Opponent review of Ph.D. Thesis

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

Author: **Ing. Jakub Solovský** (ČVUT v Praze, FJFI)

Reviewer: **doc. Ing. Milan Hokr, Ph.D.** (Technická univerzita v Liberci, NTI FM)

Introduction

The work covers various particular topics related to the title – modelling of the two-phase compositional flow in porous media. For numerical solution, this belongs to challenging problems in porous media physics due to non-linearity and complex system of constitutive relations.

The Thesis is written in a monograph form, with chapters corresponding to partial topics, coarsely how they set sequential steps in mathematical modelling – formulation of equations based on physics, deriving and analyses of numerical schemes, their implementation, verification on artificial problems, study of efficiency, and examples of problems solution analogue to real-world cases.

Some of the chapter topics are published as journal papers. Such situation could be easier for the author to choose the Thesis form of the paper collection. The monograph form in this case appears far more challenging to assemble, with a lot of links between different parts, but with appropriate value for reader to get a complete image about the modelling work and relations between the subtopics. Some problems are commented below.

Topic choice

Numerical simulation of porous media processes is a well-established field, with strong demand from practice related to big problems of current society, including groundwater contamination and energy resources. In addition to extensive development in the last decades in numerical algorithms and hardware resources, author defines and solves specific problems aiming to improve the accuracy of physical system modelling – equation formulation with realistic details of physics leading to more challenging solution, using numerical solution oriented on efficiency, and comparison of numerical results against laboratory experiments for model verification.

Methods

Methods used for problem solution are appropriate and considering the full range of topics in the Thesis, the author needed to cover several different topics to high level of expertise. The problem of two-phase compositional flow is highly nonlinear and the groundwater problems often feature complex heterogeneity in 3D, so the solution time is an issue, and the parallel computation is an implied choice. Also, the studies with comparison of laboratory experiments and numerical solution can bring useful novelty in the cases of problems with observed difficulties in numerical solution. This is even better with the configurations tailored to produce the expected complicated behavior, especially if it can be interpreted as an analogue of real-world processes.

It should be noted that the complex task of model and experiment comparison was a team work and the Thesis author's contribution is declared in particular for the published papers (section 1.5) but not explicitly in the related chapters (e.g. ch.7 introduction). The international cooperation of the "experimental team" and the "numerical team" is an inspiring starting point (likely provided by the supervisor or the faculty), to get more application-related research together with novel numerical schemes. I understand the situation that author did not personally participate on the experiments and took the resulting measurement for model evaluation, while it is not clear if he had an opportunity to contribute to the experiment design, so that the measurement could focus to problematic physical and numerical phenomena as much as possible. The understanding of personal contribution becomes even more uncertain with the use of plural verb form in most of the text (commented also below as a formal issue).

Meeting of goals

The goal was defined as investigation of gas and water behavior in subsurface, in particular the development of a numerical model and application to selected quasi-real-world problem. As mentioned above, it included all the relevant steps from mathematical problem formulation to computer code implementation and verification. As such, the goals were fully met, in all the intermediate steps.

Results and scientific contribution

This was in pieces commented above. The value of author's results is in complexity of the work, combining state-of-the-art ideas and solutions in numerical mathematics to a challenging problem resulting from practical needs of groundwater processes study. Therefore, several relevant issues are answered, as e.g. observation of the solution efficiency and options for high-performance computing and accuracy and physical meaning of the solution both against close-form solution problem and laboratory experiment with design according to real-world problems.

Formal and technical issues

With the extent of the work and combination of different topics, it was challenging to keep the text correct and consistent. I did not find generic typing errors in text, but several cases of likely insufficient attention in data compiling for the presentation: (the first two points, it should be better to confirm that the eventually wrong data are only case of the tables, not the calculations)

- In Tab.7.1, 8.2, 8.3, wrong values of M are printed (I guess a reverse unit conversion by 1000).
- In 5.1. wrong value of water viscosity (one order of magnitude, maybe wrong rounding?)
- In several table headers, errors in unit exponents: Henry constant Tab. 7.2, viscosity Tab. 5.1, 7.1, 8.2
- In some cases, subscripts are wrongly typeset (eq. (5.8), headers of tab. 5.3-5.6)
- Figures referred from 7.2 are shown far inside 7.3, I would recommend eventually not to typeset the text below the large figures if it helped to control the start of 7.3. after them.
- I find the term "tracer" questionable in chapter 8, in the context of variable-density effects (as tracing in strict sense should "visualize" the flow field without any effect to the velocity pattern).

- I find the term "radial symmetry" not accurate for the case in 3D which is in fact spherical.

Despite the large effort to compile the notation list, there are still cases not covered. I also find references from inside a chapter to the whole chapter by a number as undesired. As effect of compilation, there are unnecessary repetitions like Helios cluster detailed features.

In section 1.5., papers in impact journals are listed with Thesis author's contribution. On the other hand, there some other author's works (with coauthors) in the reference list, without such comments, and used for the Thesis compilation. It would also help if the links from 1.5. to numbers in the reference list were shown.

Considering language, there are combinations of passive voice and first person plural, sometimes within the same paragraph (abstract). The first person plural can be convenient for some kind of procedure explanation, but it can cause misleading interpretation in paragraphs like the partial chapter conclusions where the individual work of the graduate is expected.

Conclusion

I find the Thesis a valuable contribution to the numerical studies of porous media processes. The author has demonstrated a wide range of detailed expertise in many individual topics. The participation in the team work leading to the presented results could be better explained; there will be such opportunity at the defense discussion. Other questions and discussion suggestions are given below. The author proved his ability of independent scientific work. I recommend the Thesis to be accepted and to grant the Ph.D. degree to the author.

Questions for discussion:

- In the problem solution in Fig.5.5. what is the reason for the downwards peaks of the solid line at the lower interface (y=0.355m) – physically, mathematically? It is clear there must be a discontinuity due to different retention curve but this seem to be out from the range of the left and right limits.
- Why the very old COMSOL version (3.5a) is used as mentioned in 5.1.1? (in such situation maybe the software is not used for anything else, so rather surprising for the task of mesh generation with a lot of other choices)
- The problem in 6.2 has discontinuities in boundary conditions, leading to high solution gradients. Does it have any consequences on the efficiency evaluation and its generality?
- If the case in Fig.2.1a happened in smaller scale such that the homogenization could be considered, how would the entrapped gas project into the homogenized equations? (besides the anisotropy, the invariance to direction change seems to be lost)

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