THESIS FOR THE DEGREE OF LICENTIATE OF ENGINEERING IN THERMO AND FLUID DYNAMICS

Numerical simulations of industrial-scale packed-bed adsorbers

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Göteborg, Sweden 2020

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Thesis for the degree of Licentiate of Engineering 2020:03
ISSN 1652-8565
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Chalmers Reproservice
Göteborg, Sweden 2020

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Abstract

A common technique for removing harmful substances, for either persons or equipment, from a stream is to use the phenomenon of adsorption. This technique is used in, for example, water purification, personal protection, chemical and pharmaceutical production and biomass gasification. In a biomass gasification plant called GoBiGas in Gothenburg, Sweden, beds packed with activated carbon were used to remove light tars from the product gas, where the tars adsorbes to the carbon. This was a step in the gas cleaning train used for the production of bio-methane from forest residue streams in an effort towards a more carbon neutral future. However, the operation of packed beds for continuous substance removal both requires energy, and puts certain technological demands on the plant. For the production of bio-methane, all losses in the plant influence not only the economical aspects, but also the carbon footprint of the end product. Since carbon neutrality is a compelling reason for using bio-methane, this puts further demands on the bed operation. Here, numerical simulations offer increasing opportunities, both with respect to energy optimization, but also to bed design and operation.

In this work, we formulate a numerical model for an industrial sized adsorber, used in GoBiGas for benzene removal. The end goal includes an increased general understanding of the requirements for a successful numerical model of real-world, industrial conditions. This is done in order to be able to better design and optimize packed bed setups for industrial conditions before the actual facilities are built. However, the work also allows to better understand and optimize setups already online. The work presented here includes both analysis of industrial data from GoBiGas and an establishment of how a baseline numerical model performs.

The numerical model is based on solving the governing equations for the system, with no industry-specific parameter tuning. This is important in order to be able to use the models as a predictive tool, useful in e.g. bed design. A finite volume method is used to numerically simulate the flow, mass- and heat-transport in both time and space. The temperature at different axial positions in the bed is used to compare the numerical simulations with the industrial data. We show that a baseline formulation captures the main characteristics of the temperature signals in a bed but there are dynamics of the industrial data that are not captured. Three areas are identified that require additional development for a better predictability. Those are that a more complete description of the actual gas composition and a more realistic evaporation rate are required and a model for water drainage would benefit the model.

Keywords: Packed Bed, Finite Volume Method, Temperature Swing Adsorption, Industrial Scale, Numerical Modeling

To my wife

Acknowledgements

First of all, it would take far too many pages for me if I were to try to give a somewhat complete acknowledgement of everything people have done, and are doing for me. I neither have that kind of space, nor would I be able do them justice. However, I will at least try to mention some things about the people close to me and this project.

I would like to begin by thanking my supervisor Henrik Ström and my examiner Srdjan Sasic for their invaluable support in all matters, research related or others. Without you this endeavour would not be possible. I would further want to thank my co-supervisors Dario Maggiolo and Henrik Thunman, your inspiration, input and assistance makes me a better PhD student with better results.

I would also like to extend my gratitude to all my co-workers. You make life at the division significantly nicer and I am very grateful for having the opportunity to work with you. To the people in the multi-phase group, thank you for all the interesting lunches, all fantastic trips to conferences and what ever else we have been up to. I would also want to thank Elias, my roommate, who has had to endure my messy desk and mountains of coffee cups. We have had many interesting conversations and more will come. Another special thank you is to Klas. You have, and continue to, inspire me to be a better researcher and engineer. I always feel refilled with inspiration and aspiration after having discussed something with you.

Finally, I would like to thank my family, both the one I was born into and the one I married into. Your support is invaluable to me and I feel incredibly lucky to have you all so close. Most importantly, thank you Malin, my life partner and wife. Words cannot describe what you mean to me, you are the reason I can do this at all.

This work has been financially supported by the Swedish Energy Agency and the Swedish Centre for Biomass Gasification. The industrial data was provided by Göteborgs Energi from the GoBiGas facility.

Adam Jareteg
Göteborg, January 2020

List of abbreviations

Abbreviations

FVM	–	Finite Volume Method
DFB	–	Dual Fluidized Bed
TSA	–	Temperature Swing Adsorption
PSA	–	Pressure Swing Adsorption
LDF	–	Linear Driving Force

Thesis

This thesis consists of an extended summary and the following appended papers:

Paper A A. Jareteg, D. Maggiolo, S. Sasic, and H. Ström. Finite-volume method for industrial-scale temperature-swing adsorption simulations. *Submitted to a scientific journal* (2019)

Paper B A. Jareteg, D. Maggiolo, A. Larsson, H. Thunman, S. Sasic, and H. Ström. Industrial-scale benzene adsorption: assessment of a 1D temperature-swing model against on-line industrial data. *Submitted to a scientific journal* (2019)

Other related publications, not included in the thesis

Publication I A. Jareteg, D. Maggiolo, H. Thunman, S. Sasic, and H. Ström. "The influence of particle shape on the capacity of packed beds - a numerical investigation using the Lattice Boltzmann Method". *Proceedings of the International Conference on Multiphase Flow (ICMF2019).* Rio de Janeiro, Brazil, 2019

Publication II A. Jareteg, D. Maggiolo, H. Thunman, S. Sasic, and H. Ström. "Detailed simulations of heterogeneous reactions in porous media using the Lattice Boltzmann Method". *EFMC12 – 12th European Fluid Mechanics Conference.* Vienna, Austria, 2018

Publication III A. Jareteg, D. Maggiolo, H. Thunman, S. Sasic, and H. Ström. "Finely resolved numerical simulations of reactive flow in porous media". *8th International Energy Conference & Workshop REMOO.* Venice, Italy, 2018

Publication IV A. Jareteg, M. Israelsson, S. Sasic, H. Thunman, and H. Ström. "Packed-Bed Reactor Characterization of Steam-Regenerated Solvent Adsorbers for Raw-Gas Cleaning". *14th International Conference on Multiphase Flow in Industrial Plant.* Desenzano del Garda, Italy, 2017

Contents

Part I
Extended Summary

Chapter 1
Introduction and background to the project

1.1 Introduction

Chalmers has a focus on sustainability that permeates most of its activities [7]. Everything from research, education and society services is performed within a framework for a sustainable future. Numerous courses are taught in sustainability, PhD students are obliged to reflect on how their project could aid a sustainable future and pilot projects are continuously launched to try new technological solutions. Even the slogan contains wording that Chalmers is "Making an impact for a sustainable future". It was in this spirit that the Division of Energy Technology started a collaboration with Göteborg Energi to address the sustainability of the future transport fleet in Sweden [8].

The aim was to create bio-fuel from forest residue streams through gasification. After a significant amount of research, proof-of-concepts and much more [9, 10], Göteborg Energi finally built a state-of-the-art industrial-scale pilot plant, called GoBiGas, for creating bio-methane from wood products.

The current research project was started in collaboration with Göteborg Energi and GoBiGas. The goal is to increase knowledge of how to better perform and use numerical modeling of packed bed adsorbers. They are a part of the gas cleaning technology found in the GoBiGas facility and they remove certain substances from the product gas. Targets include to identify key phenomena that are required for adequate modeling for predictions of industrial-sized beds, understand what is required in the transition from modeling lab-scale systems to industrial-sized systems and improve upon current modeling.

1.2 GoBiGas and the background to the project

GoBiGas was a gasification plant situated in Göteborg, Sweden, designed for transforming forest residue streams into bio-methane [8]. It began its operation in 2013 and it had to close in 2018 due to a variety of reasons, most of them economical [8]. The production target was to produce bio-methane of such quality that it could directly be distributed on the high-pressure gas infrastructure. The plant produced 20 MW product gas with a gasification capacity of 32 MW. The purpose of the plant was to demonstrate that the technology could indeed be used, with success, to commercially produce bio-methane while simultaneously mature the technology enough to be able to build a second plant, of roughly 200 MW size [11].

Figure 1.1 shows a schematic of the plant. It was essentially comprised of two different sections with distinct functions. The first one was a gasification and cleaning section (1-5

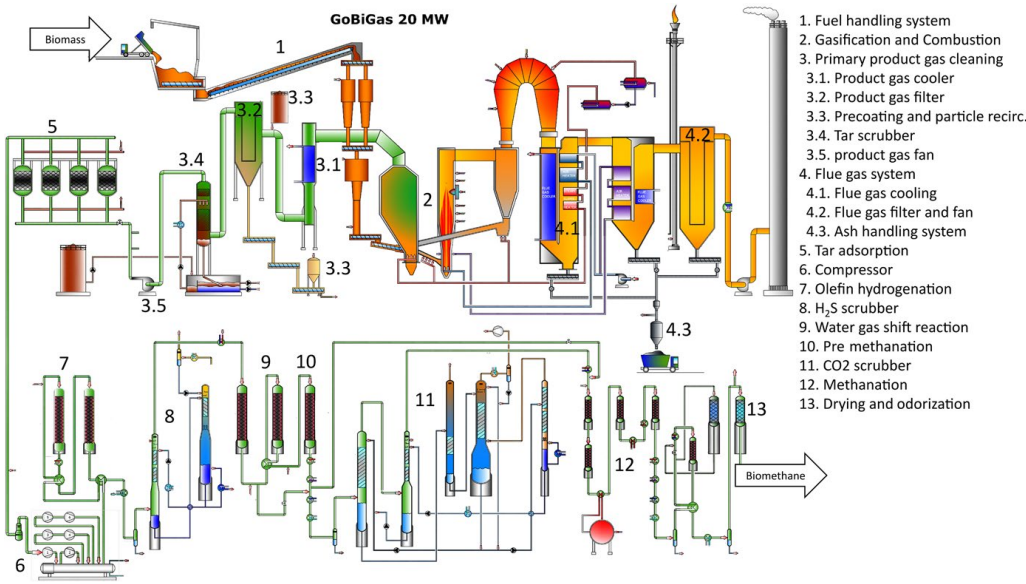

Figure 1.1: *GoBiGas schematics, where steps 1-5 are a part of the gasification and cleaning section whereas steps 6-13 are a part of the methanization part. Figure adapted from [11].*

in Figure 1.1) while the second a methanization section (6-13 in Figure 1.1). Depending on the quality targets for the product gas, for some purposes, the first part of the plant would suffice. The first part created a clean syngas suitable for e.g. internal combustion engines. However, since the target of the plant was to produce a high quality bio-methane, also the second section of the plant was required [8].

In the facility, forest residue was gasified in a dual fluidized bed (DFB) gasifier. The product gas was thereafter run through a series of cleaning steps and finally synthesized into methane [8]. The final step in the gas cleaning train was that the gas was run through packed bed adsorbers (5 in Figure 1.1). Their purpose was to remove the final tar components from the product gas, mainly benzene, that could not be scrubbed out. Some residual larger compounds were also removed, most notably naphthalene, in what began as a three-step process, where three out of the four available beds were used in sequence. The first bed served as a pre-adsorber, which caught scarce heavier tars and it was always online. The second bed in the sequence acted as the main adsorber. In it, the bulk removal took place and a bed working in this mode had to be continuously regenerated as it rapidly saturated with benzene. The third bed in the sequence acted as a safe guard to capture any trace amount of benzene that leaked out of the main bulk adsorber.

Since the two different sections were designed and delivered by two different suppliers, the beds also became the interface between the two suppliers. For several reasons, the original plan of operation and size of the beds ended up under-performing and the setup became

the bottleneck for the plant. Efforts were done by Göteborg Energi in collaboration with Chalmers to find a better operational mode for the four beds [10]. This was done to increase the capacity of the bed-setup in order to allow for maximum plant production. After some numerical simulations of the operation of the beds it was found that lowering the gas stream temperature to the beds, in conjunction with operating in a two-step mode, where the guard bed was removed and used as bulk adsorber instead, would increase the capacity enough.

The use of activated carbon for removal of harmful substances is, naturally, not limited to GoBiGas or gasification. It is a widespread technology used in, for example, personal protection, water treatment, chemical production and climate control [12, 13, 14]. However, GoBiGas is a good example of the need and usefulness of utilizing numerical simulations to better understand and optimize the use of activated carbon beds in industrial settings. This is where the current project comes into the picture, as there are still questions regarding numerical simulations of industrially-sized adsorbers [15]. Amongst others, what species are relevant to include, how to handle the long physical times and cyclic operation of the beds, what additional information one can get from a numerical simulation and how to incorporate this information in the design of the bed system.

This project aims to answer some of the above mentioned questions. To achieve this, a one-dimensional (1D) finite volume (FVM) tool is developed. The governing equations are solved in both space and time, and the entire operation of a bed is simulated. This includes correctly sized bed with enough simulated physical times to achieve a cycle-steady operation. A baseline model is developed, with the standard design aspects included, and evaluated against industrial data from GoBiGas. This to determine how much of the industrial bed behaviour that is explained by standard design considerations, and how much that is still missing. The intention is then to gradually add the missing physics in order to more precisely capture the real-world data.

Chapter 2
Methodology

Industrial-sized adsorbers have some distinct differences from the more common lab-scale ones that need to be taken into consideration when performing numerical simulations. Notably the gas composition is far more complex, the beds are continuously cycled and, due to the larger size of the beds, the ratio between the activated carbon and the actual container is significantly different [15].

The increase in complexity of the product gas in industrial units compared to controlled lab-scale experiments has several implications. Firstly, the product gas contains several species that, as with the target substance benzene, adsorb to the activated carbon. Commonly, lab-scale experiments, and also their numerical simulation counterparts, deal with a single adsorbing species [16, 17, 18]. Secondly, there are likely complex interactions between the different species during the adsorption process, such as competitive adsorption and different site interactions [18], posing questions into how important these interactions are and how viable they are to simulate.

There are also some effects from the fact that the beds are of industrial size and used in an industrial setting. Firstly, the beds will never be in a fresh state, i.e. they will, before the active stage, never be empty but rather always be in some form of inter-cyclic steady state condition. This puts requirements on the numerical simulations to be able to handle real-world cycling times. The simulations must be able to handle simulated physical times in the order of days, possibly weeks. Secondly, the physical size of the beds will shift the main thermal mass more towards the activated carbon itself. In lab-scale the container itself may in several cases have significantly more thermal mass than the carbon. Incidentally, this simplifies the numerical simulations since the inclusion of support systems, such as the containing geometry, loses significance [15].

2.1 Packed beds for gas cleaning

The concept of using packed beds of activated carbon to remove substances from a stream is based on the fact that the targeted substance adsorbs to the activated carbon. If that is not the case, the beds cannot remove it. Adsorption is the phenomenon where molecules, the adsorbate, attach, or adhere, to a solid surface, the adsorbent [19]. In the case of benzene removal, benzene molecules adhere to the surface of the activated carbon. Adsorption is a consequence of surface energy, and the fact that the adsorbate is in a lower energy state when attached to the adsorbent [19]. This means that adsorption is an exothermic process and will release heat. The reverse process, desorption, where molecules are moved from the surface back to the fluid or gas phase again, is thus endothermic.

Adsorption is not a process that continues indefinitely. To describe the basics of the

process it is convenient to introduce the concept of adsorption sites [12]. A site is a place where a molecule can attach and it is a feature of the microscopic surface properties of the adsorbent. This also means that there are different sizes and strengths of sites, making it so that molecules of different sizes might stick to different sites, and there are only a finite number of these sites available [12]. In addition, there are several different interactions between molecules and sites, e.g. molecules can stack on each other [20]. The fundamental restriction of a finite amount of locations for molecules to stick to is, in the end, limiting. When there are no more sites available, the adsorbent is saturated and, for the conditions, equilibrium is achieved.

However, whether a molecule actually sticks to a site is not only a function of the type of the molecule and site, it is also a function of the amount of molecules in the surrounding fluid that are eligible and the energy of those molecules [19]. In macroscopic terms, that would correspond to the concentration and temperature in the fluid. A higher concentration of adsorbates in the fluid leads to more adsorbed substance and a higher temperature leads to the opposite, a lower amount of adsorbed substance.

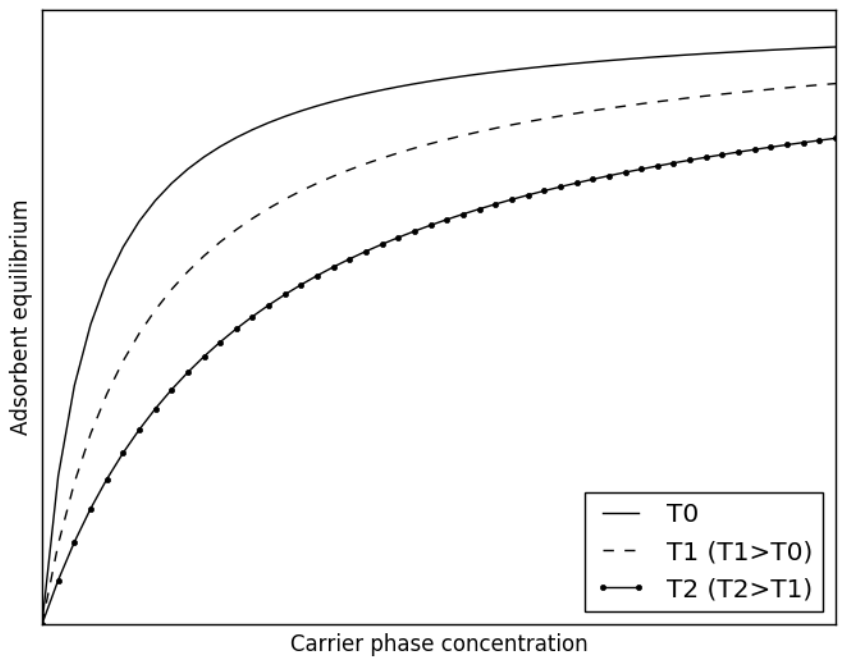

Figure 2.1: *Example of adsorption isotherms for three temperatures T0 < T1 < T2.*

The equilibrium between the amount of substance adsorbed to the adsorbent and the amount in the carrier phase is, as mentioned, a function of both carrier phase concentration and temperature. This relation is normally described by adsorption isotherms [21] where each isotherm describes the equilibrium, for that given temperature, between the concentration in the carrier phase and the amount of substance on the adsorbent (Figure 2.1 is an example of such isotherms). Such isotherms are used in the simulations as they describe the driving force for the adsorption, or desorption, of the adsorbate.

The ability to use activated carbon for the removal of a substance from a stream, in industrial applications, is heavily dependent on the ability to remove the adsorbed substance from the adsorbent [22]. Otherwise, any activated carbon would have to be replaced after saturation occurred. That might be fine in consumer goods, such as breathing masks, however for industrial use it is not feasible. The industrial process of desorbing a substance from the adsorbent is what is referred to as regeneration of the adsorbent. It is mostly done in one out of two ways. Either through increasing the temperature of the bed while simultaneously flushing it with a purge gas, often referred to as temperature-swing adsorption (TSA). Or, through decreasing the pressure in the bed, often referred to as pressure-swing adsorption (PSA). By doing either, the equilibrium shifts so that the adsorbed substance desorbs from the adsorbent and is released into the purge gas, which transports the substance out of the beds.

2.2 Model choices

Due to the complex multi-scale and multi-physics nature of system, the modeling choices naturally include assumptions around what are and are not important phenomena to include. The choices done here are based on, what seems to be, the most accepted model choices. Initially, the choices also align with the design considerations for GoBiGas.

First, there are some general assumptions around the flow and the bed. More specifically, any radial or tangential variations are assumed to be small in comparison to the main direction, thus the transport is only solved for the axial direction. The bed is also considered to be homogeneously packed, thus it can be characterized by a single scalar porosity. This corresponds well with efforts done in the industrial beds, where care is also taken to ensure that the flow through the bed is as homogeneous as possible in the two off-directions. Inert particles are spread below and above the activated carbon to disperse any flow heterogeneity and the activated carbon is itself raked to level.

Besides the flow assumption, some assumptions are also made with regards to the active species in the model, where the major ones include a restriction of the gas composition, the fact that the species do not interact (e.g. no competitive adsorption), no homogeneous reactions and there is no diffusive gas transport. The rationales for these assumptions vary slightly, there are by experience limited effects of homogeneous reactions in the bed for example. However, the restriction in the modeled gas composition is a modeling choice

that for the results and papers presented is limited to only include benzene. The reason is that benzene is the targeted substance to be removed and the substance for which the beds are designed for. However, as presented in Paper B, the scope of the included species will be increased in future work, thus making the exact number of included species somewhat arbitrary and a judgement call. The exclusion of the diffusive term is due to the dominant source terms in the equations, representing the adsorption/desorption phenomena. These phenomena completely dominate the dynamics of the bed, where substance will be transported by the gas to an adsorption front and there adsorb abruptly thus effectively limiting the effect of diffusion, see Paper A.

The last subject area for the assumptions is about the steam and condensed water. It is assumed that steam does not adsorb to the activated carbon but only condenses. The condensed water will then stay condensed at the same location or be evaporated again, it will however not flow anywhere. These assumptions are currently more of a necessity to be able to model the system at all [23], rather than expectations that adsorption of steam or water movement is completely negligible. It is known that steam will adsorb to the carbon and it is also known that it might affect the isotherm for the other species [24]. However, the extent and influence of the interaction between steam and the other species are not well established, making it difficult to find appropriate models. It is, for GoBiGas, also known that some of the condensed water flows out of the bed. However, calculations of the theoretical water content of the carbon, if all water is absorbed (i.e. the process of liquid water penetrating into the carbon particles) by the carbon, show that the carbon is more than capable of simply absorbing all of the condensed water. This all makes predictions of the actual amount of liquid water drainage troublesome and the assumption that no water drains out of the bed is then a more conservative option.

2.3 Governing equations

Taking the assumptions and model choices into consideration, the equations that model the system are gas continuity, energy conservation for the bed and gas and transport of substances in the gas and to the bed.

The gas phase total continuity is described by,

$$\frac{\partial \varepsilon \rho_g}{\partial t} + \frac{\partial \rho_g u}{\partial x} = \sum \frac{\partial \rho_b q_x}{\partial t} \tag{2.1}$$

where ε is the bed porosity (-), ρ_g the gas phase density (kg/m^3), u the linear gas velocity (m/s), ρ_b the bed density (kg/m^3) and q_x the mass fraction of a species x in the bed (-).

Mass transport in the gas phase for species x is described by,

$$\frac{\partial \varepsilon \rho_g \omega_x}{\partial t} + \frac{\partial}{\partial x}\left(\rho_g u \omega_x\right) = \frac{\partial}{\partial t}\left(\rho_b q_x\right) \tag{2.2}$$

where ω_x is the mass fraction of species x in gas phase (-) and the source term on the right-hand side represents the transport to, or from, the bed.

Mass transport processes to, or from, the bed are described by the conventional linear driving force (LDF) model [15, 25, 18, 26] as,

$$\frac{\partial}{\partial t}\left(\rho_b q_x\right) = ak\left(c_{x,eq} - \rho_g \omega_x\right) \tag{2.3}$$

where a is the specific surface area of the carbon ($\mathrm{m}^2/\mathrm{m}^3$), k is the mass transfer rate (m/s), and $c_{x,eq}$ is the equilibrium concentration (kg/m^3).

The temperature in the gas phase is obtained from the energy balance,

$$\frac{\partial}{\partial t}\left(\varepsilon \rho_g C_{p,g} T_g\right) + \frac{\partial}{\partial x}\left(\rho_g u C_{p,g} T_g\right) = ah\left(T_b - T_g\right) \tag{2.4}$$

while the solid phase energy balance is,

$$\frac{\partial}{\partial t}\left(\rho_b C_{p,b} T_b\right) = -ah\left(T_b - T_g\right) + \sum\left(\Delta H_x \frac{\partial}{\partial t}\left(\rho_b q_x\right)\right) \tag{2.5}$$

where $C_{p,g}$ and $C_{p,b}$ is the specific heat capacity for the gas mixture and solid phase respectively (J/kg,K). T_g and T_b are the gas and bed temperature respectively (K) and h is convective heat transfer coefficient (W/m,K). ΔH_x is the heat release associated with the mass transport to/from the bed (J/kg).

2.4 Numerical discretization and implementation details

To solve the governing equations the finite volume method (FVM) is used. It is a versatile and inherently conservative method, suitable for solving conservation equations [27]. It also allows for easy manipulation of the solved equation in terms of what terms that are included, e.g. it is rather straightforward to include any dispersion effects or additional sources of heat. These properties are important due to the initial uncertainty of exactly what is required to include in order to satisfactorily simulate the industrial conditions.

The FVM reformulates terms in the governing equations into a discrete numerical approximation. Depending on the exact way this is done, the numerical system will have different properties. Since the transport in the gas phase, through the bed, is solely based on advection, the method of discretizing the advective term is important. However, the simplest and possibly most common method for discretizing the term, the upwind scheme, is notoriously diffusive (Paper A). Since the dominating physical phenomena in a bed happen in a rather sharp front, false diffusivity is a problem. For that reason, several other, higher-order, schemes were tested in Paper A where the ULTIMATE QUICKEST

[28] scheme was eventually selected as an appropriate advective scheme.

The code for simulating the system is written in C++ with a fully object-oriented layout. Since the project aims at understanding what is required to satisfactorily simulate industrial conditions, there is a need for a setup which allows full and accessible flexibility of the number of equations, variables and terms included in the system. In the same time, it is important that the code performs well enough to simulate the several days of physical time required for capturing the cycles. The code was therefore written to, potentially, simulate an arbitrary amount of equations in a coupled system.

2.5 The GoBiGas beds

GoBiGas uses a regeneration scheme which may be categorized as a TSA setup where steam is used as the regeneration agent. Utilizing steam is, for an industry like GoBiGas, convenient since it is readily available.

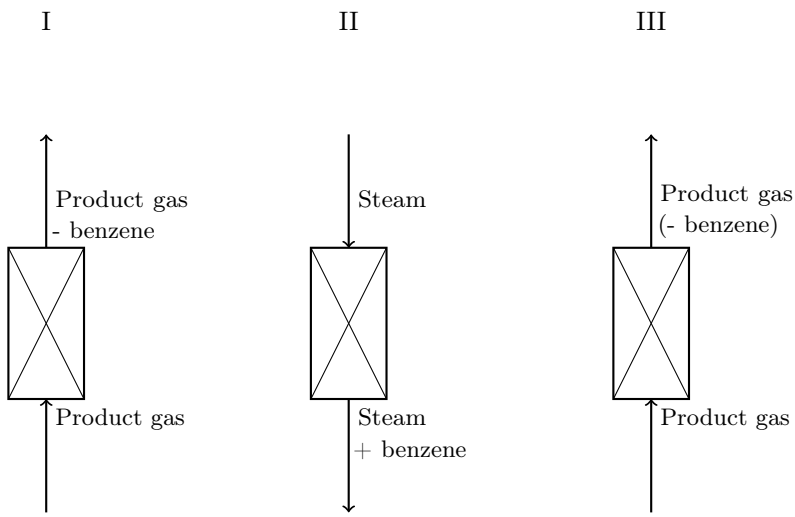

Figure 2.2: *Illustration of the three stages a bed undergoes during a cycle. I) An active stage, II) a regeneration stage and III) a cooling stage.*

The specific operation procedure for GoBiGas was that any bed operated as a bulk removal bed would go through three different stages (Figure 2.2): I) An active stage, where the product gas entered the bed from the bottom and flowed upwards. During this stage the bed removed the targeted species from the product gas. II) Thereafter a regeneration stage, where the steam entered the bed from the top and moved downwards. During this stage, the adsorbed substance desorbed from the bed and was transported out of it. III) Finally a cooling stage, where the bed was cooled with product gas that entered from the

bottom of the bed and flowed upwards.

The beds were all fitted with temperature sensors in order to better be able to monitor the beds online. These sensor readings are the only industrial data from GoBiGas that is available from within the beds. However, it is significantly more detailed data than, the more common, inlet and outlet measurements. From the temperature readings, the information about the state of a bed can be deduced, together with the information about where exo- or endo-thermic processes take place. Most of the important processes in gas cleaning are in fact exo- or endo-thermic so that the temperature profiles acquired show a relatively complete image, even though exact influences from the different phenomena might be difficult to conclude. However, this is invaluable information when attempting to determine the predictability of numerical models.

Chapter 3
Results

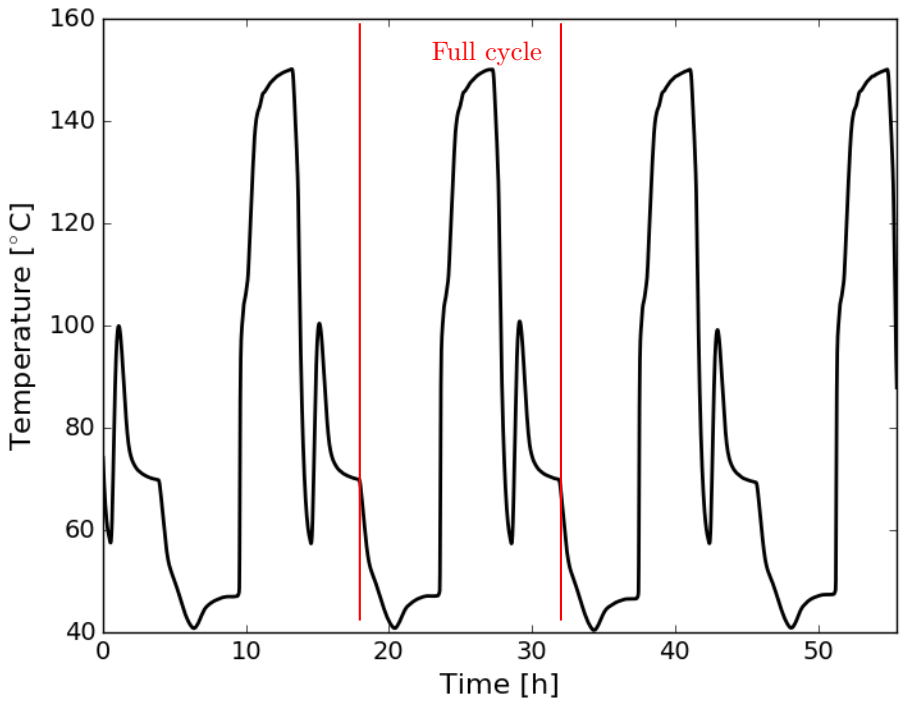

Figure 3.1: *Example of temperature signal of several cycles during industrial temperature-swing adsorption cycling.*

Figure 3.1 is an example of how the temperature varies at a position in a bed during continuous operation. However, since the operational conditions are relatively steady it is sufficient to compare a single cycle. Therefore, the data for both the simulations and industrial measurements are presented (Figure 3.2 and Figure 3.3) for a single, representative cycle. The first part in the figures is the active stage (up to ca. 300 min). The middle part of the figures is the regeneration stage and it is between ca. 300 min to ca. 580 min into the cycle. The final part of the figures is the cooling part. However, the industrial data includes two periods where the beds are passive and no flow goes trough them; a short break between the active and regeneration stage and a longer passive period after the cooling stage. Since no flow goes through the bed during these

periods, and no diffusive terms are included in the models, these periods are not simulated.

3.1 Results from the simulations

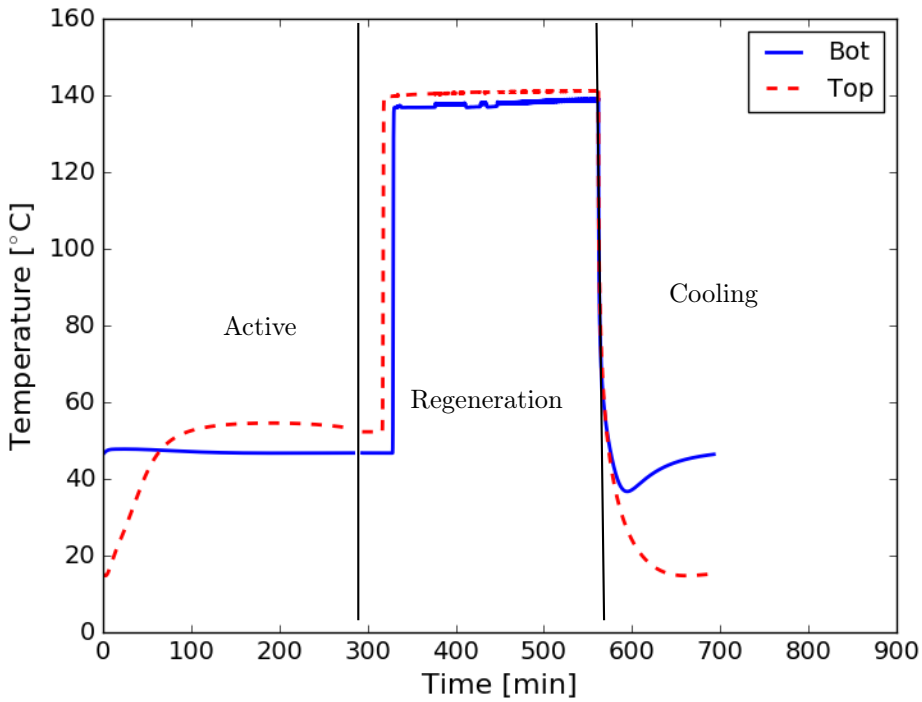

Figure 3.2: *Temperature signals for two positions in the bed of a simulated cycle. Bot is the bottom-most sensor position in the bed and Top is the top-most position.*

Figure 3.2 shows the simulated cycle and the temperature profile for the bottom-most and top-most sensor positions in the bed. The active stage is mostly dominated by three things: the inlet temperature, the temperature from the cooling stage of the previous cycle and the adsorption in the bed. The adsorption, or the heat release associated with it, can be seen in the difference of temperatures between the two positions (denoted *Bot* and *Top*). The increased temperature at the top is a result of the heat release due to the adsorption of benzene in the bed.

During the regeneration stage the temperature quickly goes up to, at least, saturation

temperature of the steam. Since the steam is slightly overheated, the top profile gets even higher than saturation. This is due to the highly effective heat transfer of steam condensing to liquid water. Due to this, there is in the beginning of the stage a steam front moving through the bed. At the front, steam condenses and heats the bed to saturation temperature. The delay between the temperature increase in the two positions is a consequence of the front moving through the bed. There is, similar to the active stage, also a temperature effect due to the presence of benzene in the bed. The difference between the top and bottom position for the majority of the stage is an effect of the energy required for desorption.

During the cooling stage, the temperature quickly reduces again in the bed. During this stage there are mainly three temperature effects. Firstly, the inlet flow temperature which will drive the bed temperature towards the inlet temperature. Secondly, as the condensed water evaporates it also cools the bed. Thirdly, the benzene in the gas starts to adsorb to the newly regenerated bed material, thus heating it up again. As seen in Figure 3.2, the bottom position reaches the inlet temperature, after a brief dip below it, by the end of the stage. However, the top position displays a substantially lower temperature during most of the stage. As mentioned, the only mechanism that may lower the temperature below the inlet temperature is the evaporation of condensed water. The assumption that no water drains out of the bed means that all condensed water eventually evaporates. And, as seen, the evaporation has a dominating effect on the bed for the entire stage.

3.2 Results from the industrial data

Generally, the temperature profiles from GoBiGas exhibit more dynamical behaviour compared to those of the simulated data set. That in itself is expected due to the presence of other substances that interact with the carbon, however the impact the other substances have on the thermal behaviour of the bed is substantial compared with the impact of the species that the bed is to remove, that is benzene.

The impact of the full gas complexity of the industrial data set can be seen affecting the thermal profiles during all stages, most notably though in the regeneration and cooling stages. In the cooling stage, there is a sharp temperature peak that is not visible at all in the simulated data. In the simulated data set, the temperature rapidly drops, even below the inlet temperature and there is a large difference in temperature between the top and bottom positions. The difference is similar in the industrial data set, only shifted to higher temperature. The only process that can heat the bed at this point is adsorption so there must be a substantial adsorption of the gas components to the carbon, releasing many times more heat than that of benzene adsorption alone.

This additional adsorption also manifests in the regeneration stage. Since more substance is adsorbed to the carbon, also more is desorbed during the regeneration. This, in turn, requires more heat during the regeneration stage, thus the halt in temperature increase

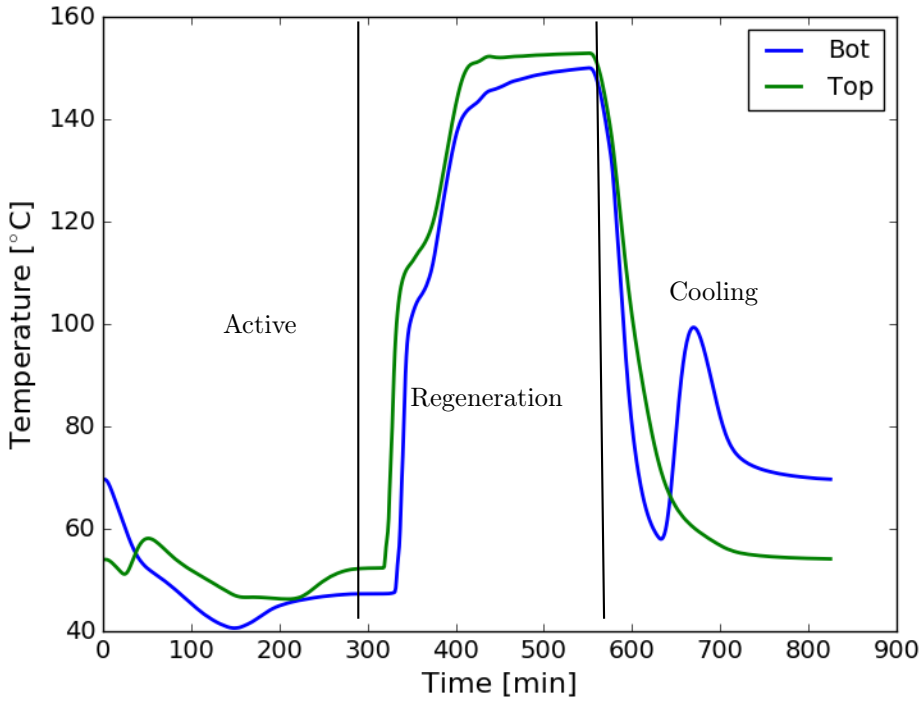

Figure 3.3: *Temperature signals for different bed positions of an average cycle during industrial temperature-swing adsorption cycling. Bot is the bottom-most sensor position in the bed and Top is the top-most position.*

during the initial period of the regeneration stage.

The only major difference between the simulated and industrial data set that cannot be explained by the presence of other active species in the product gas is the dip in temperature during the active stage. As mentioned earlier, the only process that cools the bed during this stage is evaporation of condensed water. Thus, in the industrial data there must be significant evaporation happening during a majority of the active stage. This was not seen in the simulations, where a majority of the condensed water had already evaporated back into the gas stream during the cooling stage.

Chapter 4
Conclusions

The aim of this work was to establish how well common modeling methods and choices represent real world industrial conditions of a packed bed adsorber. The industrial data comes from the biomass gasification plant of GoBiGas which uses a TSA setup for benzene removal.

While the simulation accurately captures the main characteristics of the temperature signals observed in a bed, there are dynamics in the industrial data that are not captured. The main reasons for this is that too few of the species in the product gas composition are included in the simulations. Most of the discrepancies between the simulation and the industrial data may be explained by adsorption and desorption of additional species, besides benzene. Inclusion of more substances in the simulation would allow a more dynamic temperature signal and it would also likely better reproduce the industrial data. Accurately capturing and tracking the species in the product gas are both very challenging for real-world processes and at the same time of limited interest. Instead, to still take the product gas composition into account a lumped species approach could prove valuable. In such an approach, the product gas mixture is represented as a single average species with benefits both with regards to computational effort, as well as to keeping the focus of the simulation on the targeted species.

Besides that additional species have to be taken into consideration to better predict the dynamics of the bed, improved models are required with regards to the condensed water, both with respect to water drainage and transport rate to and from the gaseous phase. It is seen that the evaporation rates are too fast in the simulation compared to the industrial data. This fact, together with the observed water drainage in the GoBiGas plant, suggests that more research on the topic is needed.

Chapter 5
Future work

As hinted in the conclusions, additional work on including more species into the simulations is required. The additional species, together with improved model for the condensed water will improve the model accuracy to better capture real-world data. However, the strength of numerical modeling lies beyond just capturing real-world data to the best ability. Therefore, future work also includes studies on regeneration schemes, which is the main operational cost for the beds. With the help of numerical models, insights into how to best regenerate the beds could be drawn with parameter studies, and other optimization schemes. This could improve future design and decision making for using a TSA setup.

Besides work on the 1D model, there is also ongoing work on comprehensive 3D modeling of packed beds. Initial simulations have been done both on the difference between liquid and gaseous transport in packed beds [6], as well as mass-transport differences between particles of different shape. Hopefully, this work can contribute to both identify better bed configurations as well as to provide insights into how to incorporate, e.g. liquid drainage.

Chapter 6
Summary of papers

6.1 Paper A

A. Jareteg, D. Maggiolo, S. Sasic, and H. Ström. Finite-volume method for industrial-scale temperature-swing adsorption simulations. *Submitted to a scientific journal* (2019)

6.1.1 Division of work

I developed the code, did the simulations and analyzed the results. I wrote the first draft, together with Henrik Ström. The other co-authors supervised the work and contributed with feedback and ideas.

6.2 Paper B

A. Jareteg, D. Maggiolo, A. Larsson, H. Thunman, S. Sasic, and H. Ström. Industrial-scale benzene adsorption: assessment of a 1D temperature-swing model against on-line industrial data. *Submitted to a scientific journal* (2019)

6.2.1 Division of work

Besides being main author, I developed the code, did the simulations and analyzed the results. The industrial data was provided by GoBiGas and the co-authors supervised the work, contributed with feedback and ideas.

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