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A generic methodology for processing route synthesis and design based on superstructure optimization

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ABSTRACT

In this paper, a systematic framework for novel and sustainable synthesis-design of processing routes is presented along with the associated computer-aided methods and tools. In Stage 1, superstructure optimization is used to determine the optimal processing route(s). In Stage 2, the design issues are resolved and targets for improvement are identified through the use of integrated tools. In Stage 3, new alternatives are generated using the selected route and the previously identified targets. In addition to the various computer-aided tools, two special tools are presented: (1) a database employing a specially developed knowledge representation system, and (2) Super-O, a software interface that guides users through the formulation and solution of synthesis problems. Super-O transfers data between the different tools, including a library of generic models, representing a wide range of processing options. Application of the synthesis and design stages is highlighted through two case studies (biorefinery and carbon capture-utilization).

1. Introduction

Finding novel and more sustainable production systems is an important step towards addressing the grand challenges of energy, water, environment and food currently faced by modern society. Significantly better and/or new processing routes are needed to, just to name a few, convert available resources to useful products, recycle unused material, and reprocess used material, without negatively impacting sustainability of modern society. The synthesis-design of processing routes is receiving increasing attention, not only due to the scope and significance of the problems that it covers, but also because of its industrial relevance. A processing route is a combination of raw materials, a series of processing steps to convert them, and products which they can be converted to; each processing step has various alternatives in terms of processing technologies, giving rise to a superstructure of alternatives. The synthesis-design problem is formulated as a superstructure optimization problem, solved to obtain the optimal network topology along with the values of continuous variables (such as operating conditions), from a superstructure of alternatives. Due to its decision-making nature, the synthesis-design problem involves a combination of continuous and discrete variables, hence leading to its formulation as a mixed-integer nonlinear programming (MINLP) problem.

From a process systems engineering point of view, the wide application range of the synthesis-design of processing routes provides opportunities to develop and employ systematic and generic solution approaches. This class of problems involve data (sometimes large amounts of data) coming from different sources; generation and evaluation of all possible alternatives; mathematical representation of the alternatives; solution of the mathematical programming (optimization) problem. That is, a computer-aided tool to solve such problems is ideal and important and should: support efficient data-management; provide versatile superstructure generation and flexible generic modeling; allow for fast and robust numerical solution; and implement the workflows and data flows corresponding to synthesis-design methodologies.

Abbreviations: BR, Brazil; CA, Canada; CN, China; DMC, dimethyl carbonate; DME, dimethyl ether; EC, ethylene carbonate; EG, ethylene glycol; EO, ethylene oxide; IN, India; MEA, monoethyl amine; MeOH, methanol; MILP, mixed-integer liner programming; MINLP, mixed-integer nonlinear programming; MX, Mexico; NC, number of components; NDV, number of discrete variables; NEQ, number of equations; NF, number of feedstocks/raw materials; NI, number of processing intervals; NL, Number of geographic locations; NP, number of products; NR, number of reactions; NS, number of processing steps; NU, number of utilities; NV, number of variables; PC, propylene carbonate; PG, propylene glycol; PO, propylene oxide; PSIN, Processing Step-Interval Network; TH, Thailand; US, United States.

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Nomenclature

Subscripts

CO_2	Carbon dioxide
i	Component
j	Utility
k	Processing interval
kk	Processing interval (alias)
l	Geographic location
r	Reaction
react(i)	Subset of key reactant components
step	Processing step

Superscripts

AC	Added chemicals and solvents
CAP	Capital expenditures
D	Disaggregated flow
IN	Inlet in a processing interval
L	Lower bound
M	Outlet of mixing task
OUT, P	Primary outlet of product separation task
OUT, S	Secondary outlet of product separation task
P	Primary
PROD	Product
R	Outlet of reaction task
RAW	Feedstock/Raw material
S	Secondary
U	Upper bound
UT	Utilities
TR	Transportation
W	Outlet of waste separation task

Continuous variables

C	Cost
f	Component flow rate
F	Total flow rate
g	Added/removed component/utility flow rate
Indirect	Indirect emissions (resulting from energy, for example heating, compression)
Net	Overall emission balance
S	Sales
UtilizedUtilized	Utilized emissions
Z	Objective function (profit)

Binary variables

x	Allocation of process interval in location (binary)
y	Selection of process intervals (binary)

Parameters

AVAIL	Availability
DEM	Demand
S	Superstructure connection (binary)
M	Large number for Big-M
MW	Molar weight
P	Price
β	Specific consumption of utility with respect to stream flowrate in utility point
δ	Fraction separated as waste
γ	Stoichiometric coefficient
μ	Ratio of chemical consumption with respect to reference compound
υ	Allocation of intervals to a process step (binary)
σ	Fraction separated as primary product
θ	Conversion
τ	Project lifetime

The shift from crude oil to biomass feedstocks for the production of chemicals and fuels requires suitable methods and tools for synthesizing, evaluating and selecting process alternatives, and for designing promising processes. Systematic process synthesis and design methods have been developed for traditional chemical processes. Systematic frameworks with a mathematical programming approach have been applied to synthesis-design of biorefineries by various authors: thermochemical fuels from biomass (Gassner and Maréchal, 2009), bioethanol production from lignocellulosic biomass (Martín and Grossmann, 2010), a multi-product biorefinery problem including gasoline production (Zondervan et al., 2011) and biodiesel production from microalgae (Rizwan et al., 2015). Generic frameworks for synthesis of processing networks have been proposed (Baliban et al., 2011 and Quaglia et al., 2012a). Supply chain considerations have been included in synthesis problems for biorefinery networks (Cucek et al., 2013, 2010; Garcia and You, 2015). Recently, González-Delgado et al. (2015) suggested a combined method for the synthesis of a microalgae-based biorefinery, starting with identification of promising pathways via a hierarchical approach and continuing with superstructure optimization. The synthesis and design of downstream processes in biorefineries was addressed by Corbetta et al. (2016) through an interface between an optimization environment and a process simulator. In terms of modeling, a library of equation-based models for design of biofuel production processes using superstructure optimization was developed by Martin and Grossmann (2012). With regard to data management for biomass processing networks, Trokanas et al. (2015) designed and implemented an ontology in the domain of biorefining. However, an important issue not considered in detail is the issue of economic feasibility of biorefinery products versus variations in availability, characteristics and costs of biomass in different geographic locations. Moreover, unlike crude oil, each different biomass source provides a different feedstock in terms of chemicals, their composition and properties, and even the same feedstock varies in its characteristics based on the region and climate. Therefore, unlike the optimal petrochemical refinery, the optimal biorefinery network problem needs to have location-dependent solutions.

In addition, as the global population increases, demands for products, energy, and natural resources continue to rise (United Nations Population Fund, 2015). As a result of the growing consumption and production, there is more waste and emissions being produced and emitted into the atmosphere (United Nations Population Fund, 2016), and, carbon dioxide (CO_2) is the most prevalent greenhouse gas constituting over 80% of greenhouse gas emissions (IPCC, 2014). Methods to reduce the concentration of carbon dioxide in the atmosphere, including carbon dioxide capture, utilization and storage, are needed. Carbon dioxide capture and utilization is a promising method, in addition to carbon capture and storage, which removes the carbon dioxide from emission streams and reuses it or transforms it to commercial products. Superstructure optimization has been performed to optimize carbon capture processes to determine: the adsorbents for pressure/vacuum swing distillation (Leperi et al., 2015), the best capture method (chemical absorption, membrane, pressure swing adsorption, vacuum swing adsorption) for an emission source (Hasan et al., 2012), and the optimal supply chain for carbon capture, utilization and sequestration (Hasan et al., 2014). These works reflect progress in the optimization of the types of capture depending on the source and what quantities to utilize and sequester. However, they represent a fixed utilization scenario, enhanced oil recovery (EOR) and sequestration scenario; superstructure optimization has not been applied to determining the optimal utilization path considering chemical conversion.

An integrated business and engineering framework was developed by Quaglia et al. 2012a consisting of a step-by-step procedure