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Review of the PhD thesis

Author: Marek Nedoma

Title: Low-temperature adsorption for post-combustion CO2 capture from fossil fuel combustion

Bratislava, 5. October, 2023

About the achieving of the dissertation objectives:

The general goal of the thesis was to find and investigate the potential of a suitable method for the post-combustion CO2 capture (PCC) from industrial flue gases. The physical adsorption with a zeolite-based adsorbent was chosen and three main steps had to be carried out: 1. Development of a simplified non-linear dynamic mathematical model of the fixed bed adsorption, 2. Development of a complex non-linear dynamic model of the 4-step vacuum swing adsorption (VSA), 3. Design of adsorption PCC system integrated into an urban-scale energy system. In summary, the main steps and objectives were achieved and the operation of the 4-step VSA was simulated, its theoretical concept was designed together with other flue-gas treating sub-systems.

About the level of analysis of the current state of the problem being solved in dissertation:

The literature research presented in thesis is very detailed, the list of references contains 164 items including research papers, patents, books, PhD theses, handbooks. Very helpful is the fact that for the majority of references, the web pages are also available. A minor comment here: the citation [103] is invalid.

About the theoretical contribution of the dissertation

I think that the main theoretical contribution of the thesis is the development of mathematical models of different complexity for simulation of adsorption-desorption phenomena and their application for prediction of breakthrough curves and for design and economy assessment of the PCC. A high level and complexity has also simulation of the full combined heat and power plant summarized and illustrated in Figure 21.

About the practical contribution of the dissertation

I appreciate that author focused also on practical aspects of the problem, performed useful adsorption experiments and provided economy assessment of the recently commercially unavailable PCC using a 4-step VSA which can be compared with other technologies.

About the solution methods used in dissertation

Solution methods used in the dissertation represent a smart combination of simpler and faster mathematical models with more complex and expensive fully dynamic models of the adsorption phenomena and with commercially available models of the ASPEN Plus software package.

How the solution methods were applied

The solution methods were developed and applied logically starting from the simplified mathematical models and identification of the weaknesses of such approach and then developing and applying more sophisticated and complicated models and finally employing the complex models for simulations of the 4-step VSA and combining such simulations with the ASPEN Plus simulations of the whole plant.

Whether the author has demonstrated adequate knowledge in the given field

The author has definitely demonstrated adequate knowledge of physics, mathematics, engineering and effectively combined such knowledge for analysis of unit operations and synthesis of several sub-systems into a full plant.

About the formal level of the dissertation

I enjoyed reading the thesis. It is written logically, in very good English almost without formal errors, technical and graphical content is clear and extensive

(22 figures, 14 tables, 4 Appendices -available electronically). I appreciate also the detailed nomenclature and list of acronyms.

Comments and questions:

In summary, the thesis has high theoretical and technical level. What follows are some comments and questions for my better understanding of the work.

1. What is the key advantage of passing the gas mixture in the breakthrough apparatus from top to bottom?
2. Sensitivity analysis is indeed a useful tool to better understand the impacts of some uncertain model parameters and flux limiters on the simulated breakthrough onset times. After understanding the impacts what would be the main recommendations for employing different correlations and flux limiters for the simulations ?
3. I expect that a key challenge of the modelling and simulation of the 4-step PCC VSA cycle was to reach the cyclic steady state (CSS) and it needed more than 100 cycle simulations. Indeed, the CSS solution depends on the input values and boundary conditions of the VSA unit mathematical models. Have you simulated different scenarios, i.e. CSS for different combinations of inputs and boundary conditions, similarly as it was done for a single adsorber and summarized in Figure 15?
4. The process flow diagram for the combined heat and power (CHP) plant shown in Figure 21 contains several sub-systems and several recycles which are interconnecting different sub-systems. What kind of methodology was used to achieve convergence of the recycle streams properties? In other words, were the inputs into the VSA-unit modelling changing as a consequence of gradual convergence of properties of other streams of the whole process?
5. Different amounts of adsorbent are needed for the TSA column depending on the cooling water temperature. Is there any universal amount of adsorbent or some practical approach how to operate the TSA unit during the whole year without need to change amount of adsorbents in columns?

I confirm that I reviewed the thesis and recommend the dissertation for defense and award of the PhD title under Act 111/1998 Sb.