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

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).

A Generic Methodology for Superstructure Optimization of Different Processing Networks

In this paper, we propose a generic computer-aided methodology for synthesis of different processing networks using superstructure optimization. The methodology can handle different network optimization problems of various application fields. It integrates databases with a common data architecture, a generic model to represent the processing steps, and appropriate optimization tools. A special software interface has been created to automate the steps in the methodology.
A Generic Methodology for Superstructure Optimization of Different Processing Networks

A large focus is placed on sustainability and sustainable practices as a result of the arising environmental issues. As an element of this, sustainable process synthesis and design becomes important. A generic, systematic methodology is proposed for solving the problem of optimal design of sustainable processing networks containing three stages: (i) synthesis stage, (ii) design stage, and (iii) innovation stage. In this work, a focus is placed on the first stage, the synthesis stage. Process synthesis becomes necessary in determining the appropriate processing routes to produce a selection of products from a set or feedstock. The problem to be solved here is the following: for a given set of raw materials, products and a network of processing routes, determine the optimal processing route from a sustainability point of view. Three different processing networks arising from chemical processes, biorefineries, and carbon dioxide utilization are considered. In the synthesis stage, the processing alternatives are represented in a superstructure and the associated data is collected and stored in a database. Once a specific process synthesis problem is formulated, the existing superstructure is retrieved and reduced in order to include only the relevant alternatives. New alternatives can easily be added and stored in the database. The superstructure of alternatives in the network is then represented using a generic data-independent process model, which yields a mixed integer linear or nonlinear programming problem. The proposed methodology involves the use of additional methods and tools, such as a database and an external software for solving the network optimization problem. The database has been created using an ontology-based knowledge representation consisting in various layers of data and interconnections between them. Using a common database structure for any process synthesis problem allows for easy data collection, storage and retrieval, as well as giving the possibility of solving combined problems that have been previously solved independently. The step-by-step methodology has been implemented in a software interface that guides the user through the problem formulation and solution steps and integrates the various methods and tools for efficient flow of information between them. By using this interface, the user can retrieve and/or modify existing networks and alternatives from the database, as well as add new alternatives and connections between them. With the generated superstructure of alternatives and the corresponding data, an input file for GAMS is automatically created. This input file contains values of all the parameters of the generic process model. Then, the problem is solved in GAMS and the interface shows the results and allows for the selection of alternatives. The output from the synthesis stage (the first stage) is the optimal processing route for the defined problem and scenario, which can be transferred to a rigorous process simulator for the second stage (design stage). Here, the selected route needs to be further designed, simulated and analyzed. Then, more sustainable innovative designs can be developed in the third stage based on the output design from the second stage. This generic methodology and software interface can be applied to an array of problems within synthesis of processing networks. This is illustrated through case studies from two applications: the synthesis of biorefinery networks and the synthesis of sustainable carbon dioxide utilization processes.
A grand model for chemical product design

Chemical engineering has been expanding its focus from primarily business-to-business products (B2B) to business-to-consumer (B2C) products. The production of B2B products generally emphasizes on process design and optimization, whereas the production of B2C products focuses on product quality, ingredients and structure. Market and competitive analysis, government policies and regulations have to be explicitly considered in product design. All these considerations are accounted for in the Grand Product Design Model, which consists of a process model, a property model, a quality model, a cost model, a pricing model, an economic model as well as factors such as company strategy, government policies and regulations. This article introduces the model and highlights selected aspects of the model with two case studies. One is a die attach adhesive that illustrates how pricing affects profitability, and how product composition changes with market conditions. Another is a hand lotion that illustrates how product quality affects the profit. (C) 2016 Elsevier Ltd.

General information
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Hong Kong University of Science and Technology
Contributors: Fung, K. Y., Ng, K. M., Zhang, L., Gani, R.
Pages: 15-27
Publication date: 2016
Peer-reviewed: Yes

Publication information
Journal: Computers and Chemical Engineering
Volume: 91
ISSN (Print): 0098-1354
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1 SNIP 1.616
Web of Science (2016): Impact factor 3.024
Web of Science (2016): Indexed yes
Original language: English
Keywords: Product design, Product ingredients, Product structure, Product price, Government policies


This work proposes an integrated model-based framework for chemical product design and evaluation based on which the software, VPPD-Lab (The Virtual Product-Process Design Laboratory) has been developed. The framework allows the following options: (1) design a product using design templates, such as, single molecule products, formulated products, blended products, emulsified products and devices; (2) analyze the product by performing virtual experiments (product property and performance calculations); (3) create and add new product property and product performance models; (4) create new product design templates when the desired template is not available. The product design templates follow the same common steps in the workflow for a product type but have options to employ product specific property models, data and calculation routines, if necessary. This paper highlights the application of the templates for three case studies: (i) the design of a refrigeration cycle, (ii) a mixtureblend design problem involving lubricant design and (iii) a tailor-made product design of jet-fuels (blended chemical products).

General information
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Kalakul, S., Cignitti, S., Zhang, L., Gani, R.
Publication date: 2016

Host publication information
Title of host publication: Proceedings of the 26 European Symposium on Computer Aided Process Engineering - ESCAPE 26
Publisher: Elsevier
ISBN (Print): 978-0-444-63428-3
Keywords: Chemical product design, Blended product, Refrigeration cycle
New Vistas in Chemical Product and Process Design

Design of chemicals-based products is broadly classified into those that are process centered and those that are product centered. In this article, the designs of both classes of products are reviewed from a process systems point of view; developments related to the design of the chemical product, its corresponding process, and its integration are highlighted. Although significant advances have been made in the development of systematic model-based techniques for process design (also for optimization, operation, and control), much work is needed to reach the same level for product design. Timeline diagrams illustrating key contributions in product design, process design, and integrated product-process design are presented. The search for novel, innovative, and sustainable solutions must be matched by consideration of issues related to the multidisciplinary nature of problems, the lack of data needed for model development, solution strategies that incorporate multiscale options, and reliability versus predictive power. The need for an integrated model-experiment-based design approach is discussed together with benefits of employing a systematic computer-aided framework with built-in design templates.

A New Optimization Model for Computer-Aided Molecular Design Problems

Computer-Aided Molecular Design (CAMD) is a method to design molecules with desired properties. That is, through CAMD, it is possible to generate molecules that match a specified set of target properties. CAMD has attracted much attention in recent years due to its ability to design novel as well as known molecules with desired properties. The attention is in particular targeted at the design of chemical based products, such as solvents, refrigerants, active pharmaceutical ingredients, polymers, surfactants, lubricants, and more [1]. Property prediction methods are needed in molecular design, as they enable the prediction of the target properties of the generated candidate molecules from there structural information. Here, CAMD methods can be regarded as the reverse engineering approach to property prediction, as the target properties are known while the molecules that match them need to be determined. In this way, CAMD problems can be formulated as a Mixed Integer Linear/Non-Linear Program (MILP/MINLP). With the advent of connectivity-based prediction methods, several researchers have developed new strategies for embedding it with CAMD method. Constantinou et al. [2] proposed a systematic strategy for generating isomers from a set of groups. Harper et al. [3] proposed a framework for CAMD method, where the pre-design phase defines the basic needs, the design phase determines the feasible candidates (generates molecules and tests for desired properties) and the post-design phase performs higher level analysis of the molecular structure and the final selection of the product. Samudra and Sahinidis [4] proposed a new optimization model using relaxed property targets and refined property targets with structural corrections. It is usually difficult to model and solve the MILP/MINLP problem with structure information considered due to the increased size of the mathematical problem and number of alternatives. Thus, decomposition-based approach is proposed to solve the problem. In this approach, only first-order groups are considered in the first step to obtain the building block of the designed molecule, then the property model is refined with second-order groups based on the results of the first step.
However, this may result in the possibility of an optimal solution being excluded. Samudra and Sahinidis [4] used property relaxation method in the first step to avoid this situation, but it is not always easy for the users to find the appropriate relaxations. On the other hand, the feasible region of the optimization problem will become larger when relaxations are applied, which makes the solution of the problem harder. In this paper, a new model for CAMD problems is proposed. The model has been developed for the consideration of higher order groups in the molecular generation step of CAMD through mathematical optimization [5]. The model can consider both first and second order groups simultaneously in the MILP/MINLP formulation through a set of mathematical constraints. Structural constraints are defined through a set of linear mathematical equations for the feasible generation of molecules and the connectivity of molecular groups through the adjacency matrix. Property constraints are defined from a set of linear constraints based on the group contribution method [2]. The structural information of the molecule is obtained from the solution of the adjacency matrix. The adjacency matrix provides the adjacent connectivity of first order molecular groups. From this, the second order group description is found, which increases the structural information and property prediction accuracy. This will avoid the possible situation in which the optimal point is excluded from the feasible region due to inaccurate property prediction and ensures the obtainability of a global optimal solution. The model is implemented into a GAMS-based environment for the efficient optimization of a given problem. The model applicability will be demonstrated through the solution of a range of product design problems from literature, such as design of simple molecules (solvents and refrigerants) to design of complex molecules (polymers, lipids and surfactants).

**General information**
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Cignitti, S., Zhang, L., Gani, R.
Number of pages: 1
Publication date: 2015
Peer-reviewed: Yes
Event: Abstract from 2015 AIChE Annual Meeting, Salt Lake City, United States.
Electronic versions: Abstract_A_New_Optimization_Model_for_Computer_Aided_Molecular.pdf
Research output: Contribution to conference › Conference abstract for conference – Annual report year: 2015 › Research › peer-review

**Computer-Aided Chemical Product Design Framework: Design of High Performance and Environmentally Friendly Refrigerants**

Refrigerants are widely used in household and industrial applications, such as processes for energy transfer from low grade heat sources. Refrigerants are utilized in heat pump cycles for moving heat from one source to another with the task to heat or to refrigerate. Environmental issues have been a driving force for the industry to continuously seek novel refrigerants as current refrigerants risk phasing out due to environmental regulations. This trend has been seen since the Kyoto Protocol in 1997 and recently from the EU regulations from 2014, which will restrict the use of some known refrigerants today (Mota-Babiloni et al., 2015). However, design of new refrigerants poses a great challenge and finding an optimum solution for a given application often faces trade-off issues between cycle performance and environmental criteria. In addition, following issues are still to be addressed. What target properties and needs should carefully be selected for a given heat pump cycle to ensure that an optimum refrigerant is found? How can cycle performance and environmental criteria be integrated at the product design stage and not in post-design analysis? Computer-aided product design methods enable the possibility of designing novel molecules, mixtures and blends, such as refrigerants through a systematic framework (Cignitti et al., 2015; Yunus et al., 2014). In this presentation a computer-aided framework is presented for chemical product design through mathematical optimization. Here, molecules, mixtures and blends, are systematically designed through a decomposition based solution method. Given a problem definition, computer-aided molecular design (CAMD) problem is defined, which is formulated into a mixed integer nonlinear program (MINLP). The decomposed solution method then sequentially divides the MINLP into smaller sub-problems; (i) MILP for molecular structure generation, (ii) LP for pure property constraints, (iii) NLP for mixture/blend constraints, (iv) NLP for process constraints. With this, it is ensured that the MINLP is feasible to solve and that a global optimum is reachable. The method is applied on refrigerant design for a heat pump cycle. It is shown how the presented framework can generate optimal novel refrigerants that are high performing and environmentally friendly. This is achieved through integrated product-process based optimization objective, namely, target physicochemical and environmental properties for refrigerant design and target heat pump cycle performance.

**General information**
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Computer Aided Process Engineering Center
Contributors: Cignitti, S., Zhang, L., Gani, R.
Number of pages: 1
Publication date: 2015
Peer-reviewed: Yes
Event: Abstract from 10th European Congress of Chemical Engineering, Nice, France.
Computer-aided Framework for Design of Pure, Mixed and Blended Products

Design of novel chemical products with process and application considerations is an emerging topic in the field of chemical and biochemical engineering. Methods, such as Computer Aided Molecular Design (CAMD) [1] and Computer-aided Mixture and Blend Design (CAMbD) [2], provide the possibility of designing such products. However, these product design problems can quickly become large and difficult, if not infeasible, to solve through mathematical optimization. In addition, considerations of process, application, special product attributes, economic feasibility, environmental and sustainability metrics that must be included in today's product designs, consequently makes the problem harder to mathematically formulate and to solve. In this work, a framework for computer-aided design of pure, mixed and blended chemical products has been developed. The framework is a systematic approach to formulate and solve CAMbD problems through four sequential steps. In the first step, the needs, target properties and product type are defined. In the second step, the CAMbD is formulated together with objectives and process/application model. In the third step, the formulation is then converted into a mixed integer non-linear program (MINLP). In step four, the MINLP is directly solved (if possible) or sequentially solved through a decomposed optimization approach. The decomposed approach can solve a large MINLP by decomposing it into a smaller set of sub-problems. The framework application is highlighted through a solvent design case study.

General information
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Cignitti, S., Zhang, L., Gani, R.
Number of pages: 1
Pages: 234
Publication date: 2015

Host publication information
Title of host publication: Book of abstracts for PSE-2015/ESCAPE-25
Editors: Bertran, M., Bisgaard, T., Frauzem, R.
Article number: 1130
ISBN (Print): 978-87-93054-72-1

Bibliographical note
Track 9.1. Molecular Systems Engineering

Research output: Contribution to conference › Conference abstract for conference – Annual report year: 2015 › Research › peer-review

Computer-aided Framework for Design of Pure, Mixed and Blended Products

This paper presents a framework for computer-aided design of pure, mixed and blended chemical based products. The framework is a systematic approach to convert a Computer-aided Molecular, Mixture and Blend Design (CAMbD) formulation, based on needs and target properties, into a mixed integer non-linear program (MINLP). The MINLP is sequentially solved through a decomposed optimization approach to solve the possibly large MINLP in a smaller set of sub-problems. The framework application is highlighted through a solvent design case study.

General information
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Cignitti, S., Zhang, L., Gani, R.
Number of pages: 6
Pages: 2093-2098
Publication date: 2015

Host publication information
Title of host publication: Proceedings of the 25th European Symposium on Computer Aided Process Engineering
Volume: 37
Publisher: Elsevier
Editors: Gernaey, K. V., Huusom, J. K., Gani, R.
(Computer Aided Chemical Engineering).
Keywords: Product Design, Mixture, Blend, CAMD, MINLP
DOIs: 10.1016/B978-0-444-63576-1.50043-1
Generic Mathematical Programming Formulation and Solution for Computer-Aided Molecular Design

This short communication presents a generic mathematical programming formulation for Computer-Aided Molecular Design (CAMD). A given CAMD problem, based on target properties, is formulated as a Mixed Integer Linear/Non-Linear Program (MILP/MINLP). The mathematical programming model presented here, which is formulated as an MILP/MINLP problem, considers first-order and second-order molecular groups for molecular structure representation and property estimation. It is shown that various CAMD problems can be formulated and solved through this model.

General information
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Zhang, L., Cignitti, S., Gani, R.
Pages: 79-84
Publication date: 2015
Peer-reviewed: Yes

Publication information
Journal: Computers & Chemical Engineering
Volume: 78
ISSN (Print): 0098-1354
Ratings:
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.04 SJR 1.108 SNIP 1.49
Web of Science (2015): Impact factor 2.581
Web of Science (2015): Indexed yes
Original language: English
Keywords: Molecular design, CAMD, Chemical structure, Group contribution, MILP/MINLP
Electronic versions:
1.s2.0_S0098135415001234_main_2_.pdf. Embargo ended: 01/05/2017
DOIs:
10.1016/j.compchemeng.2015.04.022
Source: PublicationPreSubmission
Source-ID: 108552667
Research output: Contribution to journal › Journal article – Annual report year: 2015 › Research › peer-review

Systematic Computer-Aided Framework for Sustainable Chemical Product Design

Computer-aided product design (CAPD) is a method for the generation and selection of novel pure, mixed and blended chemical products [1]. In CAPD, the chemical product is generated and selected based on defined structure, property and process/application constraints. Several challenges exist for CAPD, including the accuracy of the property estimation, molecular structure generation, inclusion of sustainability, process and application targets and needs in the problem formulation. CAPD has been widely utilized for the synthesis of several types of products, such as solvents, polymers, fuels and formulated products [2]. However, for product design problems where the process needs and sustainability possess demanding constraints, the complexity of the problem is increased as the relation between product property, sustainability and process criteria is difficult to mathematically define. In this work, a generic computer-aided framework for chemical product design is presented through a systematic framework. A CAPD problem for the generation of novel pure, mixed and blended chemical products is formulated and solved through the application of four sequential steps. In step (1), the product design problem is defined together with the process and/or application boundaries. In step (2), the CAPD problem is formulated through property constraints for pure, mixed and blended products, process/application constraints and objective function. The property constraints are carefully selected for the thermophysical property needs and the process/application needs. Process/application and property needs are connected through an analysis of the property influence on the process/application models and thermodynamic relations. The sustainability is considered through product and process/application performance, economics and environmental impact. In step (3), the CAPD formulation is converted into a mixed-integer nonlinear program (MINLP) by set-up of constraints, objective and boundaries defined in step (2). In step (4), the MINLP is solved through a decomposed approach [3]. The decomposed approach breaks down the MINLP problem into a sub-set of programs to manage the complexity: mixed-integer linear program (MILP) for molecular generation, linear program (LP) for property constraints, non-linear program (NLP) for mixture/blended property constraints, and NLP for process constraints and objective function. This approach ensures that the optimal chemical product can be found through systematic generation and screening of alternatives based on the problem definition. The framework is implemented into a GAMS-based tool. The application of the framework is demonstrated through sustainable working fluid design for a heat pump cycle. Working fluids used in heat pumps are continuously regulated due to the environmental issues, such as ozone depletion or global warming potential. Many of the currently used working fluids are soon to be phased out [4]. The design of novel working fluids is a challenging task as retro-fitting as well as re-designing demand increased sustainability and minimal trade-off with system performance. In the CAPD formulation, the product properties are related to the needs of heat pump cycle and its components through sensitivity analysis of the
thermodynamic models and energy balances of the system. Furthermore, simple models are included for efficient
evaluation of the sustainability and design criteria of both the cycle and its components. It will be demonstrated that the
working fluid product designed is optimal with respect to the sustainability and the heat pump cycle performance.

General information
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Cignitti, S., Zhang, L., Kalakul, S., Gani, R.
Number of pages: 1
Publication date: 2015
Peer-reviewed: Yes
Event: Abstract from 2015 AIChE Annual Meeting, Salt Lake City, United States.
Electronic versions:
Abstract_Systematic_Computer_Aided_Framework_for_Sustainable_C.pdf
URLs:
Research output: Contribution to conference › Conference abstract for conference – Annual report year: 2015 › Research › peer-review

Projects:

THERMCYC: Advanced thermodynamic cycles utilising low-temperature heat sources
Energy sources at a low temperature level are available from a variety of sources ranging from waste heat from ships, industry and refrigeration plants, to renewable energy in the form of biomass, geothermal and solar.
There is significant potential for improving the use of these sources in developing new cycles based on new multi-
component fluid mixtures. These improvements will not only increase the efficiency of today's technology, but they will also make it possible to use low-temperature sources which, due to lack of technical feasibility or economy is not used today. This ambitious, interdisciplinary project will lead the way to innovative thermal system for electricity generation, heat pumping and cooling by utilization of low value sources, at efficiencies that surpasses today’s level significantly. The project will develop advances in the design of both processes and media so that energy savings of 15% can be achieved.
The analysis will include numerical simulation and advanced thermodynamic methods based on energy and exergy analysis and experimental verification of component performance. The development of a systematic approach to the optimization of cycle and the working medium in the given application. The results will provide a scientific basis for choosing the future use of low-temperature resources in Denmark. This may contribute significantly to the development of the future society using no fossil resources, but large amounts of fluctuating renewable energy.
Elmegaard, B., Project Manager, Department of Mechanical Engineering, Thermal Energy
Haglind, F., Project Participant, Department of Mechanical Engineering, Thermal Energy
Clausen, L. R., Project Participant, Department of Mechanical Engineering, Thermal Energy
Kærn, M. R., Project Participant, Department of Mechanical Engineering, Thermal Energy
Markussen, W. B., Project Participant, Department of Mechanical Engineering, Thermal Energy
Sin, G., Project Participant, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Gani, R., Project Participant, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Meroni, A., PhD Student, Department of Mechanical Engineering, Thermal Energy
Andreasen, J. G., PhD Student, Department of Mechanical Engineering, Thermal Energy
Cignitti, S., PhD Student, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Frutiger, J., PhD Student, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Babi, D. K., Project Participant, Department of Mechanical Engineering, Thermal Energy
Mancini, R., Project Coordinator, Department of Mechanical Engineering
Pierobon, L., Project Participant, Department of Mechanical Engineering, Thermal Energy
Zühlsdorf, B., Project Participant, Department of Mechanical Engineering, Thermal Energy
Zühlsdorf, B., Project Participant, Department of Mechanical Engineering, Thermal Energy
Collaborators: Maersk Group, Technical University of Munich, Danfoss AS, Arla Foods, Alfa Laval AB, MAN Diesel and Turbo, Viegand Maagée A/S, Delft University of Technology, Alfa Laval Copenhagen A/S, Aalborg University, Danish Technological Institute
Project: Research