DIFFUSE INTERFACE MODELS IN THEORY OF INTERACTING CONTINUA

BY MARTIN ŘEHOŘ

My cooperation with Martin Řehoř started during his undergraduate studies when I supervised his master thesis entitled *Behaviour of new types of material models in a squeeze flow geometry*. The topic of his research was numerical simulation of squeeze flow of a piezoviscous fluid, and the problem was solved numerically using a spectral collocation method. Martin wrote a nice master thesis, and the results obtained in the thesis were later published in Řehoř and Průša (2016). At that time Martin has already clearly shown his programming skills and the ability to work independently.

When looking for a topic of his PhD thesis, we were thinking about the project entitled *Mathematical modelling within the framework of implicit constitutive theory with application in food science*, which was supposed to be co-advised by professor Willi Jäger (Ruprecht-Karls-Universität Heidelberg). Unfortunately, this project did not materialise. In the mean time the mathematical modelling group at Charles University was contacted by the company Glass Service, which is a company providing expert counselling the the field of glass manufacturing. This started our affair with the float glass forming process (Pilkington process).

By courtesy of Glass Service we were allowed to attack the problem via two approaches. The first one was rather straightforward one. It was based on a quasi two-dimensional model based on a thin film approximation, and it is currently tested in a semi-commercial regime. The other approach—the more speculative one—was based on a full three-dimensional Cahn–Hilliard–Navier–Stokes type model, and it partially became the topic of Martin's thesis entitled *Diffuse interface models in theory of interacting continua*. The thesis has been again written in the framework of a *co-tutelle* study programme, this time co-supervised by professor Peter Bastian (Ruprecht-Karls-Universität Heidelberg). This allowed Martin to spend some time at Heidelberg University, and work there at the Interdisciplinary Center for Scientific Computing.

Martin's thesis is focused both on the modelling as well as the computing. In the modelling part Martin carefully discusses the thermodynamical background of the Cahn–Hilliard type models, see Cahn and Hilliard (1958). Partly motivated by Souček et al. (2014), Martin focuses on role of the diffusive flux (relative motion of the constituents). In the fundamental texts on Cahn–Hilliard type models it is usually assumed that "the relative momenta and the kinetic energies of the constituents are negligible when computed relative to the gross motion of the fluid", see Gurtin et al. (1996), or Abels et al. (2012) who "assume that the inertia and kinetic energy due to the motion of the fluid relative to the gross motion is negligible". In this respect, Martin's survey provides, to my best knowledge, the first comprehensive analysis of the role of the "relative momenta and the kinetic energies" in the diffuse interface models.

After the analysis of the kinematic assumptions behind the Cahn–Hilliard type models, Martin continues with the thermodynamical analysis and derives several models for diffuse interface. In particular, Martin focuses on *multi-component models with non-matching densities under non-isothermal conditions*. In the latter aspect, his contribution is again essential, since the works focused on the non-isothermal setting started to appear only very recently, see for example Freistühler and Kotschote (2017).

The second part of the thesis is devoted to the development of numerical schemes for the solution of the corresponding governing equations. The problem that motivated the work—Pilkington process—requires one to consider a three-component mixture with non-matching densities and high viscosity and density contrast, which makes the problem quite intricate to solve numerically. (The mixture is composed of the nitrogen, molten tin and molten glass.) In order to solve the problem Martin—*on its own initiative and without my guidance*—applied several state-of-the-art approaches. In particular, he implemented an advanced preconditioning technique to the Navier–Stokes part of the system of governing equations. (Since the specific role of the varying density and viscosity, this required original changes in the available state-of-the-art approaches designed for the incompressible Navier–Stokes equations.) The developed code is now available as a library for open-source computing platform FEniCS. Some results are summarised in the already published work Řehoř et al. (2017).

Besides the aforementioned papers, Martin has also published two papers focused on the mechanics of viscoelastic rate-type fluids, see Průša et al. (2017) and Řehoř et al. (2016).

In my opinion, Martin Řehoř has clearly proved the ability to work independently and creatively, to work on long term projects, and to develop code for the numerical solution of complex systems of partial differential equations. The thesis documents that he is able to handle equally well *theoretical* (mathematical modelling, numerical mathematics) as well as *implementation* challenges, and that he is able to present his results in a concise and well-organised form. For me it was a pleasure to work with him, and I strongly recommend Martin Řehoř to be awarded by PhD degree.

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Vít Průša

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