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Designing optimal bioethanol networks with purification for integrated biorefineries

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ABSTRACT

Bioethanol networks with purification for processing pathways in integrated biorefineries are targeted and designed in this work by an analytical approach not requiring graphical constructions. The approach is based on six fundamental equations involving eight variables: two balance equations for the stream flowrate and the bioethanol load over the total network system; one equation for the above-pinch bioethanol load being picked up by the minimum fresh resource and the purified stream; and three equations for the purification unit. A solution strategy is devised by specifying the two variables associated with the purifier inlet stream. Importantly, continuous targeting is then possible over the entire purifier inlet flowrate range on deriving elegant formulae for the remaining six variables. The Unified Targeting Algorithm (UTA) is utilized to establish the minimum fresh bioethanol resource flowrate and identify the pinch purity. The fresh bioethanol resource flowrate target is shown to decrease linearly with purifier inlet flowrate provided the pinch is held by the same point. The Nearest Neighbors Algorithm (NNA) is used to methodically synthesize optimal networks matching bioethanol demands and sources. A case study of a biorefinery producing bioethanol from wheat with arabinoxylan (AX) coproduction is presented. It illustrates the versatility of the approach in generating superior practical designs with up to nearly 94% savings for integrated bioethanol networks, both with and without process constraints, for grassroots as well as retrofit cases.

1. Introduction

Process integration tools broadly aim at minimizing external resource requirements through maximizing internal material reuse/recycle and energy recovery [1–3]. In turn, they endeavor to minimize adverse environmental impact and maximize profitability through sustainable process designs [4,5].

Process integration using pinch analysis as well as mathematical programming has been applied to various biorefinery configurations [6–10] including value added production pathways and combined heat and power generation [11,12]. However, as pointed out by Martinez-Hernandez et al. [13] in their seminal work, biorefinery mass integration at the product level for potential utilization of various products within the biorefinery processes to reduce material utilities and/or feedstocks has not been explored. Thus, targeting as in pinch analysis for the minimum utility [14–16] is valuable for screening and scoping of different product allocation networks as more complex and advanced process technologies emerge in biorefining.

Biofuels, being renewable or green fuels, potentially provide a sustainable way to satisfy the world's ever-increasing energy demands [17,18]; however, their production processes must be cost-effective and process designs optimal in terms of efficient use of resources. Bioethanol, a gasoline additive/substitute, is by far the most widely used biofuel for transportation worldwide [19,20]. Recently, Martinez-Hernandez et al. [13] have emphasized the need to develop new tools for the integrated processing of starch and lignocellulosic feedstocks in bioethanol production, wherein ethanol can be used as utility for biomass fractionation or pretreatment as well as chemical reactant. Their methodology, adapted from hydrogen pinch analysis [21], seeks to minimize the bioethanol requirement within the biorefinery using a graphical approach based on composite curves and a surplus diagram. However, the surplus diagram method requires transferring of data from one plot to another and is iterative [22]. Their analysis for bioethanol network design thus involves graphical construction, tedious calculation and typically several iterations; so, it is adapted to a spreadsheet tool using Excel–VBA. In general, graphical

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targeting methodologies can often be unwieldy although graphical representations in process integration can provide valuable visual insights. A purely analytical method offers various advantages including easy implementation to real-world problems with big data sets, speedy what-if analysis and high accuracy.

The aim of this work is to develop a straightforward non-iterative methodology to continuously target and design bioethanol networks over the entire purifier inlet flowrate range. The totally analytical approach proposed here requires no graphical constructions and is based on two versatile algorithms along with a set of six fundamental equations. This work thus extends the unified conceptual approach developed by Agrawal and Shenoy [23] for water and hydrogen management to biorefinery integration [24]. It involves a systems engineering methodology for the holistic understanding of the flow of a species within a process to determine its optimal allocation between sources and demands. The overall goal is to optimally allocate resources (e.g., water, hydrogen, energy, and component species) that have both a quantity (load) and a quality (level) by matching demands and sources (after appropriate mixing, if necessary). In the present context, the flow of bioethanol in a biorefinery is studied to target the minimum makeup fresh resource, and optimal bioethanol networks are designed with and without purification under known process constraints.

Here, the classic two-stage approach of pinch analysis [25,26] is followed: first, minimum bioethanol flow targets are established by the Unified Targeting Algorithm (UTA); and, second, optimal bioethanol networks are systematically designed by the Nearest Neighbors Algorithm (NNA). The major advantage of the UTA [27] and the NNA [28] is that they both provide a unified methodology. The UTA is applicable to a diverse range of process integration problems [29], including those of heat/mass exchange, water, hydrogen, nitrogen, oxygen, carbon emission, and property-based material reuse networks. Similarly, the NNA has been extensively applied for the synthesis of various resource conservation networks [2] including water networks [30,31], hydrogen networks [23], carbon emission networks [32,33], and material reuse networks [34]. Some practical applications of the NNA include industrial water conservation in a steel plant [35], zero wastewater discharge in an alumina plant [36], ultrapure water recovery scheme for wafer fabrication section in a semi-conductor plant [37], sustainable energy planning using agricultural-land/water/carbon footprint [38], and property integration in a metal degreasing process as well as hydrogen integration in a petroleum refinery [39].

In what follows, fundamental equations for bioethanol networks with purification are presented and used to study the continuous variation of the optimal targets as a function of the purifier inlet flowrate. The UTA is utilized to determine the minimum fresh bioethanol flowrate target and the pinch. The NNA is then fruitfully used for designing networks to meet the targets with and without a purifier as well as with and without process constraints. A case study is analyzed of a complex biorefinery with arabinoxylan (AX) extraction, wherein ethanol is a biorefinery product as well as a process stream, resulting in demands and sources at different purity levels. Finally, a graphical explanation of the targeting methodology is provided.

2. Methodology

2.1. Fundamental equations for bioethanol networks with purification

The fundamental balance equations for stream flowrate and component load [23] over the total network system with purification (Fig. 1) are

$$F_R - F_E = \Delta_1 \quad \text{where } \Delta_1 \equiv \sum F_d - \sum F_s \tag{1a}$$

$$F_R y_R - F_E y_E = \Delta_2 \quad \text{where } \Delta_2 \equiv \sum F_d y_d - \sum F_s y_s \tag{1b}$$

where F denotes stream flowrate, y denotes bioethanol component purity fraction, and subscripts R and E denote fresh resource and excess/waste, respectively. The net system flowrate (Δ_1) and the net system component load (Δ_2) are obtained as deficits by taking the sum of all demands (denoted by subscript d) and subtracting the sum of all sources (denoted by subscript s). Defining such net quantities (Δ) that are constant for a given network system is advantageous in resource optimization [40].

For the purification unit, the inlet stream entering at purity y_{in} is considered as a demand and the streams leaving at y_{pr} (product stream of high purity) and y_r (residue stream of low purity that typically goes to waste) as two sources [41]. For a purification process starting at an inlet purity y_{in} and achieving an outlet purity y_{pr} (at or above the pinch purity y_p), the component load balance over the above-pinch region [23] yields

$$F_R(y_R - y_p) + F_{pr}(y_{pr} - y_p) = M_p \tag{2}$$

where M denotes component load, and subscripts p and pr denote pinch and product stream of high purity, respectively.

For the purifier, the flowrate and bioethanol component load balances are simply given by

$$F_{in} = F_{pr} + F_r \tag{3a}$$
$$F_{in} y_{in} = F_{pr} y_{pr} + F_r y_r \tag{3b}$$

Further, the product purity y_{pr} and the component recovery R, as defined below, are usually specified for the purifier:

$$R = F_{pr} y_{pr} / (F_{in} y_{in}) \tag{3c}$$

Since Eqs. (1)-(3) constitute six equations in eight unknowns (F_R, F_E, F_{in}, F_{pr}, F_r, y_E, y_{in} and y_r), there are two degrees of freedom. Therefore, two variables may be specified and the equations then solved to determine the targets as discussed next.

2.2. Solution strategy for continuous targeting

Let the two variables corresponding to the purifier inlet (i.e., F_{in} and y_{in}) be specified. Then, the equations may be written in terms of F_{in}, y_{in} and other known quantities (Δ_1, Δ_2, y_R, y_p, M_p, y_{pr} and R) as follows.

Eq. (2) is rearranged using Eq. (3c) to establish the minimum flowrate target for the fresh bioethanol resource as

$$F_R = F_{R0} - K F_{in} \tag{4a}$$

where $F_{R0} = M_p/(y_R - y_p)$ and $K = (R\, y_{in}/y_{pr})(y_{pr} - y_p)/(y_R - y_p)$. Notably, the form of Eq. (4a) specifies F_{R0} as the fresh bioethanol flowrate target in the absence of a purifier.

Eqs. (1) and (4a) then yield the flowrate and purity of the excess/waste as

$$F_E = F_{R0} - \Delta_1 - K F_{in} \tag{4b}$$

$$y_E = (F_{R0} y_R - \Delta_2 - K y_R F_{in}) / (F_{R0} - \Delta_1 - K F_{in}) \tag{4c}$$

Eqs. (3a)–(3c) may be combined to obtain the outlet flowrates and the residue purity for the purifier as

$$F_{pr} = (R y_{in}/y_{pr}) F_{in} \tag{4d}$$

$$F_r = (1 - R y_{in}/y_{pr}) F_{in} \tag{4e}$$

$$y_r = y_{in}(1 - R)/(1 - R y_{in}/y_{pr}) \tag{4f}$$

As per Eq. (4a), the fresh bioethanol resource flowrate target F_R varies (decreases) linearly with the purifier inlet flowrate F_{in} provided the pinch is held by the same point [i.e., (M_p, y_p) and