Optimization-Based Design of Rotating Packed Beds with Zickzack Packings

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Abstract

Due to the fast development of the market in the chemical industry, more flexible and efficient equipment is obligatory. High-gravity contactors in form of Rotating Packed Beds (RPBs) have the potential to meet these needs since they offer an enhanced mixing by imposing centrifugal forces resulting in an intensified mass and energy transport. With the rotational speed as an additional degree of freedom, RPBs offer faster start-up times and an enlarged operating window. Despite the increasing scientific work in the areas of experimental investigations and modeling, industrial applications are still limited due to a lack of reliable methods for scale-up and design. In respect to the latter, this work presents a nested superstructure approach for the optimization-based design of RPBs with zickzack packings that is further demonstrated for the dehydration of methanol.

Keywords: optimization, process intensification, rotating packed bed, zickzack packing

1. Introduction

During the last decades, the chemical industry started to face a transition to more flexible production plants motivated by a constant change in feedstock towards sustainable resources, as well as a more fluctuating market caused by globalization and steady cultural development. In the same period, high-gravity contactors, like Rotating Packed Beds (RPBs), have gained increasing attention to meet these challenges via process intensification (Neumann et al., 2018). RPBs enable intense mixing, as well as heat and mass transfer intensification between the contacted phases through the application of centrifugal forces, several times larger than earth’s gravity. Besides shorter residence time and reduced equipment size, RPBs have considerably shorter start-up times compared to gravity-based static contactors. The rotational speed in an RPB offers an additional degree of freedom that enlarges the operating window and aids flexibility during operation.

While substantial research on RPBs is conducted with particular emphasis on feasibility studies, general process development and operation in absorption, stripping, and distillation, with a steadily increasing number of publications, most studies focus on experimental evaluation (Cortes Garcia et al., 2017) Only a few articles address general design guidelines (Agarwal et al., 2010; Sudhoff et al., 2015), while so far, only a single optimization-based design approach for RPBs was introduced by Qian et al. (2017). The presented method focused on the design of a single-stage rotor equipped with a wire-mesh packing for H₂S-removal by absorption. However, especially for complex separation problems, the necessary rotor sizes may result in impractical designs and high uncertainty related to the varying loadings along the radial distance in the annular-shaped packing.
Especially for distillation, an alternative rotor design termed Rotating Zigzag Bed (RZB) has been promoted by Wang et al. (2008), which contrary to the single block packing, implements a tray-like structure of alternating baffles mounted on a rotating and a stationary disc. For the RZB, several hundred industrial applications for distillation have been reported primarily in Asia (Xu et al., 2012). The possibility of adjusting the distance between the baffles as well as the baffle size allows for the establishment of more uniform hydrodynamic conditions. However, the alternation of static and rotating baffles results in an increased pressure drop and power consumption. To overcome the latter limitations, Qammar et al. (2019) have recently introduced a single block Zickzack (ZZ) packing, which employs the same tray-like structure as in an RZB but can be implemented in a single-block RPB (see Figure 1), allowing for a reduced pressure drop and approximately constant F-Factors along the radial length. It was shown that the pressure drop for a 3D-printed ZZ packing was reduced by ten times compared to the equivalent RZB setup, also resulting in a considerable decrease in the electrical power consumption.

![Figure 1: Schematic depiction of an RPB with a single block packing and an RPB with a ZZ packing including vapor (dashed lines) and liquid (solid lines) flows](image)

Unlike the superstructure model of Qian et al. (2017), which evaluates the performance of a single stage RPB based on an HTU-NTU approach without further discretization along the radial length, the current work introduces an optimization-based approach for the conceptual design of a multi-stage RPB with ZZ packing, building on an efficiency-based equilibrium stage approach to represent the tray-like contacting in the ZZ packing. Therefore, a nested superstructure is developed, which enables the sizing of an RPB with a variable number of rotors and a variable diameter of each rotor, based on a rigorous equilibrium-tray model in combination with classical Murphree efficiencies. Additionally, the model is further complemented by general sizing constraints (Agarwal et al., 2010; Sudhoff et al., 2015) as well as an economic model, which allows for the minimization of the total annualized costs (TAC). The developed approach is further demonstrated for the dehydration of methanol.

2. Methodology

The optimization-based design approach for the RPB with ZZ packing builds on four elementary parts. First, a superstructure needs to be defined, which allows for a flexible sizing of the RPB in terms of the number and size of rotors, while the number of iterating baffles in the ZZ packing has to be matched to the number of equilibrium stages via an efficiency model and the specific hydrodynamic. Furthermore, a cost model and a strategy for initialization and optimization need to be specified.
2.1. Superstructure Model

The ZZ structure of the considered packing allows for a modeling approach based on equilibrium trays where two baffles are termed as a baffle pair represented by one equilibrium tray with a certain efficiency. Figure 2 illustrates the respective nested superstructure, showing only a radial intersection through the axisymmetrical RPB. While vapor streams are indicated by dotted lines, liquid streams are depicted by solid lines. There is an outer superstructure representing the number of rotors and an inner superstructure accounting for the number of baffle pairs in each rotor. This leads to the possibility of bypassing single stages in a rotor and bypassing of complete rotors resulting in different rotor diameters and different overall rotor setups, respectively. Analogously to the superstructure of a conventional column (CC) (see e.g. Kraemer et al., 2009), the reflux and the reboil stream can enter each rotor in the rectifying and stripping section, respectively, which is modeled by additional binary decision variables. The size of each rotor is determined by a decision variable for the location of the vapor stream coming from the rotor below. Since the rotor diameter can vary significantly, the current design assumes that the rectifying and stripping sections are implemented in separate housings, which however requires additional motor and shaft work. For the RPB design, the feed is always introduced at the eye of the rotor since the rotor is in constant rotational movement, while in an RZB, the upper plate is stationary, such that an intermediate feed position would be feasible.

2.2. Murphree Efficiency

Referring to Qammar et al. (2019), the efficiency of a baffle pair in a ZZ packing with 25 baffles is assumed to be about 15% - 30%. Therefore, the concept of Murphree stage efficiencies (ME) is utilized (Murphree, 1925), in order to account for the respective mass transfer limitation by a departure of the vapor composition from the equilibrium composition for each baffle pair. As a result, the vapor composition \( y \) leaving a baffle pair is determined from the equilibrium composition \( y^* \) and the ME \( \eta \), cf. Equation (1).

\[
y_{n,i} = y_{n+1,i} + \eta (y^*_{n,i} - y_{n+1,i})
\]  

(1)

The ME is specific for the considered equipment and the investigated mixture, but also the considered rotational speed. For the explicit packing design, investigated system and specified hydrodynamics it is assumed to be constant. Aside from the mass transfer inside
the packing, each existing rotor provides additional mass transfer in the casing, for which a ME of 90% is assumed, based on the experimental results by Qammar et al. (2019).

2.3. Sizing and costing
In order to appropriately design the multi-stage RPB, different aspects of the equipment have to be considered apart from the external heat exchangers and heat duties, which are common to the design of a distillation column, i.e., the rotors and casing, as well as the motor and the respective electrical power consumption.

Initially, the rotor geometry is determined based on the inner diameter at the eye of the rotor as well as the desired F-Factor within the rotor, which are required as model inputs. Based on the F-Factor and approximated vapor flowrates, the spacing between the baffles and the height of the rotor are calculated. The outer radius of the rotor is determined by the sum of the baffle radii depending on the superstructure decision variables. A correlation between the rotor and casing heights and diameters links the two geometries. With these geometric constraints, the cost for the RPB body is calculated based on an adjusted form of the cost correlations for a pressure vessel according to Biegler et al. (1997). The rotor costs are currently based on lab-scale equipment due to a lack of reliable data for industrial-scale applications. The costs for the motor and the drive are calculated by correlations from Woods (2007), as suggested by Sudhoff (2015).

2.4. Optimization approach
The initialization and optimization of the superstructure model is conducted similarly to the design of distillation columns, according to the approach presented by Skiborowski et al. (2015). The model was implemented in the optimization software GAMS and solved as a sequence of successively relaxed nonlinear programming problems with additional nonlinear complementary constraints, in order to solve the mixed-integer nonlinear programming problem. The thermodynamic models, including flash and enthalpy computations, are integrated via the use of external functions, as described in Skiborowski et al. (2015).

3. Results
The proposed optimization-based design approach is used to investigate the well-known case study of methanol dehydration with an equimolar feed flow of about 6.7 mol·s⁻¹ (600 kg·h⁻¹) introduced as boiling liquid. A purity of 99 mol-% methanol for the distillate and 99 mol-% water for the bottom product are set as constraints. For the calculations, a depreciation time of five years with an interest rate of 6% is assumed. The necessary utilities are cooling water at 288 K (0.05 €·t⁻¹), 3 bar steam with a temperature of about 406 K (12 €·t⁻¹), and electricity (0.076 €·(kWh)⁻¹). For the RPB, a ME within the rotor of 30% is assumed, while the casing has an efficiency of 90%. As an initial setup for the RPB, four rotors for the rectifying section, two rotors for the stripping section, a maximum diameter of 1.2 m, and maximum F-factors within the rotors of up to 6 Pa⁰.⁵ (Wang et al., 2019) are chosen, resulting in 15 baffle pairs per rotor based on approximated vapor flowrates. In contrast, the initial column setup consists of 30 trays per section and an ME of 70% per tray (Bausa and Steimel, 2018).
The optimization results for the RPB with ZZ packing are presented in Figure 3 with an additional comparison of the TAC of both RPB and CC. The structural depiction of the RPB indicates the bypassed regions (grey) and the used rotors and baffle pairs (white). For this case study, the rectifying section consists of three rotors with 15 baffle pairs each, and the stripping section comprises two rotors with 7 baffle pairs. Note that an additional constraint enforces equal sizes for the rotors in one section, in order to avoid empty casing volume. Besides the depicted structural decisions, the optimization also considers continuous operational degrees of freedom, i.e. the reboiler and the condenser duty. Based on the current cost correlations, the RPB is evaluated as the more expensive option in terms of operational and capital expenditures (CAPEX, OPEX). The increase in OPEX is about 8.9% compared to the CC related to the additional electricity input for the motor, while the necessary reboiler and condenser duties are comparable. The increase in CAPEX for the RPB compared to the CC is about 31.5% and almost entirely related to the rotors within the RPB. They account for an increase of 45.4% of the CAPEX, while the smaller casing saves about 18.6% of the costs. It should be noted that the cost increase for motor, drive and electricity is further enlarged by the consideration of two separate RPBs for rectifying and stripping section.

Despite the cost deficiency, a significant reduction in the apparatus height and volume can be achieved by the RPB. The height was reduced by approximately 91.6% considering a combined height for both RPBs (rectifying; stripping), while the overall equipment volume of the column shell is reduced by 13.4% through the RPBs.

4. Conclusion
The current work presents for the first time an equilibrium-stage based superstructure optimization approach for the design of RPBs with ZZ packings, which may also be used for the design of an RZB. The approach considers multiple rotors in individual RPBs for rectifying and stripping section. Furthermore, the model was extended by Murphree efficiencies in order to consider the characteristics of RPBs with ZZ packings. Applying a reliable polyolithic modeling and solution approach similar to that of classical distillation columns, the approach effectively determines locally optimal solutions to an intricate multi-stage RPB design for the dehydration of methanol. The results indicate a potential for size reductions by means of the RPB, however, the applied cost model for the RPB needs further refinement since it is based on a currently available limited data set for sizing and costing of lab-scale equipment. Therefore, it is suggested that not too much emphasis is placed on the economic comparison. Besides the refinement of the cost model, additional pressure drop correlations, as well as an extended ME model should be
considered in future improvements of the model for deriving a more general and reliable model for RPB design. Apart from these modifications, the superstructure model already presents a suitable platform that can further be exploited in the development of RPB-based processes.

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References