Theses of doctoral (PhD) dissertation

# Optimisation of gas purification process

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Institutional Department of Process Engineering
Veszprém
2025

## INTRODUCTION AND THE AIM OF THE WORK

Nowadays, industrial companies are facing a variety of challenges, such as rising energy prices, a shortage of skilled labour and tightening environmental regulations. These problems can be significantly reduced by optimising technology, developing an appropriate process control structure and effectively training operating staff. For this purpose, the aim of my doctoral dissertation was to develop tools based on process simulation methods to reliably and optimally operate the coke oven gas purification technology of an existing coke oven plant under varying operating conditions and malfunctions.

I developed a steady-state simulator for the investigated technology and demonstrated that a rate-based model is the most suitable for describing the absorption processes taking into account the kinetics of the reactions taking place. As a result of sensitivity studies, I determined the parameters that most influence the cleaning efficiency, which were used to define an energetically optimised and an environmentally optimised working point.

I used the dynamic process simulator to compare the control options of the H2S scrubbing column. Furthermore, I developed an emulated and a stimulated operator training simulator (OTS), which allow training of operators without disturbing the real technology and testing of intervention methods during hypothetical malfunctions.

A life cycle assessment (LCA) based on operational data was used to demonstrate the importance of the investigated part of the plant and the environmental impact of optimised work points implemented with the steady-state simulator on the whole production process. The applied methodology helps to better understand and identify environmental factors related to the plant and to support technological decision making while identifying improvement opportunities.

## EXPERIMENTAL TOOLS AND METHODOLOGIES

The data used for my research were collected from the daily sampling results, reports and declarations of the investigated coking plant. In addition, to validate the models, I also carried out more accurate sampling under different plant conditions.

I built the steady-state simulator in Aspen Plus process simulation software, using MATLAB software for the related sensitivity analysis and optimisation tasks. The dynamic simulator was created using Aspen HYSYS software. The operator training simulators were

developed using Aspen Operator Training software. For the life cycle assessment, the calculations were performed using Sphera's LCA for Experts software.

## NEW SCIENTIFIC RESULTS (THESES)

**Thesis 1.:** I have demonstrated that the equilibrium model is less suitable for describing the absorption processes during the purification of coke oven gas, therefore the use of a rate-based model is necessary with consideration of the reaction kinetics.

a) I have demonstrated that process simulation can be effectively used to analyse the impact of specific process parameters on the composition of the outlet gas. I have found that the temperature and the volume flow rate of the deacidified water have the greatest influence on the efficiency of the purification.
b) I have investigated the optimisation potential of a real coke oven gas purification technology using its steady-state simulator. The developed objective function was applied to identify both an energetically and an environmentally optimal operating point.
c) I have shown that the developed steady-state simulator is suitable for describing similar technologies, provided that appropriate measured data are available

Related publications: 1, 2, 5, 6, 7

**Thesis 2.:** I have demonstrated that dynamic simulation of existing technology is an ideal tool for investigating system dynamics, designing and testing control structures, and developing operator training simulators.

a) I have developed an emulated operator training simulator to investigate the case of a pump failure. Furthermore, I have tested how long it takes for individuals with different levels of professional experience to detect and eliminate the generated malfunction depending on whether or not the display contains a fault alarm. My findings indicate that the presence of a fault alarm significantly shortened participants' intervention time.
b) I have connected the whole technology dynamic simulator to the DCS of the plant, creating a stimulated operator training simulator. I have observed that

in the familiar environment, the operator detects the fault significantly faster than the other participants in the test.

Related publications: 3, 10, 11

**Thesis 3.:** I have conducted a life cycle assessment based on real coking plant data and demonstrated that, for a given technology, a process simulator-based life cycle analysis can effectively support the sustainable operation of existing plants amid dynamically changing energy prices and tightening environmental regulations. Additionally, it serves as a valuable tool for making informed decisions under unexpected operating conditions.

a) I have concluded that the life cycle assessment of coke production can be more efficiently examined by using the subdivision method to identify the environmental impact of each sub-processes, which can identify the most environmentally damaging part of the plant. Coking, followed by transportation, gas purification, cooling and tar recovery have the highest impact, so these sub-processes should receive special attention.
b) I have identified that, among the auxiliary materials used in the production process, electricity contributes the most to the environmental impact categories, followed by steam and process water.
c) Using life cycle assessment, I have demonstrated the importance of coke oven gas purification through four different cases and found that the energetically optimized operating point, as determined by the steady-state model of the technology, is the best scenario in terms of environmental impact.

Related publications: 4, 8, 9

# PUBLICATIONS OF THE AUTHOR

## *Articles:*

1. Radó-Fóty, N., Egedy, A., Nagy, L., Hegedűs, I. (2021) Comparison of Equilibrium-Stage and Rate-Based Models of a $H_2S$ Scrubber for Purification of Coke Oven Gas, Chem. Eng. Trans., 88, 217-222, https://doi.org/10.3303/CET2188036 **Q3, IF:-**
2. Radó-Fóty N, Egedy A, Nagy L, Hegedűs I (2022) Investigation and Optimisation of the Steady-State Model of a Coke Oven Gas Purification Process. Energies 15, 4548. https://doi.org/10.3390/en15134548 **Q1, IF: 3.2**
3. Radó-Fóty N, Egedy A, Nagy L, Hegedűs I (2023) Dynamic Modelling and Process Control System Development of a $H_2S$ Scrubber Used in a Coke Oven Gas Purification Technology, Chem. Eng. Trans., 99, 649-654. https://doi.org/10.3303/CET2399109 **Q3, IF:-**
4. Radó-Fóty, N., Egedy, A., Nagy, L., Domokos, E., Sebestyén, V., (2025) Life Cycle Assessment of Coke Production Based on Real Plant and Model-optimised Data, Int J Life Cycle Assess, https://doi.org/10.1007/s11367-025-02455-6 **Q1, IF:4.9**

## *Oral Presentations:*

5. Fóty, N.; Egedy, A., Nagy, L. (2020) Study of reducing $H_2S$ and $NH_3$ content in coke oven gas. Pannon Egyetem, Mérnöki Kari Tudományos Konferencia, pp 8. ISBN: 978-963-396-153-7
6. Fóty, N.; Egedy, A., Nagy, L. (2021) Kamragáz $H_2S$-tartalmának csökkentésének vizsgálta. Kárpát-Medencei Fiatal Magyar Kutatók Konferenciája, pp 34-35.
7. Fóty, N.; Egedy, A., Nagy, L. (2021) Modelling of $H_2S$ scrubber used for coke oven purification. Műszaki Kémiai Nap 2021 Konferencia.
8. Radó-Fóty, N., Egedy, A., Nagy, L., Domokos, E., Horváth, T. (2023) Comparative Life Cycle Analysis of a Coking Plant. 11th International Mardin Artuklu Scientific Researches Conference.
9. Radó-Fóty, N., Egedy, A., Nagy, L., Domokos, E., Sebestyén, V., (2024) Kokszoló üzem összehasonlító életciklus elemzése a gáztisztítás szempontjából. Műszaki Kémiai Napok 2024 Konferencia.

10. Radó-Fóty, N., Egedy, A., Nagy, L., Horváth, T., (2024) Dinamikus szimuláció alkalmazásai kamragáztisztító technológiákban. Műszaki Kémiai Napok 2024 Konferencia.
11. Radó-Fóty, N., Egedy, A., Nagy, L., Horváth, T., Balaton, M., Tóth, L.R. (2025) Operátor tréning szimulátor kifejlesztése kamragáz-tisztító üzemhez. Műszaki Kémiai Napok 2025 Konferencia.