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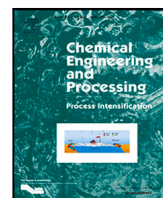
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Investigation of steam regeneration strategies for industrial-scale temperature-swing adsorption of benzene on activated carbon

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ABSTRACT

Large-scale separation of substances present at low concentrations is readily performed by adsorption in packed beds that requires recurring energy-intensive regeneration of the adsorbent. The present work uses numerical simulations previously developed for industrial-scale packed-bed benzene sorption on activated carbon with temperature-swing regeneration by steam to investigate the influence of steam properties and regeneration strategy on total energy performance and breakthrough behaviour.

It is shown that using saturated steam lowers both the steam mass and energy consumption during regeneration of a fixed amount of benzene, whereas using superheated steam returns the bed to a more fresh-like state after each regeneration stage. The most promising variation tried implies a 19% reduction in the energy consumption. Furthermore, the importance of accounting for the real industrial cycling conditions in the optimization of packed-bed adsorbers is highlighted. It is shown that the participation of different sections of the bed during adsorption varies with the regeneration strategy, but is never as localized as predicted from a model for a fresh bed without cycling. Finally, the present results also show that the effluent purity attained during regeneration increases when high-temperature saturated steam is used, e.g. a 60-degree increase in steam temperature raises the purity by 11%.

1. Introduction

The purpose of the current work is to study how to optimize a gas-cleaning process based on packed-bed adsorption using numerical simulations. Separation processes represent an important technology branch within the chemical process industry [1]. At the same time, it is currently estimated that separation processes account for about 10%–15% of process industry energy consumption [2], making efforts to optimize their energy use of very high priority. One prevailing technology, used to separate low concentrations of undesired substances from large-scale gaseous or liquid streams, is packed-bed adsorbers [3,4]. Common applications are found in air and water purification [5], solid fuel gasification [6] and the chemical industry [7], where beds packed with activated carbon have been shown to perform well in removal of volatile organic compounds (VOCs) specifically [8].

In the removal of VOCs by activated carbon beds, the contaminated stream is led through the bed and the VOCs adsorb to the carbon. However, this process eventually saturates the carbon with the VOCs, effectively preventing further separation. At that point, the carbon has to be either replaced or regenerated back to a state where it can

again adsorb the VOCs. For industrial applications, there are often incentives to regenerate the carbon rather than replace it [9] (most notably lowered running costs and the possible value of the adsorbate), and a multitude of technologies exist that facilitate saturated carbon regeneration [10].

The most common methods for regeneration are based on either elevating the temperature of the bed, called temperature-swing adsorption [10] (TSA) or elevating the pressure in the bed, called pressure-swing adsorption [11] (PSA). Both are found in industry, however, for VOC removal specifically, it is common to use a TSA approach [10,12]. This approach requires the plant to have some means of heating up the bed and flush it with a clean gas to remove the adsorbed VOCs. Both these purposes can be accomplished at the same time with steam, and since steam is often readily available in process industries, or can be retrofitted at relatively low cost, it is therefore commonly used [9].

High-quality industrial data on VOC removal by activated carbon beds are scarce, and most research has therefore been performed in lab settings [13], where it is more common to regenerate the beds with an inert gas, such as nitrogen [20]. Steam, however, has the

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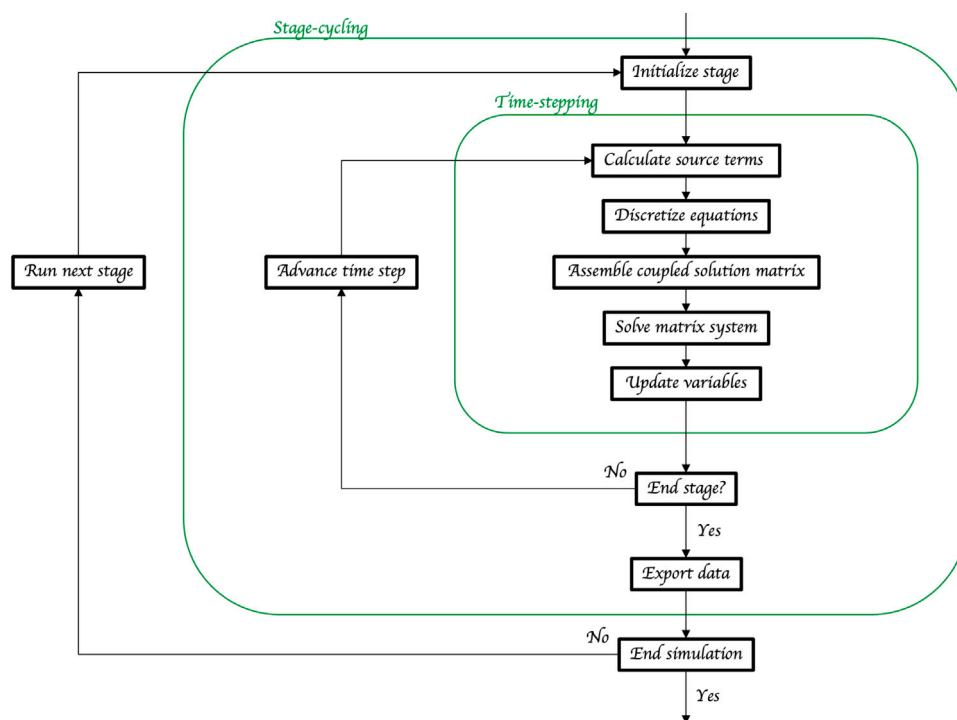


Fig. 1. Illustration of the algorithm employed by the numerical model.

Table 1

Steam temperatures for different adsorbates and the corresponding equivalent steam temperatures for benzene at the ΔT .

Reference	Substance	Steam temperature	Boiling point	ΔT	Equivalent steam temperature for benzene
Jareteg et al. [13]	Benzene	160 °C	80 °C	80 °C	160 °C
Tavan et al. [14]	Ethanol	120 °C	78 °C	42 °C	122 °C
Tavan et al. [14]	Diethyl ether	120 °C	34 °C	86 °C	166 °C
Ramalingam et al. [15]	Dichloromethane	140 °C	40 °C	100 °C	180 °C
Schweiger and LeVan [16]	<i>n</i> -hexane	127 °C	69 °C	58 °C	138 °C
Germerdonk and Wang [17]	Toluene	130 °C	110 °C	20 °C	100 °C
Gu and Bart [18]	Toluene	140 °C	110 °C	30 °C	110 °C
Pelech et al. [19]	1,2-dichloroethane	100 °C	84 °C	16 °C	96 °C
Pelech et al. [19]	1,2-dichloroethane	160 °C	84 °C	76 °C	156 °C

added complexity of possibly undergoing phase change during the regeneration, which increases the range of possible interactions with the carbon and the adsorbate, while also introducing additional mechanisms of heat transfer [18]. Several approaches of modelling steam regeneration have been proposed, with varying degrees of complexity. Among others, Schweiger and LeVan [16] used standard balance equation formulations with a Linear Driving Force (LDF) model, whereas Germerdonk and Wang [17] proposed an 11-step model, and Gu and Bart [18] proposed a model called the Double-Two-Mechanism-Model. The appropriate choice of steam model will vary depending on both the application and its uncertainties as well as the associated modelling uncertainties. Overall, the simpler models produce results in reasonably good agreement with experiments, with the exception of cases where trickling of condensate becomes important [16]. The more comprehensive models require measurements of adsorbate and water content profiles in the carbon particles during adsorption and desorption along the height of the bed [17], information which is not readily accessible in industrial systems. In our previous work [13], we successfully used an LDF-approach to describe the main characteristics of an industrial TSA system.

Besides the model description for the steam regeneration, the cyclic process operation is also an important factor to consider. Scaemhorn [21] discussed the importance of the initial bed state in determining the outcome of a single cycle, while several later works

have covered cycling for longer times [22,23]. Our previous research has also shown the importance of adequately simulating the correct cycling (adsorption–desorption) protocol in assessments of industrial performance [13,24]. More specifically, conclusions reached by analyses or simulations on loading and regeneration of fresh beds may not at all reflect the internal states of the beds correctly in the industrial setting, and thus lead to erroneous conclusions with regard to energy performance. Furthermore, the many available design options for a TSA process imply that there is potential for optimization [12]. There is therefore a need to investigate energy optimization performance of various regeneration strategies at the relevant industrial scales and using industrial cycling protocols.

When designing packed-bed steam regeneration systems, not only the energy requirements for heating the bed material and the desorption of the VOCs need to be considered, but also the conditions at which the energy is provided [21]. It must be established whether or not the steam is to be superheated or saturated, and at which conditions it is to be provided. These decisions depend on the complex behaviour of the full system upon cycling. The rules for determining the duration of the adsorption and the desorption stages must also be chosen. The purpose of the current work is to shed light on these design choices from an energy optimization point of view, by performing numerical simulations of different cycling protocols at varying steam conditions. As a basis for this analysis we use a previously developed and validated

numerical simulation model [13]. The main contribution of the present work is thus an in-depth analysis of TSA performance with respect to energy efficiency and effluent purity, performed at realistic industrial length and time scales and embodying the full complexity of steam condensation and evaporation.

Two different regeneration schemes (i.e. set of rules for determining the onset and duration of the regeneration stage) will be evaluated for a variety of steam conditions. The first set will span the spectrum of relevant temperature conditions for low-temperature steaming, chosen so as to represent industrially relevant conditions [6,9] and with intermediate points to capture trends. This analysis is focused on the effect of the chosen steaming conditions on the energy efficiency. The second set is selected as a subset from the first, to investigate the effect on breakthrough performance. The work concludes with a summary of the benefits and drawbacks of the various regeneration strategies tested.

2. Methodology

2.1. Model and numerics

The packed bed is modelled using our previously developed baseline one-dimensional model for temperature-swing adsorption at industrial scale [13]. This model describes a single species (benzene) that is alternately loaded and removed from an activated carbon bed in a cyclic operation. The benzene adsorbs to the bed during the loading stage, where benzene is streamed through the bed together with a carrier gas that does not react with the bed material. Benzene is thus removed from the stream. After a certain amount of time, the loading stage is aborted and the regeneration stage commences. In this stage, pure steam is introduced at the other end of the bed and streamed through in a counter-current fashion. This elevates the temperature in the bed, causing the adsorbed benzene to desorb from the bed material, and flushes the bed with clean gas. After a certain amount of time the regeneration is halted and a new loading stage begins. These cycles are repeated until the so-called cyclic steady state has been attained, i.e. when each new loading/regeneration stage pair is predicted to be the same as the previous one.

To model the operation of the bed, the governing conservation equations are solved in time and space. This involves solving for mass conservation of benzene and water (in both the gas and the bed) and energy conservation (in both the gas and the bed), together with gas continuity. Several assumptions also have to be made in order to incorporate enough of the relevant physical phenomena while still having a tractable and reliable model. The major assumptions are as follows: The solid- and fluid conservation equations are only resolved in the axial direction of the bed, axial dispersion is neglected, and the steam does not adsorb to the carbon but only undergoes a phase change (local condensation or evaporation). In our previous work [13], a thorough discussion is presented together with a comparison against industrial data.

Under these assumptions, the gas phase conservation equation is written as:

$$\frac{\partial \epsilon \rho_g}{\partial t} + \frac{\partial \rho_g u}{\partial x} = \sum \frac{\partial \rho_b q_x}{\partial t} \quad (1)$$

where ϵ is the bed porosity (–), ρ_g the gas phase density (kg/m³), u the linear gas velocity (m/s), ρ_b the bed density (kg/m³) and q_x the mass fraction of a species x (benzene or steam/water) in the bed (–).

Mass transport in the gas phase for species x is written as:

$$\frac{\partial \epsilon \rho_g \omega_x}{\partial t} + \frac{\partial}{\partial x} (\rho_g u \omega_x) = \frac{\partial}{\partial t} (\rho_b q_x) \quad (2)$$

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 [15,20,25,26] as:

$$\frac{\partial}{\partial t} (\rho_b q_x) = ak (c_{x,eq} - \rho_g \omega_x) \quad (3)$$

where a is the specific surface area of the carbon (m²/m³), k is the mass transfer rate (m/s), and $c_{x,eq}$ is the equilibrium concentration (kg/m³). The microstructure of the pellets in the investigated system has not been characterized in depth, but must be expected to vary in a wide range over time and from pellet to pellet. The LDF approach does not describe intraparticle surface diffusion within the microporous network, which a more advanced model could possibly be do. However, a directed experiment of a more well-defined system would have been necessary to motivate a more elaborate modelling approach in this respect. Such endeavours are beyond the scope of the current work. Moreover, the LDF model has been shown to work well in practice due to that a complete model of an adsorption process necessarily entails averaging on several levels (particle level, column level and cyclic steady-state level) [27]. The equilibrium concentration is determined from either solid phase load (benzene) or saturation condition (steam/water).

The energy balance for the gas phase is:

$$\frac{\partial}{\partial t} (\epsilon \rho_g C_{p,g} T_g) + \frac{\partial}{\partial x} (\rho_g u C_{p,g} T_g) = ah (T_b - T_g) \quad (4)$$

while the solid phase energy balance is:

$$\frac{\partial}{\partial t} (\rho_b C_{p,b} T_b) = -ah (T_b - T_g) + \sum_x \left(\Delta H_x \frac{\partial}{\partial t} (\rho_b q_x) \right) \quad (5)$$

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), i.e. the heat of adsorption for benzene and the heat of evaporation for steam/water. The material properties used are compiled in Jareteg et al. [13] and have been found to be in good agreement with typical property data in the literature [28,29].

The conservation equations are solved with a finite-volume method, coupled semi-implicit solver written in C++ with a sparse matrix solver from the Eigen package. The advection terms in the mass and energy transport equations in the gas phase are discretized with a high-order scheme for better interface capturing. A previous work discusses the importance of this numerical discretization in cyclic simulations of packed beds [24]. Comprehensive model verification and validation against experimental data on breakthrough performance, adsorption and industrial cycling is available in Jareteg et al. [13] (with supporting information). An overview of the computational algorithm is provided in Fig. 1.

2.2. Case setup

The cases studied in the current work are carefully chosen to represent industrially relevant operating conditions. We have previously made available unique industrial data from a 32 MW biomass gasification plant in Gothenburg, Sweden [13], where benzene was the main VOC to be removed. In this process, the regeneration was performed at a steam temperature of 160 °C. According to Shah et al. [9], it is typical to regenerate with steam at 30 – 50 °C above the VOC boiling point. Following this rule-of-thumb would point to a steam temperature in the interval 110 – 130 °C as reasonable for a benzene-removal application. However, the process for which we have most data used a somewhat higher temperature (80 °C above the boiling point of benzene).

Data from other industrial steam regeneration schemes are difficult to find in the open literature. Tavan et al. [14] published an industrial regeneration scheme that was operated at 120 °C, but for other adsorbates (ethanol and diethyl ether). Several other works on steam regeneration can be found if the criterion that the data must

Table 2

Boundary conditions for regeneration for Set 1, specific to each case.

Case	Baseline	30SH	60SH	90SH	180SH	30SAT	60SAT
Velocity [m/s]	0.0113	0.0123	0.0132	0.0142	0.0170	0.0113	0.0113
Temperature [°C]	100	130	160	190	280	130	160

Table 3

Boundary conditions for regeneration for Set 2, specific to each case.

Case	Baseline	60SH	60SAT
Velocity [m/s]	0.0563	0.0625	0.0112
Temperature [°C]	100	160	160

Table 4

Boundary conditions common for all cases.

	Active stage	Regeneration stage
Temperature	60 °C	–
Velocity	0.2925 m/s	–
Concentration benzene	10 g/m ³	0
Carrier gas	Ideal gas (Air)	Steam

Table 5

Bed data.

Bed radius	1.375 m
Bed length	1.9425
Bed porosity	0.5
Characteristic particle size d_p	6 mm
Carbon type	WS-490, Chemivron
Total mass of carbon	4500 kg

be from an industrial setting is relaxed. Table 1 summarizes steam regeneration temperatures along with the corresponding equivalent steam temperatures for benzene. The latter are deduced by calculating the steam temperature that results from adding the same ΔT as for the VOC in question to the boiling point of benzene. This overview results in an interval of 96 – 180 °C with a mean of 136 °C, slightly higher than that prescribed by the rule-of-thumb discussed earlier [9] but at the same time a bit lower than that used in the best available industrial data [13].

The steam temperatures investigated in this study are based on the aforementioned works and they span from 100 °C to 160 °C at saturated conditions. A majority of the energy provided from the steam to the desorption is due to the phase change to water, which takes place at saturation conditions and makes it important to include saturated conditions in the entire temperature span. However, the effect of super-heated steam is also important [21], and therefore some cases are super-heated beyond 160 °C (the highest temperature being 280 °C). This case design enables us to study of how the sensible heat that the super-heated steam provides affects the regeneration. The full range of temperatures investigated is given in Tables 2 and 3.

We thus arrive at two sets of 10 different cases in total to investigate all relevant regeneration modes. The focus is on industrial performance during realistic cycling of the bed, and the simulations are performed in the following way: First, an input step of benzene is allowed to travel halfway into the bed (to emulate a reasonable starting point), after which a first active stage begins, followed by a regeneration stage. The active stage and the regeneration stage are then cycled for 10 times, so that the bed attains the cyclic steady state. All the data presented are extracted from either the last active stage or the last regeneration stage, depending on what is analysed. Table 4 shows the shared boundary conditions for all the cases and Table 5 shows the relevant bed properties. The baseline case is inspired by our previous works on benzene removal in gas cleaning after biomass gasification [13,24].

The first set of simulations is performed as illustrated conceptually in Fig. 2. A fixed mass of substance that should be adsorbed and desorbed during each stage is pre-specified, and when this amount has

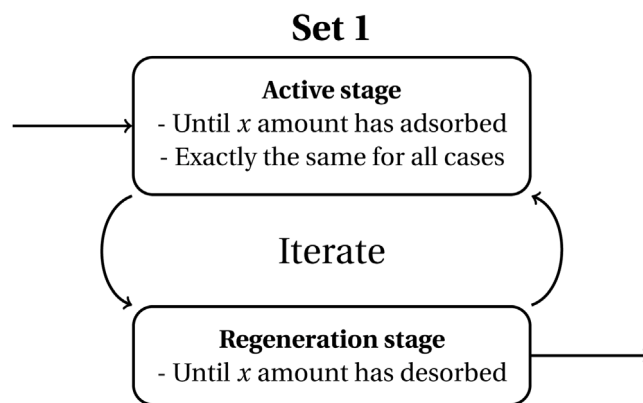


Fig. 2. Conceptual illustration of the regeneration strategy investigated in the simulations included in Set 1. The steam properties during the regeneration stage are varied between the cases in the set.

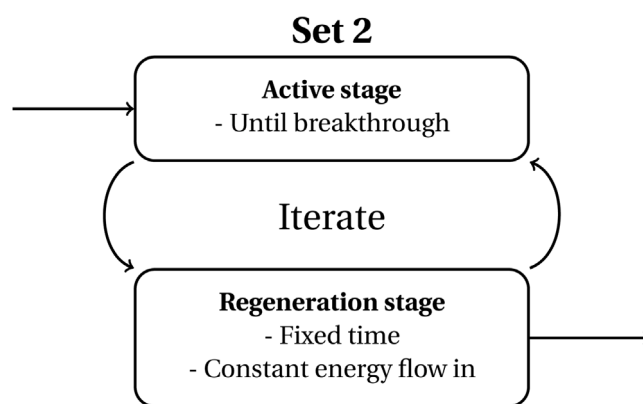


Fig. 3. Conceptual illustration of the regeneration strategy investigated in the simulations included in Set 2. The steam properties during the regeneration stage are varied between the cases in the set.

been transferred to/from the bed the current stage is aborted and the following stage is begun. Seven cases, all with constant mass flow rate of steam, are simulated: one baseline case, four cases where the steam is superheated to different degrees, and two cases where the steam is at a saturated state (elevated pressure in the bed). The boundary conditions in the regeneration stage for these different cases are presented in Table 2.

The second simulation set is performed as illustrated in Fig. 3. In these simulations, a fixed amount of energy is pre-specified, so that all regeneration stages are run with the same amount of energy. The energy considered is the heat of vaporization together with any sensible heat above the vaporization temperature. The rationale behind this approach is that, during the regeneration stage, the beds rapidly heat up to the vaporization equilibrium temperature, and at those conditions the energy for desorption is fed from the gas stream to the bed material. The subsequent active stage is run until breakthrough is detected at the outlet. Three cases (presented in Table 3) are simulated. It is only the inlet boundary conditions for the regeneration stage that varies between cases, whereas the conditions during the active stage remain the same at all times.

3. Results and discussion

The purpose of a packed-bed adsorber system is to remove a contaminant from the stream without the risk of inadvertent breakthrough. At the same time, the investment and running costs should be minimized, implying that the beds should be used as efficiently as possible

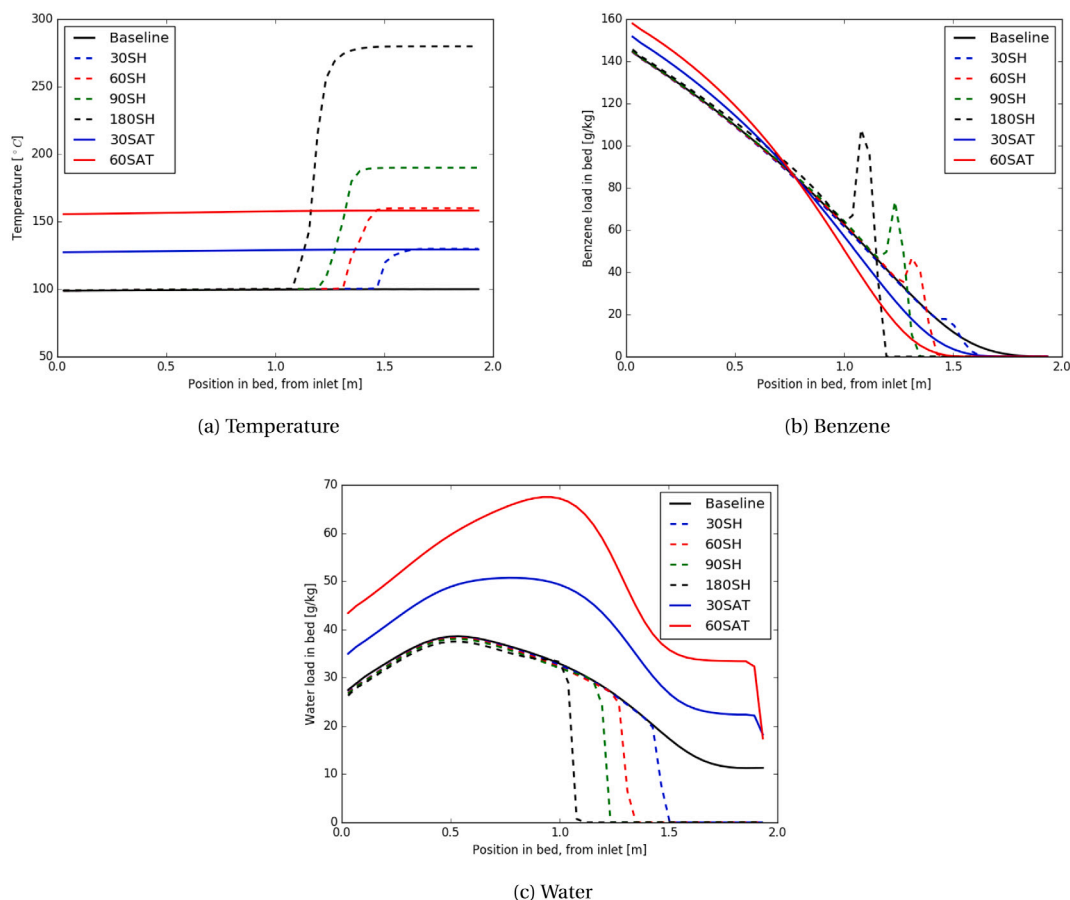


Fig. 4. Bed state by the end of the regeneration stage for the simulation cases in Set 1.

Table 6

Amount of steam required for desorbing a fixed amount of benzene from the bed. See Table 2 for case differentiation.

Case	Steam required [kg]	Steam consumption compared to <i>Baseline</i>	Energy required compared to <i>Baseline</i>
Baseline	2460	–	–
30SH	2437	–0.1%	+1.4%
60SH	2424	–1.5%	+3.0%
90SH	2413	–1.9%	+4.4%
180SH	2388	–2.9%	+8.2%
30SAT	2260	–8.1%	–11.5%
60SAT	2167	–11.9%	–18.7%

(minimization of unused installed capacity) and that the energy spent in regeneration should be kept at an absolute minimum. Here, we analyse what can be learned from the evaluation of the two different regeneration strategies (Set 1 and Set 2) for varying steam conditions.

3.1. Analysis of Set 1

3.1.1. Global performance

The first set of simulations, where a fixed amount of benzene is first adsorbed and then desorbed in each cycle, provides an opportunity to investigate the effect that the steaming mode has on the overall efficiency and the resulting internal state of the bed. Here, numerical simulations provide access to information about what happens inside the beds that is otherwise difficult to attain in an industrial setting.

Table 6 presents the amount of steam and energy required for desorbing a fixed amount of benzene from the bed in the simulations in Set 1. Most notably, it can be seen that a higher steam temperature leads to a lower steam consumption. On the other hand, if the steam is

superheated, more energy is required than if the steam is saturated at that pressure. When the steam provided is instead saturated at higher temperatures (and pressure), both the steam consumption and the total energy cost is reduced in the regeneration phase.

The increased efficiency for saturated steam with increasing temperature stems from the isotherms for sorption on the activated carbon. The larger temperature difference obtained for high-temperature steam increases the driving force for desorption during the regeneration stage. To understand why this effect is not observed for the superheated steam, the internal bed state has to be investigated in more detail.

It should be noted here that Yun et al. [20] discussed the existence of an optimal regeneration temperature for TSA systems, at which the energy requirement is the lowest. However, this temperature may be so low that the regeneration time required renders industrial cycling impossible [20], or so high that it lies outside the bounds of what is industrially feasible [30]. We also note that the optimal temperature concept does not account for regeneration with steam, where phase change plays a major role and the steam can be either saturated or superheated. It is for these reasons that we do not search for an optimum temperature, but instead seek to quantify the overall energy consumption at the given cycling conditions.

Furthermore, it is known that the adsorption kinetics plays an important role in the specific energy consumption of a TSA process [31]. The accuracy of the quantitative results obtained is therefore dependent on the model parameters used.

3.1.2. Bed state after the regeneration stage

Fig. 4 shows the bed state by the end of the regeneration stage for all the simulations in Set 1. From the temperature profiles in the bed (Fig. 4a), the cases at saturation conditions are clearly distinguishable as these show constant bed temperature throughout (corresponding

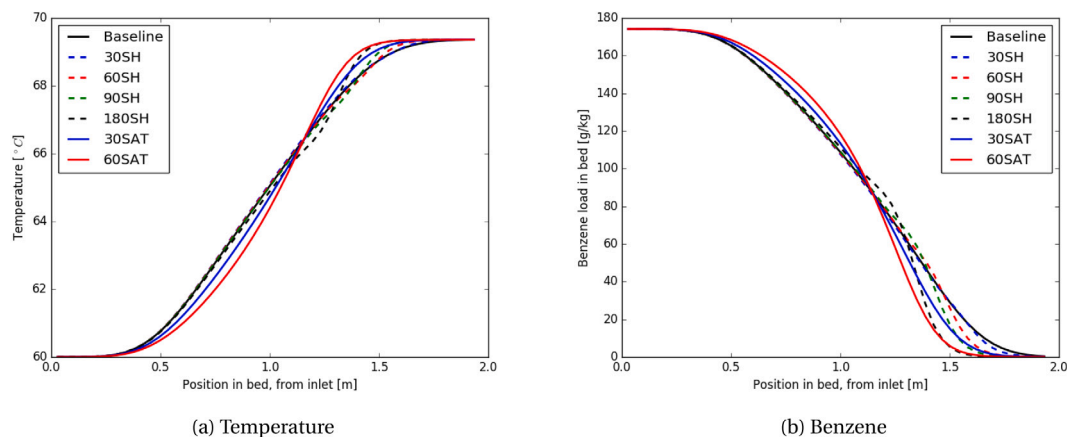


Fig. 5. Bed state by the end of the active stage for the simulation cases in Set 1.

to the saturation temperature). The superheated cases produce bed temperatures equal to the steam inlet temperatures in the region closest to the inlet (note that the regenerative flow streams from right to left), with the saturation temperature found downstream a distinct temperature front located inside the bed.

Turning to the benzene concentration in the bed (Fig. 4b), it is observed that the location of the temperature front corresponds to a local peak in the concentration of adsorbed benzene. To the right of this peak (i.e. in the region closest to the steam inlet), the benzene has desorbed completely, while after the peak all superheated cases show the same profile as the baseline case (saturated behaviour). We note that this peak in the concentration of adsorbed benzene is not found in the cases with saturated steam, where the benzene concentration is monotonically increasing with the distance from the inlet throughout the entire bed, and where the slope is sharper with increasing the temperature.

The benzene profile in the bed after regeneration is thus distinctly different in the cases with only saturated conditions, as compared to those with superheated conditions. The fact that superheated steam sharpens the front could represent a possible benefit with regards to breakthrough behaviour, as the end section of the bed has been more thoroughly regenerated and will thus adsorb new benzene more efficiently. However, as will be shown later, more research is needed to establish how to fully utilize this effect. It can also be noted that whereas the adsorption capacity may be enhanced by extending the cycle length, which would lead to a deeper regeneration of a part of the bed in the case of superheated steam, the cycle productivity would be negatively affected by such an increase of the cycle length [32].

Finally, when looking at the residual water in the bed (Fig. 4c), the only scenario where the bed is completely dry somewhere is when superheated steam is used. In these cases, the bed dries up to the desorption front and, like with the benzene profile, after the front they fall onto the curve of the baseline (saturated) case. The higher the saturation temperature, the more water content the bed will have, as it is primarily condensation of water that heats the bed and when it needs to be heated to higher temperatures, more water accumulates.

The difference in residual water between the superheated cases is a direct result of the extent of overheating. For the purpose of benzene desorption, using superheated steam to dry the bed is an unnecessary additional cost. However, it is required if temperatures above saturation conditions are desired.

3.1.3. Bed state after the active stage

Fig. 5 shows the temperature and benzene concentration profiles in the bed after the active stage (any water left after the regeneration has evaporated at this point). The pronounced differences that were observed between the cases after regeneration are found to be

Table 7

Duration of the active stage and the amount of benzene desorbed for the simulations in Set 2.

Case	Baseline	60SH	60SAT
Time in active stage [min]	154	151 (-1.9%)	182 (+18.2%)
Amount of benzene desorbed [kg]	132	129 (-2.3%)	154 (+16.7%)

significantly reduced when the active stage is completed. This homogenization is expected since the flow into the bed is identical for all cases, and the degree of homogenization will thus depend on the ratio of the cycle loading to the full loading capacity. Some minor effects from the regeneration are however still remaining, indicating that the regeneration scheme is important not only for cost-effective regeneration, but also for optimal bed performance during the active stage. It can for example be observed that higher saturation temperatures during regeneration yield a sharper front throughout the active stage, whereas higher temperatures for superheated steam yield a sharper front at the end of the bed.

Fig. 5a displays the temperature in the bed. The temperature signal is a good indication of adsorption in a packed bed, as there is no other process that causes heating of the bed [13]. This fact is important from an industrial point of view, since temperature is relatively easy to measure and could thus serve as an indicator for adsorption in the industrial setting [13]. Here, it is indicated that adsorption takes place over a smaller section of the bed for the saturated case compared to the two other cases, as observed from the steeper slope of the temperature profile. This can be interpreted as that the saturated case better restores the bed to a fresh-like state, where the adsorption front would move as a step through the bed. This conclusion is also supported by the benzene concentration profiles in Fig. 5b.

3.2. Analysis of Set 2

3.2.1. Differences in benzene loading caused by differences in regeneration

The second set of simulations is designed to assess the potential benefits with regard to breakthrough performance that different regeneration strategies might offer. The focus is here on the benzene and its movement through the bed. In Table 7, the amount of benzene desorbed, as well as the time spent in the active stage, are listed for each investigated case. Just as with the previous set of simulations, saturated conditions prove to be more efficient than superheated ones.

Fig. 6 shows the benzene profiles after the regeneration (Fig. 6a) and the active (Fig. 6b) stages, respectively. Similar to what was observed for Set 1, the sharper front in the superheated case points to an increased potential from a breakthrough perspective, as the sharper front allows the bed to adsorb more benzene before the outlet gas phase concentration reaches critical values.

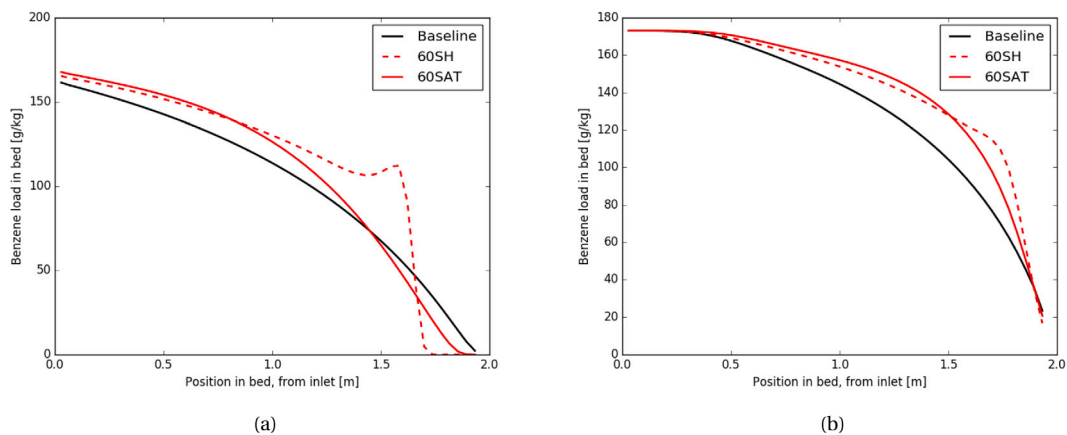


Fig. 6. Benzene concentration in the bed for the simulation cases in Set 2 at: (a) the beginning of the active stage, (b) the end of active stage.

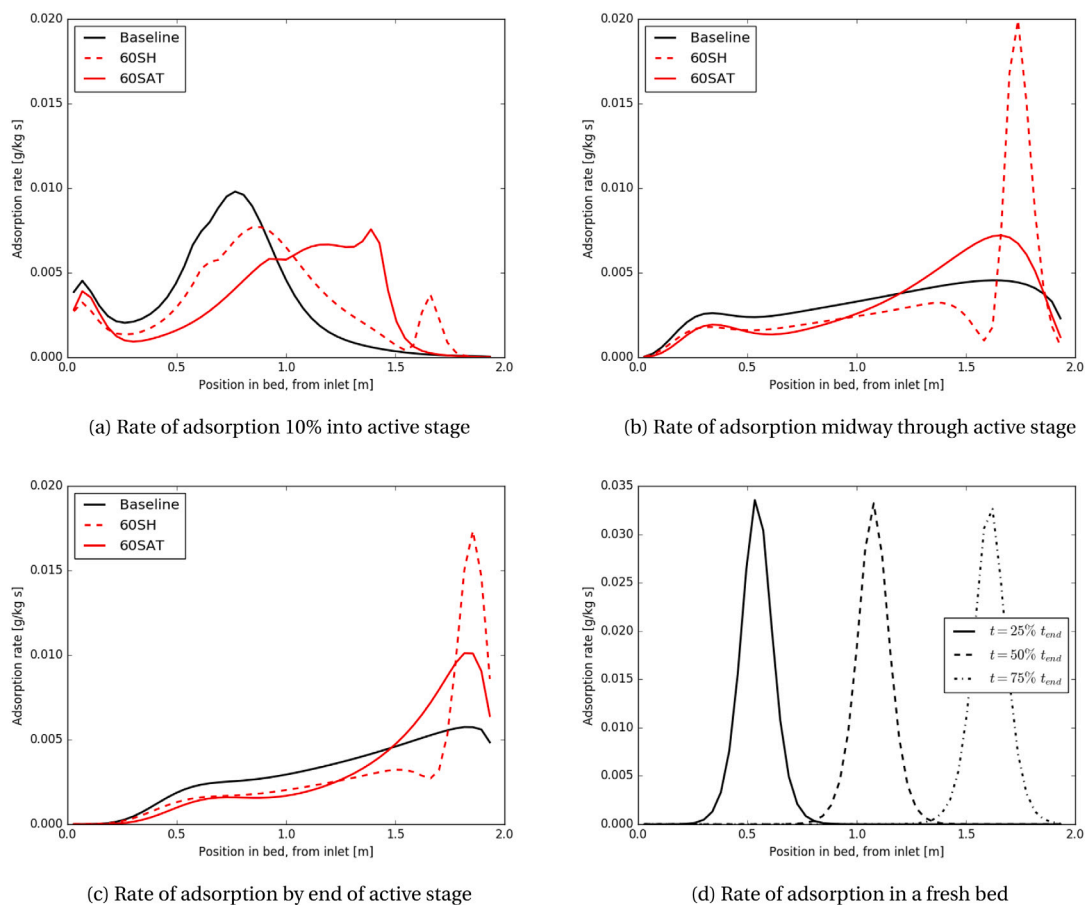


Fig. 7. Spatially resolved rates of adsorption at various times during the active stage for the simulation cases in Set 2.

3.2.2. Differences in adsorption rate caused by differences in regeneration

To highlight the differences in adsorption behaviour provoked by the different regeneration strategies, Fig. 7 compares the rates of adsorption at three different times during the active stage. Also included is a comparison to the behaviour of a fresh bed (Fig. 7d). This data represents a good example of something that would be very difficult to measure non-intrusively in an industrial setting but that is readily available from the simulations. The adsorption rate for three time snapshots is shown 10% into the stage (Fig. 7a), 50% into the stage (Fig. 7b) and at the end of the stage (Fig. 7c).

In the beginning of the stage, the adsorption front manifests as a pulse moving through the bed for all cases. At later times, it is the

section towards the end of the bed that is active in the adsorption. The behaviour of the fresh bed exhibits several differences to the behaviour of a realistic industrial bed at the cyclic steady state. In a fresh bed, the pulse shape remains the same throughout the active stage, whereas the development in panels a–c shows a much more dynamic and complex behaviour. It is also striking that a larger section of the bed is active for adsorption in a bed that is cycled. The more the bed is taken away from a pulse-like condition (the baseline case being the furthest away), the larger the section of the bed that participates in the adsorption process. This is also easily noticed at the front, where the superheated case exhibits the highest, and most fresh-like, activity.

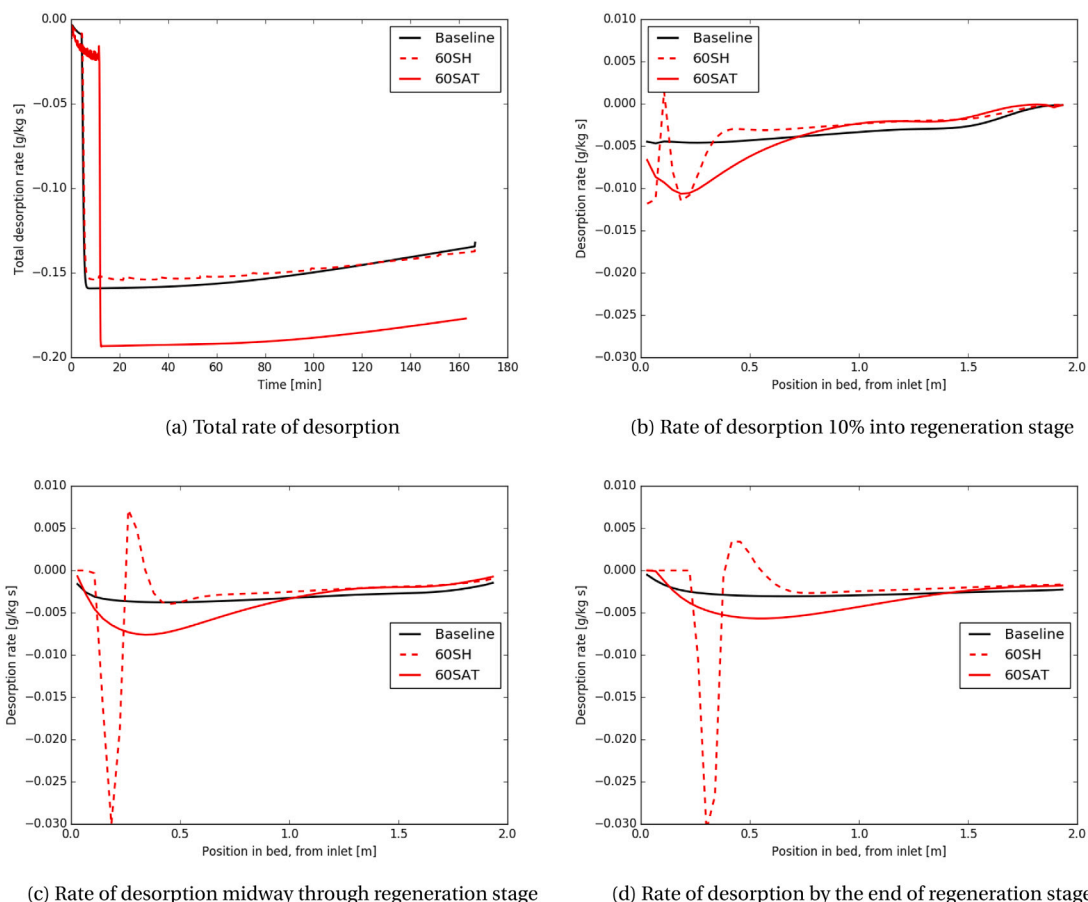


Fig. 8. Total time-resolved (a) and spatially-resolved (b–d) rates of desorption at various times during the regeneration stage for the simulation cases in Set 2.

3.2.3. Differences in desorption rate caused by differences in regeneration

Differences in the regeneration strategy do not only cause changes to the adsorption behaviour during the active stage, but also differences to the desorption behaviour during the regeneration stage itself. Fig. 8 shows the total rate of desorption in the entire bed during the regeneration stage (Fig. 8a) and the spatially resolved rates of desorption in the bed at the beginning, in the middle and at the end of the regeneration stage (Figs. 8b, 8c and 8d). From Fig. 8a, although it is seen that it takes longer before the regeneration starts for the cases with saturated steam, the regeneration is more effective once started (as also reflected in the different desorbed amounts in Table 7). The major underlying difference between saturated and superheated steam can be identified from Figs. 8c and 8d, where it is clear that the use of superheated steam leads to the formation of a region upstream the desorption front where benzene re-adsorbs to the carbon (identifiable from the positive values of the desorption rate). This effect is responsible for the local peak in the concentration curve and it can be explained by the adsorption isotherm and the presence of water. When the water dries off and the bed temperature rises to the steam temperature, more benzene is released due to that the equilibrium concentration in the bed is lowered. When the flow and bed are later cooled down due to water evaporation at saturated conditions, the equilibrium concentration is raised back up again and the now elevated gas concentrations re-adsorbs back to the bed. It is thus the drying of the bed that is the source of this loss of useful energy in the process.

3.2.4. Differences in breakthrough performance caused by differences in regeneration

One important characteristic of the behaviour of a packed-bed adsorber is the breakthrough profile (i.e. the concentration of the

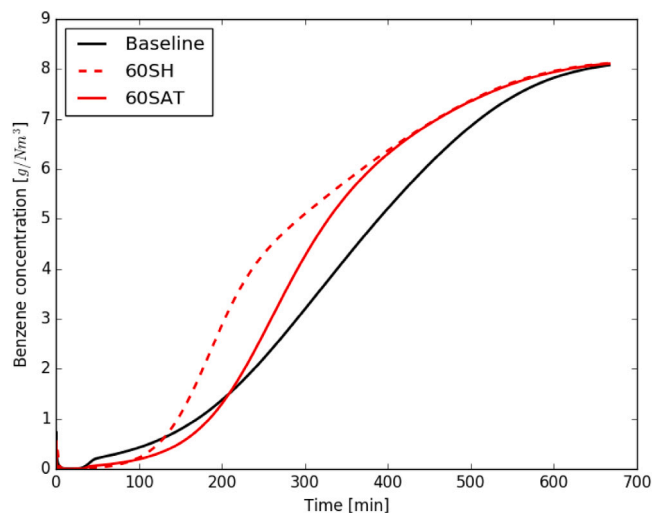


Fig. 9. Breakthrough curves (gas phase outlet concentration of benzene as a function of time) for the simulation cases in Set 2.

adsorbate at the bed outlet as a function of time). Although this profile is normally used to characterize dispersion, it is also industrially relevant to determine if there are any differences in the breakthrough behaviour between the investigated regeneration scenarios that could possibly benefit operation. Two things are relevant here: the time during which the bed maintains an outlet concentration below some threshold that is deemed acceptable, and the slope of the profile at the

Table 8

Average mass fraction of benzene on the outlet during regeneration.

Case	Baseline	60SH	60SAT
Average mass fraction [g/kg]	63.4	64.6	70.3

instance when this threshold level is surpassed (as an indicator of how severe an unintentional breakthrough would be from a process control perspective).

Fig. 9 shows the breakthrough profiles for the three cases in Set 2. As with the bed profiles, the superheated case shows the steepest initial profile, followed by the high-temperature saturated case. If a breakthrough were to happen in an industrial setting, it would be beneficial to have as long time to react as possible. From the figure, it is clear that the low-temperature saturated baseline case produces a slower breakthrough for the first half, the important one, of the breakthrough process. It is important to note here that the simulation method inherently contains numerical diffusion, which leads to uncertainties in the very beginning and end of the breakthrough curves [24].

Finally, we also investigate the purity of the effluent stream during the regeneration stage, as shown in Table 8. The purity is simply a measure of the outlet benzene concentration attained in the different scenarios. In the event that one wants to recover the benzene from the regeneration stream for secondary purposes, such as re-selling or re-using, a high concentration is much more valuable than a low one. Here, it is noticeable that the benzene concentration is higher when the saturation temperature is higher, indicating an option to favour such scenarios if secondary usage of the adsorbate is of interest. This observation is in agreement with previous studies on VOC adsorption using TSA [20,33].

4. Conclusions

This work investigates the consequences of different steam regeneration scenarios for packed-bed adsorbers designed for benzene removal from a gaseous stream. A previously developed one-dimensional model for steam-regenerated temperature-swing adsorption of industrial-scale units in cycling conditions is used for this investigation. Two sets of numerical simulations have been performed, with the intention to investigate and highlight potential upsides and drawbacks of different steaming conditions. The first set involved simulations of several steam states, both superheated and saturated. The simulations were run until a pre-determined mass of benzene had adsorbed or desorbed from the bed. This approach provided information about the overall efficiency and characteristic bed behaviour attained with the different steam modes. The second set picked a few representative modes that were simulated with a pre-determined regeneration energy and run until breakthrough. This approach made it possible to investigate differences in breakthrough performance and the variation of spatially resolved sorption rates inside the bed at the chosen conditions.

From the first set of simulations, it is clear that a primary measure for efficiency gain is to perform the desorption at higher temperatures. This is most easily achieved by raising the saturation point, since the presence of water in the bed causes most of the desorption to occur at saturation conditions. When the steam is instead superheated, even though less steam is required at a higher temperature, more energy is required. From an in-depth analysis of the internal temperature, benzene and water profiles in the bed, it is shown that the superheated steam produces a sharper benzene front and restores a larger portion of the bed to a completely fresh state. However, it also dries the bed, thus spending energy on processes other than benzene removal.

The results from the second set of simulations show that when it comes to breakthrough performance, as for efficiency, saturated conditions are to be preferred. The higher temperature case for example yields longer times in the active stage. However, if a breakthrough

inadvertently occurs, the steeper concentration profile for the higher temperature case makes the outlet concentration rise quicker. This effect is even more pronounced for the superheated case, which is even sharper in the front than the other cases. From the adsorption rates in the bed during the active stage, it is clear that most of the bed participates, irrespective of the regeneration strategy adopted. This observation is in stark contrast to what is observed for a fresh bed, highlighting the importance of realistic industrial conditions when investigating packed-bed systems for industrial use through numerical simulations.

In summary, this work highlights how numerical simulations can be used to identify optimization opportunities in steam-regenerated TSA systems. Although the present model can be used at industrially relevant conditions, we remark that operating conditions that would produce excessive flow and/or trickling of condensate inside the beds lie outside the current range of validity. A relevant area for future research is therefore model extensions to allow handling of liquid water transport in the bed. It would also be of interest to use numerical simulations to investigate possible benefits from more advanced separation systems, involving for example coupled TSA/PSA processes.

Nomenclature

Latin variables

a	Specific surface area (m^2/m^3)
C_p	Specific heat capacity ($\text{J}/\text{kg}, \text{K}$)
c	Concentration (kg/m^3)
h	Convective heat transfer coefficient ($\text{W}/\text{m}, \text{K}$)
k	Mass transfer rate (m/s)
q	Mass fraction in bed ($-$)
T	Temperature (K)
t	Time (s)
u	Velocity (m/s)
x	Space (m)

Greek variables

ε	Bed porosity ($-$)
ΔH	Heat release (J/kg)
ρ	Density (kg/m^3)
ω	Mass fraction in gas phase ($-$)

Superscripts and subscripts

b	Bed
eq	Equilibrium
g	Gas
x	Benzene or steam/water

CRedit authorship contribution statement

Adam Jareteg: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing - original draft. **Dario Maggiolo:** Supervision, Formal analysis, Writing - review & editing. **Henrik Thunman:** Supervision, Formal analysis, Writing - review & editing. **Srdjan Sasic:** Supervision, Formal analysis, Writing - review & editing. **Henrik Ström:** Conceptualization, Formal analysis, Funding acquisition, Project administration, Resources, Supervision, Writing - review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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