

## Thesis Changes Log

**Name of Candidate:** Lyudmila Khakimova

**PhD Program:** Petroleum Engineering

**Title of Thesis:** New Approaches for Numerical Modeling of Air-Injection Based Enhanced Oil Recovery

**Supervisor:** Associate Professor of the Practice Alexey Cheremisin

*The thesis document includes the following changes in answer to the external review process.*

Please, find the following changes made in the final thesis file.

Based on the Jury Member Report from Prof. Evangelos Moulas, there have been made changes according to the following suggestions

1. In the text:

In page iv the third sentence was rewritten: “During numerical reservoir modeling, the following most essential difficulties are faced: the lack of a proper reaction kinetic model and the large number of pseudo-components, more precise determination of phase equilibria and under critical conditions, porosity changes due to chemical reactions, the anisotropy of thermal properties, upscaling from laboratory to field scale and simulation time performance.” The definition of HPAI and ISC is added.

In page 1 “It has such advantages...” was substituted with “HPAI and ISC have such advantages...” to be more specific, the format of several references was corrected, “...the lack of a proper reaction kinetic model...” and “the large number of pseudo-components” were added to the last sentence.

In page 2 the sentence was rephrased: “It involves initiating the oil combustion front in the reservoir associated with the thermal front propagation through the reservoir during air injection.”

In page 3 “It gives a significant ...” was substituted with “It provides a significant ...”.

The units in page 4 was replaced with  $\text{st.m}^3/(\text{m}^2\text{hr})$ ; “under the conditions close to the real” was substituted instead of “under the conditions close to the real”.

In page 8 (Firoozabadi and Pan, 2000) reference was added.

The word “partial” was added to the first sentence in page 9.

In page 10 “...given that the compositions are sufficiently resolved” was added.

In page 13 the word order is changed in “before the numerical modeling of combustion tube (CT) test”.

The errors were corrected in the List of Tables and in page 21.

The indexes in formula was added in page 31.

In page 36 the sentence was reformulated: “These functions are assumed to be the objective functions for which the error in experimental and simulated values is minimizing during the history matching procedure.”

The word “fixed” was substituted with “detected” in page 37.

In page 40 the word “high” was added.

In page 44 (Kissinger, 1957; Taylor and Fryer, 1992) was added.

In page 69 the table were modified: the normalized differences between experimental and simulated values were added for the case of traditional and modified reaction schemes.

In page 79 the word “mentioned” was substituted with “mentioning”.

In page 84 – “used liner size” was added.

In page 91: “generation energy” - “thermal energy generation” and “start” – “starting”.

“The Helmholtz and Gibbs energy minimization algorithms consist of the following major parts: the discretization of compositional space, whose dimension is in 1 less than a number of components (and one additional volume space dimension in case of the Helmholtz energy minimization),...” was changed in page 92.

In page 93 “... technique is applicable...” was substituted with “...techniques are applicable...”.

In page 94 “Let us start with the flash calculations procedure and then move to the Helmholtz energy minimization technique.” Was substituted with “In the following part we begin with describing the flash calculations algorithm and we proceed to the free energy minimization techniques.”

In chapter 4.1.1 the third sentence were rephrased.

In page 96 “...are fed to...” was changed to “...are provided to...”.

In page 99 the word “Second” was substituted with “In the second approach” and “let us move to” – “we can proceed with”.

In page 102 “C” symbol was used instead of “Z” to denote system composition.

In page 109 “has been” was used instead of “was”.

In page 109 “gives advantages” was substituted with “has an advantage” and “Let us start with” – “To proceed, we will consider”.

In page 110 the following sentence was added:

“Note, the system volume, which is an input parameter for the Helmholtz energy minimization algorithm, is calculated in the postprocessing of the Gibbs energy minimization algorithm according to (11).”

In page 111 the second and the third sentences were rephrased.

In page 112: “second digit” – “second digit after the decimal point”.

The following text was added in page 113 to support selecting the reported limitation for a maximum number of iterations used in the flash calculations:

“...The maximum number of iterations is 100. This limitation is used to get the results of flash calculations in a reasonable time. In this case, the computational time required to obtain the vapor-liquid equilibrium parameters at constant composition is equal to 58.89s. The same calculations take 22.03s in the case of Gibbs energy minimization. The flash calculations computation time is mostly controlled by the time necessary to calculate the parameters of vapor-liquid equilibrium near the critical. Thus, the chosen limitation for a maximum number of iterations is large enough to provide an accuracy of the calculation near the critical zone that can be compatible with the one provided by the free energy minimization algorithm...”

In page 132 as “a porous media” is extended as “that can be treated as a porous medium in a multiphase problem”. The collocation “Helmholtz(Gibbs)” is substituted with “Gibbs/Helmholtz”.

The word “molecules” is substituted with “molecular species”, “technique” - “techniques”, “it” - “This approach” and the last three sentences were rephrased in page 133.

2. The following references were added to Bibliography:

“Kelemen, S.R., Afeworki, M., Gorbaty, M.L., Sansone, M., Kwiatek, P.J., Walters, C.C., Freund, H., Siskin, M., Bence, A.E., Curry, D.J., Solum, M., Pugmire, R.J., Vandenbroucke, M., Leblond, M., Behar, F., 2007. Direct Characterization of Kerogen by X-ray and Solid-

State <sup>13</sup>C Nuclear Magnetic Resonance Methods. Energy Fuels 21, 1548–1561. <https://doi.org/10.1021/ef060321h>”; “Firoozabadi, A., Pan, H., 2000. Fast and Robust Algorithm for Compositional Modeling: Part I - Stability Analysis Testing. Presented at the SPE Annual Technical Conference and Exhibition, Society of Petroleum Engineers. <https://doi.org/10.2118/63083-MS>”; “Kissinger, H.E., 1957. Reaction kinetics in differential thermal analysis. Analytical chemistry 29, 1702–1706.”; “Taylor, S.M., Fryer, P.J., 1992. A numerical study of the use of the Kissinger analysis of DSC thermograms to obtain reaction kinetic parameters. Thermochimica Acta 209, 111–125. [https://doi.org/10.1016/0040-6031\(92\)80189-4](https://doi.org/10.1016/0040-6031(92)80189-4)”

3. Articles and prepositions were changed or added:  
in page iii, 78, 79, 80, 83, 84, 86, 110, 133
4. Figure captions:  
Figure 2.6 was improved. The captions for Figure 4.1, Figure 4.14 were extended.
5. The format of references was corrected:  
in page iv, 10, 133, 134.

Based on the Jury Member Report from Prof. Raj Mehta, there have been made changes according to the following suggestions

1. The page numbering was changed to Roman in the first 21 pages.
2. Misprints and formatting errors were eliminated (e.g. “*In-situ*”, “250 K”, “Figures 4.3 (a)”, “Paragraph” was substituted with “Section”, one reference in Bibliography was changed)
3. The quality of figures 4.1 and 4.2 was improved.
4. Chapter 5 was split into three sections: Summary, conclusions, and recommendations for future research.

Based on the Jury Member Report from Prof. Dmitry Eskin, there have been made changes according to the following suggestions

1. Figure captions:  
Figure 2.5 is improved. Figures 3.15-3.17: “for carbonate oil field” was added. The details for different panels were added for Figures 4.10-4.14, 4.16, 4.18.
2. In the text:  
In Table of Content the format was corrected. “Air injection-based EOR” was substituted with “air-injection based EOR” in Pages i, 14, 23, 131. In page 79 “...Small amount...” was substituted with “...small number...”.
3. In Chapter 4:  
The following paragraph is added to describe the modern approaches used to reduce CPU time spent on phase behavior calculations in commercial reservoir simulators:  
“In order to accelerate phase behavior calculations and reveal possible instabilities rapidly, ab initio flash calculation is used. This approach is incorporated in the commercial reservoir simulator Intersect and involves the initial application of successive substitutions, eigenvalues and eigenvectors of the BICs matrix. However, in case that the calculations do not converge, the traditional iterative algorithm is used (Firoozabadi and Pan, 2000).”

Based on the Jury Member Report from Prof. Dmitri Koroteev, there have been made changes according to the following suggestions

1. Formatting errors and typos were corrected in the text.
2. The developed HPAI and ISC numerical models were validated against kinetic and combustion performance laboratory experimental results (DSC, RTO, CT tests) conducted within this research work. Since the HPAI and ISC numerical model construction involved a sophisticated analysis of experimental results, provided within this work, its description is an integral part of the dissertation.
3. The information about the application of the developed HPAI and ISC laboratory-scale numerical models for full-field simulations using commercial simulators was extended and added to Chapter 5, p. 133.

In the text:

“Notwithstanding all weaknesses of developed numerical models of HPAI and ISC have appropriate predictable power, they are adapted for a commercial simulator widely used by reservoir engineers. They are ready for being upscaled and used in full-field simulations. It was demonstrated during validation of presented numerical models against 1D laboratory-scale representation of HPAI and ISC processes, provided in CT tests. In addition, several developed numerical models, as they are, have already been used as a start model for full-field simulations in order to evaluate ISC and HPAI potential for the particular oil field. (Mukhina et al., 2020, Askarova et. al, 2020) As was mentioned in Askarova et. al, 2020, to upscale the earlier developed laboratory-scale HPAI numerical model (Khakimova et. al, 2020) and to provide full-field simulations using SMG STARS, areal heterogeneity, displacement effectivity, and numerical algorithm convergence difficulties had been considered.”

Also, a short overview of existing upscaling methodologies is added to the Chapter 5, p. 137. Although there is no comprehensive and universal routine to upscale laboratory-scale thermal EOR numerical models (including kinetic parameters modification from laboratory scale to field scale), there are approaches that can help in full-field model construction.

In the text:

“...the problem of upscaling in the thermal EOR simulations arises since considered subprocesses (reaction and evaporation front, anisotropy, local heterogeneity of porous media properties, etc.) occur at different time and length scales (from 1 day to 1 year; from 1 cm to 1 km) (Gutierrez et al., 2011). There are several upscaling routines published in the literature, which are developed to capture local-scale processes and to approximate the developed model for subprocesses description. (Christensen et al., 2004; De Zwart et al., 2008; Druganova et al., 2010; Marjerrison and Fassihi, 1992; Van Batenburg et al., 2011) For example, the dynamic gridding technique makes it possible to refine grid cells near sharp fronts and to coarse grid cells in the other region. (Christensen et al., 2004) Nevertheless, there is no straightforward algorithm to tune the model in the case of a high heterogeneous reservoir and to choose the proper size of refining blocks for dynamic gridding, which significantly complicates the upscaling procedure.”

During further research work associated with this thesis, I prefer to use another approach involving high-performance computing to resolve local-scale processes.

In the text:

“Instead of approximating the developed model for subprocesses description, one can accurately resolve these coupled processes, which requires a high-performance computing approach to achieve high spatial and temporal resolution requirements.”

“...the effectiveness of parallel computing for “upscaling candidates” has already been shown by numerical results demonstration for resolving spontaneous channeling of porous fluids owing to decompaction weakening (Omlin et al., 2018; Räss et al., 2018; Räss et al., 2019; Duretz et al., 2019) in case of hydro and thermomechanical coupled problems.”

4. The multi-GPU technique implementation is mentioned in Chapter 5 (Summary, conclusions, and recommendations for future research) to discuss the application of high-performance computing in solving the problem of upscaling. The multi-GPU technique implementation for thermal EOR modeling is promising, and it is supposed to be one of the future research directions. To approbate the high-performance computing for resolving coupled problems and study its parallel efficiency abilities, a multi-GPU numerical implementation was provided for simpler (in comparison to ISC or HPAI) hydro-mechanical problem (anisotropic elastodynamic Biot's equations).

In the text:

“In this regard, authors of the work (Alkhimenkov, Khakimova et al, 2020) developed a multi-GPU numerical implementation of the anisotropic elastodynamic equations (Biot's equations, a well-known example of a coupled system with the ability to take into account anisotropic behavior) that relied on a conservative numerical scheme to simulate in a few seconds wave fields for model domains involving more than 1.5 billion grid cells. It is possible to achieve 90% effective memory throughput and close-to-ideal parallel efficiency (98% and 96%) on weak scaling tests on multi-GPU systems. Moreover, the effectiveness of parallel computing for “upscaling candidates” has already been shown by numerical results demonstration for resolving spontaneous channeling of porous fluids owing to decompaction weakening (Omlin et al., 2018; Räss et al., 2018; Räss et al., 2019; Duretz et al., 2019) in case of hydro and thermomechanical coupled problems.”

Moreover, the text was attentively proofread; some sentences were reformulated to increase the clarity of the presented material.

I would like to thank all Jury Members for their time and consideration of the previous version of the thesis and work on it improvement!

Lyudmila Khakimova