ČESKÉ VYSOKÉ UČENÍ TECHNICKÉ V PRAZE
FAKULTA JADERNÁ A FYZIKÁLNĚ INŽENÝRSKÁ
KATEDRA MATEMATIKY

doc. Ing. Radek Fučík, Ph.D.
Trojanova 13, 12000, Praha 2

Supervisor's report of dissertation thesis

Candidate: Ing. Jakub Solovský

Thesis: Mathematical modeling of two-phase compositional flow in porous media

The submitted dissertation thesis is a result of a long-term scientific collaboration between the Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering (FNSPE), Czech Technical University in Prague (CTU) and the Center for Experimental Study of Subsurface Environmental Processes (CESEP), Colorado School of Mines (CSM), Golden, Colorado, USA in the area of multi-phase compositional flow in porous media. The thesis deals with the mathematical modeling of two-phase compositional flow in porous media with interphase mass transfer and its main focus is the investigation of gas exsolution and dissolution processes in the unsaturated zone of porous media.

The thesis is divided into nine chapters and besides the introduction and conclusion, these chapters form the following three topical parts:

I. theoretical background and mathematical model (Chapter 2),

II. numerical model, its parallelization, verification, and benchmarking (Chapters 3 to 6),

III. application to problems with experimental data provided by CESEP (Chapters 7 and 8).

In Part I, the candidate introduces the macroscopic continuum models of two-phase compositional flow in porous media with models of mass transfer between phases. He also pinpoints assumptions and simplifications of these models that allow to establish a system of governing partial differential equations endowed by appropriate initial and boundary conditions.

In Part II, the numerical method based on the mixed hybrid finite element method (MHFEM) suitable for solving the mathematical model is described in detail. The MHFEM numerical scheme has been developed by a broader group of authors (incl. the candidate) under my supervision and published in [2]. The candidate was responsible for the implementation of preconditioned iterative solvers and benchmarking of the numerical method. He also in detail studied problems in heterogeneous porous media and the correctness of the numerical solution on material interfaces in [4]. The main contribution of the candidate in Part II is the parallelization of the MHFEM scheme using the balancing domain decomposition by constraints (BDDC) approach and its implementation using his own code in C++ with MPI. Then, the numerical scheme is verified against semi-analytical solutions of two-phase flow in porous media. Both serial and parallel implementations are thoroughly benchmarked and for the parallel version, the strong and weak scalability is investigated. The convergence of the scheme is demonstrated and a good parallel efficiency is preserved up to a thousand of CPU cores. This work resulted in paper [6], of which the candidate is the leading author.

In Part III, the aforementioned numerical scheme is used to simulate several laboratory-scale problems of compositional flow with mass transfer in porous media in collaboration with

CESEP. All these experimental investigations were motivated by the fate of CO_2 in the subsurface in the context of deep CO_2 storage (sequestration) and potential leakage. In Chapter 7, the significance of the kinetic mass transfer model for predictions of multi-phase CO_2 evolution is investigated in partially saturated porous media under different conditions. In Chapter 8, a single-phase problem of tracer transport is studied in a highly heterogeneous porous medium mimicking the brine leakage from a deep aquifer. Experimental datasets have been provided by CESEP and in the case of the problem described in Chapter 8, the candidate was directly involved in the experimental work at CESEP during his stay there (September–December 2019). The work on multi-phase CO_2 evolution resulted in two papers: [5] of which the candidate is the leading author and [3] where the candidate was responsible for the mathematical modeling part. The brine leakage problem resulted in paper [1] where the candidate participated in collecting and analyzing the samples and helped to develop and verify the mathematical model.

The work on the thesis was conducted as part of the Czech-U.S. scientific collaboration within the framework of the Inter-Excellence project No. LTAUSA19021 of the Ministry of Education, Youth and Sports of the Czech Republic between CTU in Prague and CESEP, CSM Golden. During his study, the candidate visited CESEP five times: 3 short-term stays (1 week) and 2 long-term internships (16. 9. - 20. 12. 2019 and 4. 4. 2022 - 2. 9. 2022). During the long-term internships, the candidate was partially employed by CESEP, CSM. The candidate also participated in the HPC-Europa3 program: internships at CINECA, Italy (2. 9. - 30. 9. 2018) and CSC, Finland (28. 5. - 29. 6. 2019). Additionally, the candidate participated in a number of other research projects at FNSPE. He is the author or co-author of 7 impacted papers (based on Web of Science) and 5 additional papers listed in Scopus. He also participated in 18 international conferences with oral or poster contributions. In 2022, the candidate was invited to give a lecture at the Institute of Mathematics of the Czech Academy of Sciences.

The candidate also assists with the educational process at FNSPE. He has been guiding exercises in Mathematics 1 and 2 since 2016. Currently, he is a co-advisor of one master student. Further, he was involved in several promotion activities of FNSPE.

During his work, the candidate proved his ability to master difficult problems of interdisciplinary character. The submitted thesis is of high quality and represents major scientific contributions which is endorsed by a number of papers in Q1 journals. The thesis fulfills all requirements for Ph.D. theses. Hence, I recommend the candidate to the committee for the doctoral theses to bestow him the title of Doctor of Philosophy.

Praha, October 31, 2022

doc. Ing. Radek Fučík, Ph.D.

References

[1] Ahmad H Askar, Tissa H Illangasekare, Andrew Trautz, Jakub Solovský, Ye Zhang, and Radek Fučík. Exploring the Impacts of Source Condition Uncertainties on Far-Field Brine Leakage Plume Predictions in Geologic Storage of CO2: Integrating Intermediate-Scale Laboratory Testing With Numerical Modeling. *Water Resources Research*, 57(9):e2021WR029679, 2021.

[2] Radek Fučík, Jakub Klinkovský, Jakub Solovský, Tomáš Oberhuber, and Jiří Mikyška. Multidimensional mixed–hybrid finite element method for compositional two-phase flow in heterogeneous porous media and its parallel implementation on GPU. *Computer Physics Communications*, 238:165–180, 2019.

[3] Radek Fučík, Jakub Solovský, Michelle R Plampin, Hao Wu, Jiří Mikyška, and Tissa H Illangasekare. Computational methodology to analyze the effect of mass transfer rate on attenuation of leaked carbon dioxide in shallow aquifers. *Acta Polytechnica*, 61(SI):77–88, 2021.

[4] Jakub Solovský and Radek Fučík. Mass lumping for mhfem in two phase flow problems in porous media. In *European Conference on Numerical Mathematics and Advanced Applications*, pages 635–643. Springer, 2017.

[5] Jakub Solovský, Radek Fučík, Michelle R Plampin, Tissa H Illangasekare, and Jiří Mikyška. Dimensional effects of inter-phase mass transfer on attenuation of structurally trapped gaseous carbon dioxide in shallow aquifers. *Journal of Computational Physics*, 405:109178, 2020.

[6] Jakub Solovský, Radek Fučík, and Jakub Šístek. BDDC for MHFEM discretization of unsteady two-phase flow in porous media. *Computer Physics Communications*, 271:108199, 2022.