Property-based Integration for Sustainable Development

V. Kazantzi, D. Harell, F. Gabriel, Qin X., and M.M. El-Halwagi*

Department of Chemical Engineering
Texas A&M University, College Station, TX 77843-3122, USA

Abstract

This paper provides a systematic approach for optimal resource allocation, unit manipulation, and waste reduction using integrated component-less design. In particular, we identify a new procedure for determining optimal modifications in the design and operating variables of the process so as to optimize the allocation of process resources and minimize waste discharge. Interval arithmetic tools are used to derive rigorous bounds on the process performance, when all allowable changes in design and operating variables are considered. These bounds are mapped into a “trust region of clusters”, which represents the feasible search domain. In addition, material substitution strategies are considered for optimizing both the process and the fresh properties. A case study is also presented to illustrate the applicability of the proposed approach.

Keywords: property integration, sustainability, component-less design

1. Introduction

Unlike traditional process design carried out on the basis of chemical components, modern concepts on property-based integration can provide new useful tools for the development of sustainable design procedures based on key properties instead of key compounds. Higher demands for better performance of many units necessitate the optimization of targeted properties directly associated with the performance of these units and subsequently the performance of the whole process. Indeed, in the chemical processing industrial environment, there are many environmentally benign design problems that are not component dependent. Instead, they are driven by properties or functionalities of the streams and not by their chemical constituency. Therefore, the need for optimizing processes without enumerating all chemical constituents leads to the development of alternative methodologies in process design and a better understanding of the property-based allocation and manipulation of streams and sinks to achieve resource conservation and overall process integration.

2. Problem Statement

The problem to be addressed in this work can be formally 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, \( p_{pi} \), is a function of a set of design variables, \( d_{pi} \) and a set of operating variables, \( r_{pi} \)

* Author to whom correspondence should be addressed: El-Halwagi@tamu.edu
characterizing the whole process. The design variables belong to an interval \([d_{p,i}^l, d_{p,i}^u]\) dictated by design restrictions throughout the process. Similarly, the operating variables belong to another interval \([r_{p,i}^l, r_{p,i}^u]\) imposed by operating constraints throughout the system, e.g.

\[
d_{p,i}^l < d_{p,i} < d_{p,i}^u
\]

\[
r_{p,i}^l < r_{p,i} < r_{p,i}^u
\]

where \(p=1, 2, \ldots, N_p\) and \(i=1, 2, \ldots, N_s\)

Given is also a fresh source, whose cost per unit mass is \(C_f\), and a number of sinks (process units), \(N_u\), along with their property constraints

\[
p_{p,j}^l < p_{p,j} < p_{p,j}^u
\]

where \(j=1, 2, \ldots, N_u\)

In addition, there are certain constraints on the flowrates of streams that can be accepted in a sink \(j\):

\[
G_{p,j}^l < G_{p,j} < G_{p,j}^u
\]

In this paper, it is desirable to meet the objective of minimum fresh usage (and subsequently cost of fresh) using optimum strategies for process manipulation and source allocation, while satisfying all property and flowrate constraints for the sinks. In particular, our objectives are to develop visualization tools that systematically minimize the fresh consumption for the process and at the same time optimize the design and operating variables that affect the property values of the process sources. Additionally, new fresh resource substitutes will be investigated by optimizing the process variables and properties of the streams.

3. Componentless Approach

The previously stated problem can be tackled by integrating properties of streams and units throughout the process using the notion of “component-less design” introduced by Shelley and El-Halwagi (2000). This approach is based on tracking properties or functionalities by transforming them into conserved quantities known as clusters.

3.1 Clustering concept

Clusters are surrogate properties that are tailored so that both the intra- and inter- stream conservation rules hold. These main characteristics can be shown by first considering properties whose mixing rules are given by the following equation:

\[
\psi_p(p_{p,i}) = \sum_{i=1}^{N_s} x_i \psi_{p,i}(p_{p,i})
\]
where $x_i$ is the fractional contribution of the $i$th stream into the total flowrate of the mixture, $p_{p_i}$ is the property value of the mixture and $\psi_p(p_{p_i})$ is the operator on property $p_{p_i}$. This operator can be normalized into a dimensionless operator by dividing by a reference value:

$$\Omega_{p,i} = \frac{\psi_p(p_{p_i})}{\psi_p^{ref}}$$  \hspace{1cm} (6)

Also, an augmented property index (AUP) for each stream $i$ is defined as the summation of the dimensionless property operators:

$$AUP_i = \sum_{p=1}^{N_p} \Omega_{p,i}$$  \hspace{1cm} (7)

The cluster for a property $p$ in a stream $i$, $C_{p,i}$, can now be defined as follows:

$$C_{p,i} = \frac{\Omega_{p,i}}{AUP_i}$$  \hspace{1cm} (8)

One can now verify the two conservation rules for the clusters, e.g.:

$$\sum_{p=1}^{N_p} C_{p,i} = 1$$ \hspace{1cm} (intra-stream conservation)  \hspace{1cm} (9)

and

$$\bar{C}_p = \sum_{i=1}^{N} \beta_i \cdot C_{p,i}$$ \hspace{1cm} (inter-stream conservation)  \hspace{1cm} (10)

where $\bar{C}_p$ is the mean cluster resulting from mixing streams and $\beta_i$ is the cluster lever arm given by the following expression:

$$\beta_i = x_i \cdot \frac{AUP_i}{AUP}$$  \hspace{1cm} (11)

The aforementioned conservation characteristics enable the tracking of properties when mapped into the cluster domain.

It is worth mentioning here that the property mixing rules described in equation 5 apply for a system, where no reactions occur. In the case of reaction, an additional term needs to be considered for this equation to hold. However, the property mixing rules for a non-reactive system can properly be described by equation 5 for any stream or mixture whose concentration does change. The design method is component-free and therefore can apply to multiple-component streams.

3.2 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 $[a, b], a, b \in \mathbb{R}$. The inclusion isotonicity principle from interval arithmetic suggests that for $A$, $B \in I$, if $\alpha \in A$, $\beta \in B$, then $\alpha \ast \beta \in A \ast B$ (where the symbol $\ast$ stands for any operation (i.e. $+,-, \cdot, /$)).
Interval analysis will be used here to determine the limits of the property values \( p_{pl,i} \) and \( p_{pu,i} \). Knowing that any stream’s property value \( p_{pl,i} \) is a function of the design and operating variables throughout the process, we have:

\[
p_{pl,i} = f(d_{pl,i}, r_{pl,i})
\]  

(12)

Using inclusion isotonicity of interval arithmetic, we can derive the bounds on the dimensionless operator, \( \Omega_{pl} \):

\[
\Omega_{pl}^{l} \leq \Omega_{pl} \leq \Omega_{pl}^{u}
\]  

(13)

3.3 Visualization technique

Visualization tools can now be used, as have been described in previous papers, to graphically identify the minimum fresh consumption for the whole process, as well as the desirable design and operating conditions that provide the optimal strategy for resource conservation and unit manipulation. In particular, for each source interval arithmetic will be used to identify the bounds on the attainable zone for the source while allowing all design and operating variables to change. This is a one-time calculation that is guaranteed to include the attainable zone using inclusion isotonicity. Hence, the visualization rules of Shelley and El-Halwagi (2000) can be used to optimise the allocation using revised lever-arm rules. These revised rules will apply to a source zone (not a point) mapped to a sink. To illustrate the applicability of this technique a case study is presented next.

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).

4. Case Study

In this case study a metal degreasing plant is considered. A fresh organic solvent is used in the degreaser to degrease the metal parts. From the degreasing unit a process source was first flared resulting in economic loss and environmental pollution. Then, the source was recycled to the original unit at the nominal operating conditions, i.e. \( T=292K \) and \( P=0.4MPa \). It is desirable to recycle/reuse this source and minimize the fresh consumption using the optimum values for temperature and pressure. The source’s key properties for using it as fresh are vapour pressure (VP), density (\( \rho \)) and sulphur content (S). In particular, vapour pressure and density are functions of the temperature (T) and pressure (P) of the source. The equation that relates vapour pressure and temperature is Antoine’s equation:

\[
\ln(1000VP) = 12.5826 – 2553.3463/(T-4.0498)
\]  

(14)
The empirical equation that relates temperature and pressure of the process source with its density is the following:

\[ \rho = 976.9038 - 0.9937T + 1.416P \quad (15) \]

Regarding the sulphur content the following equation was derived using existing data and regression analysis:

\[ S = 359.8/T + 0.819P \quad (16) \]

In all the aforementioned equations 15, 16 and 17, T is in K and P in MPa.

Tables 1 and 2 show the property values for the fresh and the sink’s constraints on properties respectively. In addition, Table 3 shows the temperature and pressure constraints on the process source, along with the respective boundaries for the properties derived using interval analysis.

Table 1: Fresh properties

<table>
<thead>
<tr>
<th>VP (MPa)</th>
<th>Density, ( \rho ) (Kg/m(^3))</th>
<th>Sulfur content (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.068</td>
<td>621</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Table 2: Property constraints on sink’s feed

<table>
<thead>
<tr>
<th>VP (MPa)</th>
<th>Density, ( \rho ) (Kg/m(^3))</th>
<th>Sulfur content (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min</td>
<td>Max</td>
<td>Min</td>
</tr>
<tr>
<td>0.067</td>
<td>0.106</td>
<td>600</td>
</tr>
<tr>
<td>640</td>
<td>0.0</td>
<td>0.8</td>
</tr>
</tbody>
</table>

Table 3: Process variables and property constraints of process source

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Pressure (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min</td>
<td>Max</td>
</tr>
<tr>
<td>290</td>
<td>308</td>
</tr>
<tr>
<td>0.1</td>
<td>0.5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>VP (MPa)</th>
<th>Density, ( \rho ) (Kg/m(^3))</th>
<th>Sulfur content (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min</td>
<td>Max</td>
<td>Min</td>
</tr>
<tr>
<td>0.0386</td>
<td>0.0655</td>
<td>670.78</td>
</tr>
<tr>
<td>689.66</td>
<td>1.25</td>
<td>1.65</td>
</tr>
</tbody>
</table>

Then, the following mixing rules are applied to evaluate the properties resulting from mixing the source, \( s \), with fresh, \( f \):

\[ \overline{VP}^{1.44} = x_f \cdot VP_s^{1.44} + x_s \cdot VP_f^{1.44} \quad (17) \]

\[ 1/\overline{\rho} = x_f / \rho_f + x_s / \rho_s \quad (18) \]

\[ \overline{S} = x_f \cdot S_f + x_s \cdot S_s \quad (19) \]
Now, the problem can be mapped onto the cluster domain using equations (6) – (8) for
the sink constraints, the source boundaries and the fresh. As can be seen from Fig.1,
fresh can be mixed with the source at several points within source’s bounded region, but
only one point is the optimum; the point indicated in the graph that gives the shortest
lever-arm for the fresh and corresponds to the following properties: VP=0.0655MPa,
ρ=670.78Kg/m³ and S=1.25 wt%. Thus, the optimal operating variables for the unit are:
Topt=308K and Popt= 0.1MPa, as opposed to the previous non-optimal values, which
were: T= 292K and P= 0.4MPa. The optimal solution shows the replacement of the
degreaser feed with a mixture of 40% source and 60% fresh, whereas before operating
the degreaser at the optimal T and P, the fresh needed was 87.27%wt. Therefore, after
this process manipulation a reduction in fresh cost of 31.25% was achieved.

Figure 1: Ternary diagram for source/sink mapping – Case study

5. Conclusions

This paper suggests the use of property-based techniques for a sustainable integrated
design. The clustering approach was used to map the problem from the property into the
component-less cluster domain and interval analysis was employed to define boundaries
for properties that are functions of design and operating variables. Visualization tools
have provided optimum strategies for source allocation, process manipulation and
material substitution. Finally, a case study illustrated the applicability of this approach.

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