PROCESS MODIFICATION THROUGH VISUALIZATION AND INCLUSION TECHNIQUES FOR PROPERTY-BASED INTEGRATION

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Abstract

This paper provides a new systematic procedure for identifying optimal strategies for process modifications, so as to optimize the allocation of process sources and minimize waste discharge. The clustering concept is used to map the problem from the non-conserved property domain into the component-less cluster domain. Interval analysis principles are also employed to define rigorous bounds on the process properties of interest, when all allowable changes in design and operating variables are considered. Moreover, strategies for optimizing both process performance and fresh properties via material substitution are considered here. Finally, a case study is investigated to illustrate the applicability of the described approach.

Keywords

Property integration, Interval analysis, Process modification.

Introduction

While traditional process design is carried out on the basis of individual chemical components, it is worth pointing out that there are many design problems that are component-independent. These problems can be adequately addressed and solved by tracking functionalities or properties that are essential for the process performance within an integrated framework.

There are many examples of design problems that are based on properties or functionalities. For instance, there are constraints on process units that can accept recycled/reused waste and process streams based on the properties of the feeds to processing units. An example of this is a condenser that performs based on vapor pressure.

Moreover, there are common examples of streams, which are continuous mixtures that consist of numerous (almost infinite) chemical species. Tracking each chemical component of these streams is almost prohibitively difficult. Therefore, by designing the process based on properties or functionalities of these streams the numerous chemical constituents do not need to be enumerated.

The novel property-based design paradigm, which has been introduced by Shelley and El-Halwagi (2000), allows the conserved tracking of properties throughout the process by employing the new concept of clustering. Shelley and El-Halwagi (2000) incorporated the clustering technique into a mass integration approach to determine optimal strategies for the recovery and allocation of complex hydrocarbon mixtures.

Moreover, Qin et al. (2004) developed an algebraic procedure for property-based integrated design. Using constraint reduction techniques, they proposed a systematic method for the allocation of process and external sources to sinks based on property constraints that can involve more than three properties.

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The current approach uses the clustering concept to identify optimum strategies not only for resource allocation, but also for unit manipulation. In particular, stream properties here are allowed to change according to changes in process variables. However, rigorous bounds for the property search domain need to be determined and optimum allocation and unit manipulation rules are to be derived.

Problem Statement

The problem to be addressed here can formally be stated as follows:

Given is a process with a certain number of sources (process and waste streams), Ns, which possess a finite number of properties, Np. Each property value of a stream i, $p_{p,i}$, is a function of a set of design variables, $\mathbf{d}_{p,i}$ and a set of operating variables, $\mathbf{r}_{p,i}$ that characterize the whole process. The design variables belong to an interval [$\mathbf{d}^l_{p,i}$, $\mathbf{d}^u_{p,i}$] dictated by design restrictions throughout the process. Similarly, the operating variables belong to another interval [$\mathbf{r}^l_{p,i}$, $\mathbf{r}^u_{p,i}$] imposed by operating constraints throughout the system, e.g.

$$\mathbf{d}^l_{p,i} < \mathbf{d}_{p,i} < \mathbf{d}^u_{p,i} \tag{1}$$

$$\mathbf{r}^l_{p,i} < \mathbf{r}_{p,i} < \mathbf{r}^u_{p,i} \tag{2}$$

where p = 1, 2, …, Np and i= 1, 2, …, Ns.

Given is also a fresh source, whose cost per unit mass is C_f, and a number of process units, Nu, along with their property and flowrate constraints:

$$p^l_{p,j} < p_{p,j} < p^u_{p,j} \tag{3}$$

$$G^l_j < G_j < G^u_j \tag{4}$$

where j = 1, 2, …, Nu.

Our objective is to identify optimal process modification strategies in order to optimize the allocation of the process resources and minimize the fresh consumption, while satisfying all property and flowrate constraints for the process units.

Property-based Techniques

The proposed property-based approach was first introduced by Shelley and El-Halwagi (2000) and it is based on tracking properties or functionalities of streams by transforming them into conserved quantities known as clusters.

The Clustering Concept

Clusters are surrogate properties that are tailored to possess two main features: intra- and inter- stream conservation. They can mathematically be described as follows:

$$C_{p,i} = \Omega_{p,i} / AUP_i \tag{5}$$

where $\Omega_{p,i}$ is the dimensionless operator derived by dividing the actual operator $\psi_p(p_{p,i})$ by a reference value ψ^{ref}_p. The actual operator is a mathematical expression of the property, such as the property's mixing rule can be given by an expression of the following type:

$$\psi_p(\overline{p}_p) = \sum_{i=1}^{Ns} \chi_i \cdot \psi_p(p_{p,i}) \tag{6}$$

where χ_i is the fractional contribution of the i[th] stream into the total flow rate of the mixture and $\overline{p}_p$ is the property value of the mixture. Also, AUP_i is the augmented property index for a stream i given by the summation of all the dimensionless operators in stream i.

Interval Analysis

Interval analysis can be used to develop reliable inclusions for the minimum and maximum values of many functions (Ratschek, and Rokne, 1988).

Let I be the set of real impact intervals [a, b], a,b ϵ R. The inclusion isotonicity principle from interval arithmetic suggests the following:

For A, B ϵ I, if α ϵ A and β ϵ B, then α*β ϵ A*B, where the symbol * stands for any operation.

Thus, using the above inclusion isotonicity principle rigorous bounds on the dimensionless operators $\Omega_{p,i}$ can be derived, since these quantities are functions of the design and operating variables throughout the process.

Visualization Tools

Visualization tools can now be used as have previously been described by Shelley and El-Halwagi (2000). Interval analysis principles (inclusion isotonicity) can be employed to define rigorous bounds on the attainable zone for the source, while allowing all design and operating variables to change according to process restrictions. Therefore, revised visualization rules will apply to the source's attainable zone and the sink's feasibility region, so as to identify optimum resource allocation, minimum fresh consumption and waste discharge, while optimizing the operating conditions for all process units.

In addition, material substitution strategies can be considered by graphically identifying superior material properties, so that available resources can be optimally allocated to yield mixtures with desirable properties, while minimizing the cost of the fresh at the same time.

Consequently, optimal material properties can be translated into material components, which possess the optimal properties (Eden et al, 2002).

Case Study

We adopt the degreasing flowsheet of the case study described by Shelley and El-Halwagi (2000) and we revise some of the data as described below. In this work, it is desirable to recycle/reuse the process source leaving the degreaser and minimize the fresh usage, while allowing the temperature and pressure of the unit to change according to process constraints. The key properties for characterizing the suitability of a solvent as an acceptable feed for the degreaser are vapor pressure (VP), density (ρ) and sulfur content (S). In particular, vapor pressure and density are functions of temperature and/or pressure. Antoine's equation describes the relationship between the source vapor pressure, VP and temperature, T:

$$\ln(1000VP) = 12.5826 - 2553.3463/(T-4.0498) \qquad (7)$$

The following empirical equation relates temperature, T and pressure, P of the source with density, ρ:

$$\rho = 976.9038 - 0.9937T + 1.416P \qquad (8)$$

In addition, the following equation was derived using existing data and regression analysis for sulfur content, S:

$$S = 359.8/T + 0.819P \qquad (9)$$

In equations (7), (8) and (9) T is in K and P is in MPa.

Tables 1, 2 and 3 indicate the property values for the fresh, the property constraints for the sink and the property boundaries for the source, along with its temperature and pressure constraints respectively.

Moreover, the following mixing rules apply to determine the property values for any mixture:

$$\overline{VP}^{1.44} = x_{fr} \cdot VP_{fr}^{1.44} + x_s \cdot VP_s^{1.44} \qquad (10)$$

$$1/\overline{\rho} = x_{fr}/\rho_{fr} + x_s/\rho_s \qquad (11)$$

$$\overline{S} = x_{fr} \cdot S_{fr} + x_s \cdot S_s \qquad (12)$$

Table 1. Fresh Properties.

Vapor Pressure, VP (MPa)	Density, ρ (Kg/m^3)	Sulfur content, S (wt%)
0.0680	621.00	0.50

Table 2. Sink Constraints on Properties.

Vapor Pressure, VP (MPa)		Density, ρ (Kg/m^3)		Sulfur content, S (wt%)	
Min	Max	Min	Max	Min	Max
0.0670	0.1060	600.00	640.00	0.00	0.80

Table 3. Source Constraints on Properties and Process Variable bounds.

Vapor Pressure, VP (MPa)		Density, ρ (Kg/m^3)		Sulfur content, S (wt%)	
Min	Max	Min	Max	Min	Max
0.0386	0.0655	670.78	689.66	1.25	1.65

Temperature, T (K)		Pressure, P (MPa)	
Min	Max	Min	Max
290	308	0.1	0.5

Next, the problem can be mapped onto the clusters domain using the aforementioned clustering technique. Here the property constraints for a sink can be transformed into constraints on clusters, which in turn define a region of acceptable feed for the sink. In this case study, we focus on the degreaser, since there are no feasible mixtures of source and fresh that pass through the absorber. As Fig.1 shows, fresh can be mixed with the source (represented by a single point in this case) at the nominal conditions (T=292K and P=0.4MPa). The optimum mixing point is the one that gives the shortest lever-arm for the fresh and satisfies the flowrate and property constraints at the same time. This point corresponds to a mixture of 87% wt fresh and 13%wt process source at the aforementioned conditions. In this case, the cost reduction is only 13%.

However, if process modifications are considered, the source's feasibility region is obtained by using the inclusion isotonicity principle of interval analysis. In particular, each of the three properties (vapor pressure, density and sulfur content) can first be transformed into clusters. Thus, bounds on properties, which are functions of the operating variables, are transformed into cluster bounds, which define the feasibility region of the source for any pertinent changes in process variables.

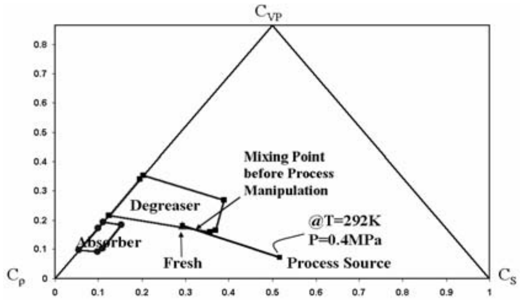

Figure 1. Ternary diagram for source/sink mapping.

Therefore, fresh can now be mixed with the source at different points within this feasibility region, as can be seen in Fig.2. There is only one optimum point, though; the point indicated in Fig.2 that gives the shortest lever-arm among all feasible source points. This point indicates the minimum consumption of fresh, while satisfying the sink's constraints on properties at the same time and corresponds to the following optimal operating conditions: Topt=308K and Popt=0.1MPa. These conditions characterize the process source with the following properties: VP=0.0655MPa, ρ=670.78 Kg/m^3 and S=1.25 %wt.

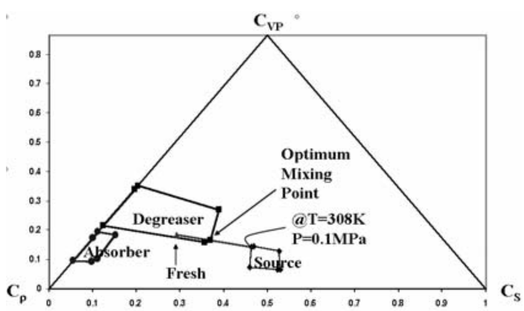

Figure 2. Ternary diagram for source/sink mapping with process modification.

Thus, the optimal solution suggests the replacement of the degreaser feed with a mixture of 40%wt source and 60%wt fresh, whereas before operating the degreaser at the optimal temperature and pressure, the fresh needed was 87%wt. Therefore, after process manipulation the additional reduction in the cost of fresh is approximately 31%, whereas after considering recycle/reuse and process manipulation the overall reduction in the cost of fresh is 40%.

The flowsheet of the metal degreasing process with the revised configuration for the optimal solution is shown in Fig.3.

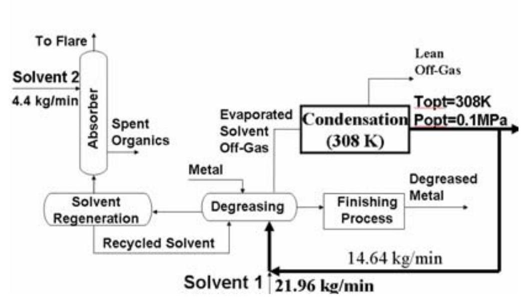

Figure 3. Process flowsheet at the optimal conditions.

Conclusions

This paper suggests the use of property-based techniques for an integrated design. In particular, visualization tools provided optimum strategies for resource allocation, unit manipulation and waste reduction.

The clustering concept was used to transfer the problem from the non-conserved property domain into the component-less cluster domain and interval analysis was employed to define rigorous bounds for properties that are functions of design and operating variables. These bounds are translated into a "trust region of clusters", which represents the feasible search domain for all possible process modifications. In addition, material substitution strategies can be considered for optimizing both the process and the material performance. Finally, a case study was presented to illustrate the applicability of the proposed method.

Acknowledgements

Financial support from the Gulf Coast Hazardous Substances Research Center and the US Environmental Protection Agency (grant# CR-831276-01-0) is gratefully acknowledged.

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