

A hierarchal approach based on reverse design algorithm for simultaneous design and analysis of product and processes.

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Abstract

In order to meet the demands of specifically architected fine chemicals it is advantageous to design the process and product simultaneously. A systematic model based approach, which consists of a framework for multilevel process and product models has been developed. The objective is to design simultaneously process and product, and, to generate design alternatives to match a desired set of performance. A design algorithm which is based on the reverse design approach will be presented together with a generic model that is able to handle a wide variety of products and processes.

Keywords

Simultaneous design, reverse design, multilevel modeling, vacuum membrane distillation (VMD), design.

1. Introduction

To satisfy the ever increasing demands for specialty chemicals, the availability of a suitable computer-aided method for identification, design and modeling of multifunctional, chemically structured products can make a big impact. The design and analysis of these chemical products and their processes require multilevel modeling, which includes macroscopic level process models and microscopic level property models. To build such a model-based design framework we use a reverse design approach, where we identify a design matching a specific target. The solution strategy based on reverse design

approach, splits the solution steps into two stages. In the first stage, the process model comprising the balance and constraint equations is solved for the property parameters of the system, which are considered as the unknown variables. In the second stage, various property models (constitutive equations of the original process model) are employed in order to determine the design variables that matches the target properties (property parameters) calculated in stage I. These are key properties of the system, which affects the performance of the process, and they depend on variables related to the process conditions and/or the product itself. In this way, the hierarchal approach converges from the inlet and outlet specifications of a process to the product and process properties, which leads to the design of the product to match the performance criteria of process, thereby providing simultaneously design for both.

2. Generic design problem

In general terms, most operations in chemical processes depend on some key properties of the system. For example, reaction rate constant or dissociation constant for reactive systems, driving force for distillation or liquid-liquid extraction etc., thermodynamic or kinetic properties for solution diffusion and, selectivity of solvents for solvent based separation. These key properties in turn depend on process parameters such as conditions (T, P, flowrates etc.), and parameters related to the equipment, chemical structure of solvent or entrainers (for azeotropic distillation), microscopic structure (for polymer membranes). Therefore, the performance of the process depends on variables related to the product as well as the process. For a given mixture to be separated, the process can thus be defined in terms of these product and/or process variables.

In order to explain the design algorithm it is convenient to use a generic model for the process. Usually, the variables in the mathematical model describing the separation process can be divided into state variables (\underline{Y}), variables defining input conditions (\underline{I}), variables defining outlet conditions (\underline{X}), which must satisfy certain performance criteria (\underline{p}), process and product design variables (\underline{d}) and constitutive model parameters ($\underline{\theta}$). The generic model (Eqn. 1) of the separation process in terms of the above variables consists of a set of differential *balance* equations (conservation laws) is represented by:

$$\frac{d\underline{Y}}{dt} = f(\underline{Y}, \underline{X}, \underline{\theta}, \underline{I}) \text{ s.t. : } I.C. : \underline{Y}(t = 0) = \underline{Y}_0; B.C. : \underline{Y}(t = t_{end}) = \underline{Y}_t \quad (1)$$

Where, the *constitutive* equations (property models) are represented by:

$$\underline{\theta} = f(\underline{d}) \quad (2)$$

and *control/definition* equations are represented by,

$$\underline{p} = f(\underline{X}) \quad (3)$$

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Equations 1-3 generally relate the desired performance criteria (\underline{p}) to the outlet variables (\underline{X}). The performance criteria could be the product purity, recovery of one constituent in the mixture, permeate flow rate etc.

3. Design algorithm

The design algorithm aims at finding or designing the set of product and/or process variables that match a desired separation defined in terms of outlet variables (\underline{X}). A conventional way to achieve this is the forward approach (Fig. 1(a)), where essentially, a trial-and-error procedure is employed. In forward approach, for specified input conditions (\underline{I}), the design variables (\underline{d}) are selected as a first step. Next, the process model is solved, using the design variables (\underline{d}) and known inlet variables (\underline{I}), to calculate the unknown outlet variables (\underline{X}). Finally, performance criterion of the whole process which is a function of \underline{X} is evaluated and compared with the desired values. If the obtained values do not match the desired (target) values, the above steps are repeated with new values for the set of design variables. This is an iterative procedure where for each iteration, all the steps need to be repeated. With this approach, the constitutive models are embedded in the process-product model and therefore, a constitutive model must be specified before the solution can be attempted. Therefore the design depends on the choice of the constitutive model.

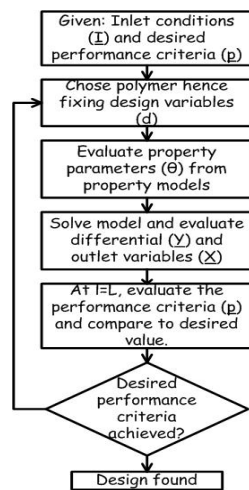


Fig 1(a) Forward approach

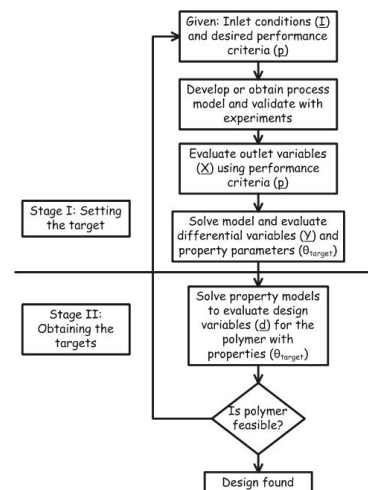


Fig 1(b) Reverse approach

This work employs a (two step) reverse design approach (Fig. 1(b)). In the first step, instead of calculating the separation achieved from a process using separation models, the separation target is fixed at the desired value. Note that for most process design problems, values for both (\underline{I}) and (\underline{X}) are assigned where the outlet variables take the values that are governed by (\underline{p}). This results in an extra degree of freedom, which is assigned to the set ($\underline{\theta}$), of the system.

So, the first step gives the value of the target properties (θ_{target}) in terms of the property parameters will ensure a separation corresponding to the desired targets for a specified inlet condition (**I**). Next, the second step in the procedure is to identify (**d**) using property models. Through this approach, since (θ) variables are the unknown variables in the first step, their solution do not need the constitutive model to be embedded in the process model, thus reducing the complexity related to the solution of the process model. Advantages include the saving of computational time and power by avoiding the iterative method of the forward approach. E.g. permeability calculations for a given system can be predicted by a group contribution method. The above mentioned calculations depend on the composition, T and P at each spatially discrete point of the membrane module. Consequently, incorporating them in the membrane model could be fairly complicated. On the other hand, many polymers may be designed (identified) without having to repeatedly solve the membrane process model coupled with the corresponding polymer property model.

4. Case study: Vacuum membrane distillation design

The model-based reverse design approach is highlighted for the design of a VMD operation. In VMD, the feed solution is brought into contact with one side of the microporous membrane, and a vacuum is maintained on the other side to create a driving force for the trans-membrane flux.

4.1. VMD model

A total mass and energy balance is established over the length of the membrane module from $z=0$ to $z=L$. The overall mass balance (feed and permeate) is:

$$\frac{du_i}{dz} = -\frac{J(z)}{h.n_c}, \text{ s.t. } u_i(z = z_0) = u_{i,0} \quad (4)$$

Since there is no change in temperature on the permeate side, the model for a temperature profile is derived only for the feed side:

$$\frac{dT_f}{dz} = \frac{1}{V_f} \left(\frac{-q_{\text{process}} \cdot w}{\hat{C}_p} + J(z) \cdot w \cdot T_f \right) \text{ s.t. } T_{bf}(z = z_0) = T_{bf,0} \quad (5)$$

The driving force for VMD is the partial pressure difference which can be calculated for feed side for component i as:

$$P_{i,wf} = P_i^{\text{sat}}(T_{wf}) \cdot \gamma_i(T_{wf}, x_{if}) \cdot x_{if} \quad (6)$$

The permeate side partial pressure for component i can be calculated as:

$$P_{i,wp} = P_{\text{vac}} \cdot x_{i,wp} \quad (7)$$

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Mass transfer through the liquid phase on the surface of the feed side membrane can be adequately described by the film theory model [1].

$$R_{total} = k_m \cdot C_t \cdot \ln \left(\frac{x_{i,wf} - x_{i,p}}{x_{i,f} - x_{i,p}} \right) \quad (8)$$

Flux in the case of Knudsen-viscous diffusion for component i is given as [3]:

$$R_i = \frac{1}{R \cdot T_{avg} \cdot \delta_m} \left(D_{a,e}^i \cdot \Delta p_i + B_0 \cdot \frac{p_{i,wf} + p_{i,wp}}{2} \cdot \Delta P \right) \quad (9)$$

The heat transfer from bulk of the feed to the permeate side of the membrane can be described by simple heat transfer equations:

$$Q_{process} = h_{film} (T_{feed} - T_{wf}) \quad (10)$$

4.2. Model validation

Simulations for the recovery of aroma compounds from Black currant juice using the VMD model was made under different conditions of operation for twelve different aroma compounds, representing various chemical groups [2]. The membrane used in the experiments was Polytetrafluoroethane (PTFE), which has a pore size of $0.2 \mu m$ and a porosity of 0.75. The module is 9.75 cm long, 3.8 cm wide and 1 mm high. The results are shown in Fig. 2, where the molar fractions of aroma compounds in permeate from the model is compared versus those obtained from experiments [2] at three different feed flow rates (300, 400, 500 l/h).

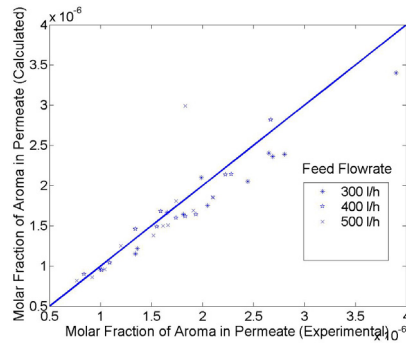


Figure 2: Comparison of molar fractions in permeate from model and experiments

4.3. Design problem

An example to illustrate simultaneous product and process design using the

reverse design algorithm is presented here. For the case of aroma recovery, we chose to study benzaldehyde recovery from water-benzaldehyde binary mixture. According to the reverse design algorithm (Step 1), the feed conditions and the separation targets are specified a priori. So, in this case, mole fraction of aroma compound in feed, $I = x_f = 1e-6$; separation targets: $p_1 =$ Concentration factor (CF) = 8.5 (corresponding to $X_1 = x_{i,p}$); $p_2 =$ Recovery (ratio of moles of benzaldehyde in permeate and in feed) = $5.3e-7$ (corresponding to $X_2 = R_i$). By specifying two additional variables, we now have two degrees of freedom that can be assigned to any two variables depending on if it is desired to design the product or the process or some aspects of both (Step 2).

4.3.1. Product design

In this case, in addition to the specified aroma concentration in feed, the temperature and flow rate are also specified ($T = 323.15$ K and $F = 300$ l/h). The unknowns in this case are, porosity and pore size, which are calculated from VMD model as $\theta_{target} = \{\varepsilon = 0.57 \quad r = 8.227e-7\text{m}\}$. A polymer with these properties will give the desired separation for the specified feed conditions.

4.3.2. Process design

In this case, we specify the polymer properties in addition to the aroma concentration in the feed. We choose PTFE as the polymer, hence fixing its porosity and pore size as given above. The unknown design variables in this case are, feed temperature and its flow rate, which are calculated from VMD model as $\underline{d} = \{T = 313$ K and $F = 400$ l/h}. Note that in product design, T and F were specified as the intention was to design the product and not the process.

5. Conclusions

From the results of the application of the reverse design approach for the specific case study, it can be seen that it is comparatively easier to formulate and solve the models for the reverse approach than adopting the forward approach. Also, no trial and error procedure was needed to obtain the targeted design. Results from this case study and others not reported here confirm that the developed methodology is efficient, robust and widely applicable.

References

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