Concept of a Flexible Wetted-Wall Column for the Distillation of Specialty Chemicals

The trend of increasing product diversity and decreasing production amounts led to the requirement of higher flexibility of production processes of specialty chemicals. Conventional distillation columns, mostly equipped with structured packings, lack the flexibility to handle product changeovers and throughput. Thus, a newly designed distillation column for specialty chemicals is presented. A numerical model was implemented to analyze the potential of the wetted-wall column. The simulation of the distillation of a binary methanol/water mixture demonstrated that the wetted-wall column can generate the desired concentration and temperature profiles. Furthermore, analyses of the pressure drop and separation efficiency with the test system chlorobenzene/ethylbenzene were conducted.

Keywords: Countercurrent flow; Distillation; Falling films; Simulation; Wetted-wall column

Received: October 09, 2020; revised: March 12, 2021; accepted: May 05, 2021

DOI: 10.1002/ceat.202000468

1 Introduction

Production processes of specialty chemicals require a high degree of flexibility. Small production amounts in the range of several 100 t y⁻¹ up to several 100 000 t y⁻¹ and short production periods imply a comparably high frequency of product changeovers [1]. Specialty chemicals are often temperature-sensitive and tend to foul or foam. These attributes of the components must be considered during the selection of suitable equipment design. Temperature sensitivity most often leads to the use of packed columns in the field of distillation processes as they generate the lowest pressure drop among the available separating internals. Nonetheless, structured packings are not an option of choice if fouling is occurring [2].

Equipment with high potential in flexibility is desired in all steps of the production process. While in the field of reaction technology several different innovative and flexible reactor designs are well developed [3], downstream processes in general and specifically distillation units are known to be the bottleneck in flexibility considerations [4].

Various approaches of flexible, small-scaled distillation units have been presented in several research projects. Microstructured distillation columns reveal a distinctive intensification in separation efficiency, but throughput and capacity are relatively low [5]. Another promising technology is zero gravity distillation. In form of short path distillation, the temperature profile is induced externally by heating and cooling the two ends of the horizontal column. The temperature profile invokes countercurrent mass transport [6]. Rotating packed beds as HiGee devices can already be found in commercial applications and promise higher flexibility and a compact apparatus design [7], but the pressure drops are significantly higher than in conventionally structured packings [8–10].

The concept of an innovative apparatus is presented that takes the challenges of the distillation of specialty chemicals into account. A first analysis of the wetted-wall column and a comparison with a packed column was already published previously [11]. The conceptional design of the proposed wetted-wall column is described in the following section. The numerical model that has been developed to analyze the wetted-wall column is presented in Sect. 3. The results of simulation studies concerning the general performance, as well as the pressure drop and the separation efficiency of the wetted-wall column, are discussed in Sect. 4.

2 Concept of the Flexible Wetted-Wall Column

The developed design and proposed dimensions of the wetted-wall column are illustrated in Fig. 1. The wetted-wall column consists of a rectangular cross section and is inclined by an angle $\alpha$ to the horizontal. To set a certain inclination angle, the wetted-wall column can be turned around an axis of rotation. For a first potential analysis, it is assumed that the liquid falling film is applied on a one-sided flat plate as a stratified flow. The surface of the flat plate is assumed to be perfectly plain.

Arnulf Reitze*, Marcus Grünewald, Dr.-Ing. Julia Riese
reitze@fluidvt.rub.de
Laboratory of Fluid Separations, Ruhr University Bochum, Universitätsstr. 150, 44801 Bochum, Germany.

1) List of symbols at the end of the paper.
Microstructured surface treatments, as typically conducted in conventional packed columns, can be beneficial concerning the wetting behavior on the plate as well as with regard to the separation efficiency [12, 13]. The vapor phase flows upwards to generate the typical countercurrent two-phase flow of distillation processes.

The dimensions of the apparatus given in Fig. 1 result in a free cross section of:

\[
A = B \cdot H = 2.8 \ldots 4.4 \text{ cm}^2
\]

which is comparable to small-scale laboratory distillation columns with diameters from 3 to 5 cm [14]. The setting of a rectangular channel allows for a modular adaption in case of increasing capacity demand.

The adjustable inclination angle allows influencing the fluid dynamics inside the column independently from the throughput. Changing the inclination angle of the wetted-wall column has two effects on the fluid dynamics of the liquid film: an increase of the inclination angle leads to a thinner film thickness \(d_L\) and to a faster liquid velocity \(w_L\). According to the film thickness derived from the Nußelt theory in Eq. (2), a change of the inclination angle from 90° to 25° results in an increase of the film thickness by 25%; see Fig. 2.

Experimental investigations using optical measurements showed that the Nußelt theory is valid for inclined smooth plates at low Reynolds numbers [13, 15].

\[
d_L = \frac{3 \sqrt{3 V_L \rho_L}}{B g \sin \alpha}
\]

High inclination angles cause small film thicknesses and consequently to a lower liquid holdup inside the column. This might improve the mass transfer as the small film thickness leads to shorter diffusion paths in the liquid phase. On the other hand, the increased film velocity at higher inclination angles can harm the mass transfer [16]. To which extent these effects influence the separation efficiency of a distillation process has not been investigated yet. The overall effect of the inclination angle on the separation efficiency of the wetted-wall column is analyzed based on a numerical model in Sect. 4.

Structured packings are categorized by the specific surface area as a degree of the interface area which they can generate for the mass transfer. In a rectangular wetted-wall column, the specific surface area is a function of the channel height:

\[
a = \frac{1}{H}
\]

As a larger specific surface area usually generates a greater interfacial area in conventionally structured packings, the separation efficiency rises with increasing specific surface area. On the other hand, a larger specific surface area also causes a higher pressure drop [17]. The influence of the specific surface area on the capacity and the separation efficiency is also analyzed in Sect. 4.

3 Materials and Methods

To identify the influences of the inclination angle and the specific surface area in a falling-film distillation process, it is necessary to calculate the countercurrent two-phase flow in the wetted-wall column. Therefore, a rate-based model that considers the heat and mass transfer rates between both phases was implemented in the software Aspen Custom Modeler®. The channel is discretized along the flow direction \(z\). A number of \(n = 100\) segments deliver reliable results. The model is based on the two-film model. As the focus in this work is on the general performance of the innovative design of the apparatus, the model is limited to the analysis of binary mixtures. Thus, the
mass and heat transfer between the liquid and vapor phase is realized by overall transfer coefficients from correlations based on the literature, which are presented and compared in Sect. 3.3. Consequently, a discretization of the film is neglected in both phases. Besides, it is assumed that uniform distributions of concentration and temperature along the width $B$ of the channel are present. These assumptions and the incorporation of models for condenser and reboiler result in a one-dimensional process model. Furthermore, it is assumed that the wetted-wall column is operated in steady state and that the plate of the wetted-wall column is completely wetted.

### 3.1 Mass and Energy Balances

In agreement with the two-film model, it is assumed that the bulk phases are ideally mixed. The model structure is based on the rate-based approach of the detailed description by Kenig and Blagov [18] and can estimate fluid dynamics, mass transport, and the pressure profile inside the presented wetted-wall channel. The resulting differential-algebraic set of equations is discretized in the orientation of the main flow direction along the $z$-axis in Fig. 1.

The mass and heat balances are deployed separately for the liquid and the vapor phase. Fig. 3 illustrates the infinitesimal control volumes of both phases inside the wetted-wall column. The mass balances per component $i$ are set up in the form:

$$
- \frac{\partial (\dot{F}_i x_i)}{\partial z} \, dz + \left[ k_{li} c_{il} (x_i^l - x_i^B) + \dot{n}_{li} x_i^B \right] Bdz = 0
$$

(4)

$$
\frac{\partial (\dot{F}_V y_B^i)}{\partial z} \, dz - \left[ k_{Vl} c_{il} (y_B^i - y_i^l) + \dot{n}_{Vl} y_i^l \right] Bdz = 0
$$

(5)

As continuity of mass transport at the interface must be valid, both phases are connected by the continuity equation that ensures equal mass transport in both phases at the interface:

$$
\dot{n}_L = \dot{n}_V
$$

(6)

![Figure 3. Control volumes in the liquid and vapor phase and adoption of the two-film model of the mass transfer according to [19].](image)

$$
k_{li} c_{il} (x_i^l - x_i^B) + \dot{n}_{li} x_i^B = k_{Vl} c_{il} (y_B^i - y_i^l) + \dot{n}_{Vl} y_i^l
$$

(7)

The flow direction from the liquid phase into the gas phase is defined as a positive flow direction; see Fig. 3. The mole fractions $x_i$ and $y_i$ in both phases have to be in accordance with the summation condition:

$$
\sum_i x_i^B = 1
$$

(8)

$$
\sum_i y_i^B = 1
$$

(9)

Like the mass balances, the energy balances for both phases are defined as:

$$
- \frac{\partial (\dot{F}_i h_i)}{\partial z} \, dz + \left[ U_i (T_i^l - T_i^l) + \sum_{i=1}^{NC} \dot{n}_{li} h_{li} \right] Bdz = 0
$$

(10)

$$
\frac{\partial (\dot{F}_V h_V^i)}{\partial z} \, dz + \left[ U_V (T_V^l - T_V^l) + \sum_{i=1}^{NC} \dot{n}_{Vl} h_{Vl} \right] Bdz = 0
$$

(11)

Likewise, continuity of heat flow at the interface is given by:

$$
\dot{q}_L = \dot{q}_V
$$

(12)

$$
U_i (T_i^l - T_i^l) + \sum_{i=1}^{NC} \dot{n}_{li} h_{li} = U_V (T_V^l - T_V^l) + \sum_{i=1}^{NC} \dot{n}_{Vl} h_{Vl}
$$

(13)

At the bottom of the column, a partial reboiler is implemented which generates the vapor stream entering the wetted-wall column. The liquid phase of the reboiler exits as a product stream the apparatus. A total condenser liquefies the ascending vapor at the top of the wetted-wall column and a splitting factor allows to set the ratio between the liquid reflux flow into the wetted-wall column and the distillate product stream of the low-boiling component.

### 3.2 Equilibrium Condition at the Vapor/Liquid Interface

It is supposed that at the interface between liquid and vapor phase the components are in equilibrium. To calculate the equilibrium mole fractions of both components, it is also assumed that the vapor phase can be described as an ideal gas. This supposition is valid as only moderate system pressures around ambient conditions or vacuum are considered for the simulation of the wetted-wall column. To describe the real mixture in the liquid phase, the activity coefficients $g_i$ are calculated by the non-random two-liquid (NRTL) model. Consequently, the equilibrium at the interface is calculated by:

$$
p y_i^l = p_i^\text{sat} x_i^l
$$

(14)
At the interface, the mole fractions of the components in both phases have to coincide with the summation conditions:

\[ \sum_{i} x_i^l = 1 \quad (15) \]
\[ \sum_{i} y_i^g = 1 \quad (16) \]

### 3.3 Interfacial Mass and Energy Transportation

The mass transport of components in binary mixtures is applied based on the film theory by Lewis and Whitman and allows the use of various correlations from the literature which were generated by experimental studies [20].

For the liquid-sided mass transport resistance the correlation by Brauer [21] is used.

\[
\begin{align*}
S_{lt} &= 0.0224Re_{l}^{0.8}Sc_{l}^{0.5} & 12 \leq Re_{l} < 70 \\
S_{lt} &= 0.08Re_{l}^{0.5}Sc_{l}^{0.5} & 70 \leq Re_{l} < 400 \\
S_{lt} &= 8.9 \times 10^{-4}Re_{l}^{2.5}Sc_{l}^{0.5} & Re_{l} > 400 \quad (17)
\end{align*}
\]

The correlation is divided into three segments representing the different flow regimes of laminar, pseudo-laminar, and turbulent film flow. The operational range of distillation columns is typically given by the gas velocity corrected by the gas density in form of the F-factor \( F \) and by the liquid loading \( u_l \). The operational conditions at total reflux are given in Tab. 1. It is obvious that the assumption of a solely laminar flow regime is valid at the investigated operating conditions. Thus, only the first part of the Brauer correlation in Eq. (17) is relevant for this study.

### Table 1. Reynolds numbers of the gas and liquid phase for the operational range of the wetted-wall column.

| \( F \)-factor | Liquid loading \( u_l \) | Reynolds number \( Re_V \) | Reynolds number \( Re_l \) |
|----------------|-----------------|-----------------|-----------------|
| \( \text{[Pa}^{0.5}] \) | \( \text{[m}^3\text{m}^{-1}\text{h}^{-1}] \) | \(-[\cdot] \) | \(-[\cdot] \) |
| 0.5 | 3.7 | 765 | 14 |
| 3.0 | 22.9 | 4595 | 84.3 |

For the gas phase the correlation by Braun and Hibi [22] is used because it is developed for countercurrent two-phase flow:

\[
S_{lt} = 0.015Re_{v}^{0.75}Re_{l}^{0.16}Sc_{v}^{0.44} \left[ 1 + 5.2 \left( \frac{L}{d_h} \right)^{-0.75} \right]^{0.5} \quad (18)
\]

\[1000 \leq Re_{v} \leq 14\,000 \quad 200 \leq Re_{l} \leq 700 \]

The correlation was generated with experimental studies at slightly higher liquid Reynolds numbers than the ones given in Tab. 1 but as the correlation covers the pseudo-laminar flow regime it is assumed that the accuracy is acceptable for this first conceptional study.

Instead of the diameter of an annular pipe, the hydraulic diameter for the rectangular wetted-wall column is employed according to Eq. (19):

\[ d_h = \frac{4BH}{2(B + H)} \quad (19) \]

A commonly used approach to calculate the heat transport coefficients \( U_L \) and \( U_V \) is the use of the Chilton-Colburn analogy [23]:

\[ U = k \rho \left( \frac{Sc}{Pr} \right)^{\frac{2}{3}} \quad (20) \]

### 3.4 Characterization of Fluid Dynamics

For the laminar flow regime, the film thickness can be determined by applying a force balance in \( y \)-direction on the liquid phase for Newtonian fluids; see Fig. 1.

\[ \eta \frac{d^2 w(y)}{dy^2} + \rho_l g \sin \alpha = 0 \quad (21) \]

Neglecting the influence of the countercurrent vapor stream on the downwards liquid stream and assuming the no-slip condition at the wall, Eq. (21) results in the Nußelt velocity profile [24]. Taking the countercurrent vapor flow into account and assuming shear stress at the phase interface of

\[ \eta \frac{d^2 w}{dy^2} \bigg|_{y=0} = -r^1, \quad \text{Eq. (21) results in}: \]

\[ w_l(y) = \frac{g \sin \alpha \delta_l}{v_l} \left[ \frac{1}{3} \left( \frac{r^1}{2 \rho_l g \sin \alpha} \right) \right] \quad (22) \]

By integrating the velocity profile \( w(y) \) over the film thickness \( \delta_l \), the average film velocity leads to:

\[ \bar{w}_l = \frac{g \sin \alpha \delta_l^2}{v_l} \left( \frac{1}{3} - \frac{r^1}{2 \rho_l g \sin \alpha} \right) \quad (23) \]

The velocity at the vapor-liquid interface, which is needed for the calculation of the interfacial shear stress in Eq. is calculated by:

\[ w_l(y = \delta_l) = w_l^1 = \frac{g \sin \alpha \delta_l^2}{v_l} \left( \frac{1}{2} - \frac{r^1}{\rho_l g \sin \alpha} \right) \quad (24) \]

Considering the continuity of mass flow, the film thickness is given by:

\[ \delta_l = \frac{\dot{M}_l}{\bar{w}_l \cdot b \cdot \rho_l} \quad (25) \]

The interfacial shear stress \( r^1 \) in Eqs. (22)–(24) is calculated by the interfacial friction factor:

\[ f^1 = \frac{2 \cdot r^1}{\rho_v \cdot (w_v - w_l^1)^2} \quad (26) \]

Lee shows that the interfacial friction factor depends on the Reynolds numbers of the vapor and the liquid phase as well as on the ratio of the liquid and vapor viscosity [25]. Experimen-
tal investigations with water-air as the test system lead to the following power-law relationship for the interfacial friction factor $f^I$:

$$f^I = 4.3 \times 10^{-11} R_{LV}^{0.96} R_{IL}^{0.31} \left( \frac{H}{\eta V} \right)^{1.86}$$  \hspace{1cm} (27)

The author states that the interfacial friction factor calculated with this correlation is valid above Reynolds numbers of $R_{IL} = 2360$. In lack of interfacial friction factors for laminar stratified flow regimes, Eq. (27) is used in this conceptional study, and the results of the two-phase pressure drop are compared to the single-phase pressure drop in Sect. 4.

For the evaluation of the pressure drop of the countercurrent stratified two-phase flow inside the inclined wetted-wall column, the momentum equation of the gas phase can be described according to Johnston as [26]:

$$\frac{\partial P}{\partial z} B (H - \delta_L) - f_{wV} \rho_V \frac{w_V^2}{2} [B + 2(H - \delta_L)] - f^I \rho_V (w_L - w_V)^2 B$$

$$- \rho_V B (H - \delta_t) g \sin \alpha = 0$$  \hspace{1cm} (28)

$f_{wV}$ denotes the friction factor of the vapor phase at the wall. The wall shear stress of the single-phase flow is not significantly affected by the interfacial shear stress [25, 27]. Thus, the wall friction factor for laminar single-phase flow can be calculated by the Hagen-Poiseuille law:

$$f_{wV, lam} = \frac{64}{R_{Ev}}$$  \hspace{1cm} (29)

Complementary to the previous study [11], the pressure drop also in the turbulent flow regime is considered. The friction factor is calculated according to Blasius [28]:

$$f_{wV, turb} = \frac{0.3164}{\sqrt{R_{Ev}}}$$  \hspace{1cm} (30)

The friction factors in Eqs. (29) and (30) can be combined to [29]:

$$f_{wV} = \sqrt{f_{wV, lam}^2 + f_{wV, turb}^2}$$  \hspace{1cm} (31)

The arrangement of the applied friction factors in the wetted-wall column is illustrated in Fig. 4.

![Figure 4](image_url)

**Figure 4.** Top view of the rectangular channel with the according friction factors at the wall and the gas/liquid interface for the momentum balance of a two-phase flow.

### 3.5 Physical Properties

The simulation studies were performed with two different test mixtures. As an example of aqueous mixtures, the system water-methanol was tested. To determine the separation efficiency of the wetted-wall column, the commonly used organic test system ethylbenzene-chlorobenzene was chosen. This is recommended because of its nearly constant relative volatility for a broad concentration range at a given temperature and pressure [30]. The characteristic physical properties of the components are given in Tab. 2. The vapor-liquid equilibria were calculated with the NRTL method.

| Component       | Density $\rho$ [kg m$^{-3}$] | Viscosity $\nu$ [$10^6$ Pa s] | Specific heat capacity $c_p$ [kJ kmol$^{-1}$K$^{-1}$] | Vapor pressure $P^v$ [mbar] |
|-----------------|-------------------------------|-------------------------------|-----------------------------------------------|-----------------------------|
| Methanol        | 789.6                         | 538.0                         | 90.3                                          | 168.3                       |
| Water           | 994.7                         | 912.5                         | 74.2                                          | 31.7                        |
| Chlorobenzene   | 1100.4                        | 755.4                         | 138.3                                         | 15.9                        |
| Ethylbenzene    | 863.6                         | 635.4                         | 188.2                                         | 12.8                        |

### 4 Results and Discussion

The developed numerical model is applied to evaluate the performance of the wetted-wall column. Therefore, simulation studies with two different intentions are conducted. First, the general separation performance of the wetted-wall column is analyzed by calculating the purification of a binary methanol/water mixture. For a detailed characterization of the separation efficiency of the wetted-wall column which allows for a classification concerning other column designs like structured packings, the separation of the test system chlorobenzene-ethylbenzene is calculated.

#### 4.1 Methanol/Water Distillation

The concentration profile of methanol in the vapor bulk phase and at the interface over the length of the wetted-wall column is displayed in Fig. 5. The equimolar feed of a methanol/water mixture enters the apparatus in the reboiler. The mixture is separated into a distillate stream at the top of the column with a methanol concentration of 0.89 mol mol$^{-1}$. The mole fraction of water in the reboiler and the bottom product stream is 0.77 mol mol$^{-1}$. The gradient of the concentration profile decreases slightly while the driving force of the mass transfer, i.e., the concentration difference between the bulk phase and the interface, gets smaller towards the top of the column.

The respective temperature profile over the length of the wetted-wall column is illustrated in Fig. 6. At the bottom of the column, the vapor temperature equals the boiling temperature...
of the mixture in the reboiler. The liquid stream cools the countercurrent vapor stream down to a temperature of 70.3°C.

In the total condenser, the vapor stream is liquified and enters at the top of the wetted-wall column with a boiling temperature of 66.3°C. Similar to the gradient of the concentration profile, the temperature gradient decreases towards the top of the column as the temperature difference between the vapor and the liquid phase gets smaller.

The results of the methanol-water distillation indicate that the numerical model can depict the separation in a distillation unit. The paths of the concentration and temperature profiles present the typical behavior as known in conventional distillation columns.

### 4.2 Fluid Dynamics

Correspondingly, studies of the pressure drop and the height equivalent of a theoretical plate as a function of F-factor, inclination angle, and specific surface area are conducted at total reflux with the test system chlorobenzene-ethylbenzene. Hence, performing a more detailed analysis of the wetted-wall column is possible. The operating conditions for the following studies of the pressure drop and the separation efficiency are given in Tab. 3.

| Parameter | Value |
|-----------|-------|
| $M_F$     | 10 kg/h^{-1} |
| $\Gamma_T$ | 10,000 |
| $\Gamma_B$ | 0.25–2.5 |
| $\beta_F$ | 100 °C |
| $\rho_C$  | 1.013 bar |

As mentioned above, the used correlation for the interfacial friction factor is only validated for larger Reynolds numbers. To classify the results according to Eq. (28), the single-phase pressure drop is calculated as:

$$\Delta p = \varphi \cdot \frac{L}{d_h} \cdot \rho_N \cdot \frac{u_N^2}{2} \quad \text{(32)}$$

The factor $\varphi$ takes the rectangular geometry into account and is set to $\varphi = 1.5$ for the given aspect ratios [28]. The pressure drop of the gas-liquid two-phase flow is significantly higher than the calculated single-phase flow pressure drop according to Eq. (32) because of the higher friction factor of the wavy interface area. However, to quantify the two-phase pressure drop more precisely, a more valid determination of the interfacial friction factor in the corresponding flow regime is required. Due to the increased relative velocity at the interface, the pressure drop reaches its maximum at a vertical inclination and decreases towards more narrow inclination angles; see Fig. 7.

The comparison of different specific surface areas demonstrates that the influence of the wall friction factor of a single-phase flow leads to a three times higher pressure drop for a surface area of $a = 500 \text{ m}^2 \text{m}^{-3}$. Considering the gas-liquid flow, the influence of the increased specific surface area is less pronounced as the pressure drop is mainly evoked by the interfacial friction factor. The absolute surface area is in both cases identical as only the channel height is changed; see Eq. (3).
4.3 Separation Efficiency

The separation efficiency is analyzed with the same operational conditions that are given in Tab. 3. The number of theoretical stages is calculated using the Fenske equation:

$$N_{\text{min}} = \frac{\log \left( \frac{y_T CB}{y_T EB} \right)}{\log w_{\text{ave}}}$$

(33)

$w_{\text{ave}}$ denotes the average relative volatility of the binary mixture, calculated by the geometrical average $w_{\text{ave}} = \sqrt{w_T \cdot w_B}$ of the relative volatility at the top and the bottom of the column. The relative volatility is calculated by:

$$w_{T/B} = \frac{x_{T/B}}{y_{T/B}}$$

(34)

The separation efficiency at total reflux can be expressed by the height equivalent of a theoretical plate HETP, which is determined by:

$$\text{HETP} = \frac{L}{N_{\text{min}}}$$

(35)

As indicated in Fig. 8, the HETP increases with rising F-factors. This effect is different from the typical behavior of structured packings in conventional distillation columns, which exhibit constant separation efficiency below the loading point.

The comparison of different specific surface area demonstrates that the duplication of the specific surface area results in the bisection of the HETP for low F-factors. However, the configuration with a specific surface area of $a = 250 \text{ m}^2/\text{m}^3$ generates a steeper gradient, which indicates that the mass transfer is less intensified in this case.

The influence of the inclination angle on the separation efficiency is insignificant. An increase of the inclination angle from $25^\circ$ to $90^\circ$ leads to an average decrease of the HETP of $3\%$. The increased efficiency for the vertical configuration of the wetted-wall column is due to the higher film velocity which results in a higher Reynolds number in Eq. (17). Physically, reduced liquid film thicknesses result in shorter diffusion paths, which improves the mass transfer. However, the influence of the liquid film thickness on the separation efficiency appears to be very limited according to this study: while the liquid film thickness changes by around $-31\%$, as
observed in Fig. 2, the separation efficiency just changes by the given 3 %.

5 Conclusion and Outlook

The characterized wetted-wall column represents a possible contribution to future flexible equipment. As short time-to-market and changeover times are getting crucial features of production processes, flexible production equipment is of high importance. Through its compact design, the innovative wetted-wall column creates the possibility of fast process characterization.

The implemented and presented model to describe the distillation process in the wetted-wall column allows first predictions about the operation of the apparatus. Studies conducted with a mixture of methanol and water proved that the separation of a binary mixture in the presented wetted-wall column is technologically feasible. The concentration and temperature profiles showed the expected behaviors that are already known from conventional distillation columns with structured packings. Further studies with the test mixture of chlorobenzene and ethylbenzene demonstrated that the pressure drop is significantly lower than in structured packings.

At low F-factors, the separation efficiency is similar to structured packings with the same specific surface area. The separation efficiency decreases with increasing F-factors, which can be explained by the absence of mixing zones which intensify the mass transport. The influence of the inclination angle on the separation efficiency is relatively small, which leads to the conclusion that the liquid film thickness has a minor impact on the separation efficiency in distillation processes. The pressure drops in the wetted-wall column are considerably lower than in structured packings, which can be beneficial for operation in vacuum.

These results illustrate that the designed wetted-wall column can be an interesting alternative for the distillation of specialty chemicals. The reduced complexity of the apparatus geometry, which simplifies cleaning the column during product changeovers, and the considerably lower pressure drop can offer advantages compared to structured packings. However, experimental studies have to be conducted to confirm the results of the presented simulation studies.

Acknowledgment

The authors acknowledge the financial support by the Federal Ministry of Education and Research, Germany in the project TransProMinC (project No. 01LN1712A). Open access funding enabled and organized by Projekt DEAL.

The authors have declared no conflict of interest.

Symbols used

| Symbol | Unit | Description |
|--------|------|-------------|
| A      | [m²] | area        |
| a      | [m²] | specific surface area |
| b      | [m]  | width of the channel |
| c      | [kmol·m⁻³] | molar density |

Greek letters

| Symbol | Description |
|--------|-------------|
| α      | inclination angle |
| Γ      | boil-up/reflux ratio |
| γ      | activity coefficient |
| Δ      | film thickness |
| η      | dynamic viscosity |
| θ      | temperature |
| λ      | thermal conductivity |
| ν      | kinematic viscosity |
| ρ      | density |
| τ      | shear stress |
| ω      | relative volatility |

Subscripts

| Symbol | Description |
|--------|-------------|
| ave    | average |
| B      | bottom |
| h      | hydraulic |
| i      | component index |
| j      | component index |
| L      | liquid phase |
| min    | minimal |
| T      | top |
| t      | total |
| V      | vapor phase |
| w      | wall |

Superscripts

| Symbol | Description |
|--------|-------------|
| B      | bulk phase |
| I      | interphase |
| sat    | saturation |
Abbreviations

| Abbreviation | Description                  |
|--------------|-------------------------------|
| CB           | chlorobenzene                 |
| EB           | ethylbenzene                  |
| MeOH         | methanol                      |
| NC           | number of components          |
| NRTL         | non-random two-liquid         |

References

[1] C. Hiller, R. Meier, G. Niggemann, A. Rix, Chem. Eng. Res. Des. 2015, 99, 220–227. DOI: https://doi.org/10.1016/j.cherd.2015.04.010

[2] G. Niggemann, A. Rix, R. Meier, in Distillation: Operation and Applications (Eds: A. Görak, H. Schoenmakers), Elsevier, Waltham, MA 2014.

[3] E. Y. Kenig, Y. Su, A. Lautenschleger, P. Chasanis, M. Grünewald, Sep. Purif. Technol. 2013, 120, 245–264. DOI: https://doi.org/10.1016/j.seppur.2013.09.028

[4] J. Riese, S. Lier, S. Paul, M. Grünewald, ChemEngineering 2019, 3 (2), 44. DOI: https://doi.org/10.3390/chemengineering3020044

[5] K. F. Lam, E. Sorensen, A. Gavrilliidis, Chem. Eng. Res. Des. 2013, 91 (10), 1941–1953. DOI: https://doi.org/10.1016/j.cherd.2013.07.031

[6] S. Ricks, M. Wende, N. Preuß, T. Gambaryan-Roisman, E. Y. Kenig, Chem. Eng. Res. Des. 2019, 147, 615–623. DOI: https://doi.org/10.1016/j.cherd.2019.05.022

[7] K. Gladyszewski, M. Skiborowski, Chem. Eng. Process. Process Intensif. 2018, 127, 1–9. DOI: https://doi.org/10.1016/j.cep.2018.02.024

[8] T. Kelleher, J. R. Fair, Ind. Eng. Chem. Res. 1996, 35 (12), 4646–4655. DOI: https://doi.org/10.1021/ie950662a

[9] G. Q. Wang, Z. C. Xu, J. B. Ji, Chem. Eng. Res. Des. 2011, 89 (8), 1434–1442. DOI: https://doi.org/10.1016/j.cherd.2011.02.013

[10] D. P. Rao, A. Bhowal, P. S. Goswami, Ind. Eng. Chem. Res. 2004, 43 (4), 1150–1162. DOI: https://doi.org/10.1021/ie030630k

[11] A. Reitze, M. Grünewald, J. Riese, Chem. Ing. Tech. 2020, 92 (12), 1968–1975. DOI: https://doi.org/10.1002/cite.202000065

[12] M. Kohrt, I. Ausner, G. Wozny, J.-U. Repke, Chem. Eng. Res. Des. 2011, 89 (8), 1405–1413. DOI: https://doi.org/10.1016/j.cherd.2011.01.010

[13] S. J. Gerke, J.-U. Repke, Chem. Eng. Res. Des. 2019, 147, 634–643. DOI: https://doi.org/10.1016/j.cherd.2019.05.043

[14] H. Schoenmakers, L. Spiegel, in Distillation: Operation and Applications (Eds: A. Görak, H. Schoenmakers), Elsevier, Waltham, MA 2014.

[15] S. Paschke, J.-U. Repke, G. Wozny, Chem. Ing. Tech. 2008, 80 (10), 1477–1485. DOI: https://doi.org/10.1002/cite.200800056

[16] S. Paschke, Experimentelle Analyse ein- und zweiphasiger Filmströmungen auf glatten und strukturierten Oberflächen, Ph.D. Thesis, Technische Universität Berlin 2011.

[17] Ž. Olujić, A. F. Seibert, J. R. Fair, Chem. Eng. Process. Process Intensif. 2000, 39 (4), 335–342. DOI: https://doi.org/10.1016/S0255-2701(99)00095-1

[18] E. Y. Kenig, S. Blagov, in Distillation: Fundamentals and Principles (Eds: A. Görak, E. Sorensen), Elsevier 2014.

[19] W. G. Whitman, Chem. Metall. Eng. 1923, 29, 146–148.

[20] W. K. Lewis, W. G. Whitman, Ind. Eng. Chem. 1924, 16 (12), 1215–1220.

[21] H. Brauer, Chem. Ing. Tech. 1958, 30 (2), 75–84. DOI: https://doi.org/10.1002/cite.330300205

[22] D. Braun, J. W. Hibi, Chem. Ing. Tech. 1970, 42 (6), 345–349. DOI: https://doi.org/10.1002/cite.330420605

[23] T. H. Chilton, A. P. Colburn, Ind. Eng. Chem. 1934, 26 (11), 1183–1187. DOI: https://doi.org/10.1021/ie50299a012

[24] W. Nußelt, Z. Ver. Dtsch. Ing. 1916, 60, 569–575.

[25] S. C. Lee, Chem. Eng. Commun. 1992, 118 (1), 3–16. DOI: https://doi.org/10.1080/009864954208936082

[26] A. J. Johnston, Int. J. Multiphase Flow 1994, 10 (3), 371–383. DOI: https://doi.org/10.1016/0301-9322(84)90027-2

[27] T. J. Hanratty, J. M. Engen, AIChE J. 1957, 3 (3), 299–304. DOI: https://doi.org/10.1002/aic.690030303

[28] W. Kast, E. S. Gaddis, K.-E. Wirth, J. Stichlmair, in VDI Heat Atlas, 2nd ed., VDI-Buch, Springer, Berlin 2010.

[29] L. Fischer, U. Bühlmann, R. Melcher, Chem. Eng. Res. Des. 2003, 81 (1), 79–84. DOI: https://doi.org/10.1205/026387603321158221

[30] M. Ottenbacher, Ž. Olujić, T. Adrian, M. Jödecke, C. Großmann, Chem. Eng. Res. Des. 2011, 89 (8), 1427–1433. DOI: https://doi.org/10.1016/j.cherd.2011.02.012