase field models has the side effect that interfaces arising e.g. in dealing with immiscible fluids are diffusive, which may lead to some difficulties in interpretation of the results. Here, one should mention a different approach used recently in multi-scale numerical methods where the dynamics of strict interfaces between fluids is coupled in critical regions, e.g. close to a solid wall, with a molecular dynamics description. The well-known difficulties with "boundary angles" of an interface intersecting a solid wall are arising here, too. However, I think that the approach presented here cannot couple the scales of molecular processes and the scale assumed in using fields.

Martin Heida is presenting in this thesis a rather general and a very substantial approach to mathematical modelling of flows, transport, reactions and phase transitions in porous media. The results obtained were essentially influenced by the cooperation between Prague and Heidelberg. Heida was very successful in combining expertise in multi-scale modelling and applications in porous media in Heidelberg with the expertise in thermodynamic modelling of a system of fluids available in Prague and to obtain new insights. Here especially the cooperation with Josef Malek, his advisor in Prague has to be mentioned.

The thesis of Martin Heida is exceptional in several aspects. Heida has the aim to develop a general theoretical framework and is a substantial contribution to modelling using profound analytical techniques. Even proper formal expansions are an art by itself and very useful, especially if the situation is so complex as it is the case here. He is presenting a colourful bunch of specific results, each of which can be used for starting new investigations. Despite the fact that basic existing concepts for multi-scale and multi-component systems are used, the thesis is providing several new, original ideas deserving more detailed follow-up analysis.

Martin Heida deserves high appreciation for this PhD thesis.

I am evaluating the thesis with grade

1,00

following the examination rules of the University of Heidelberg.
The final degree for the whole PhD examination has to be decided by the examination committee taking into account all ratings.

Heidelberg, June 13, 2011

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Willi Jäger