Integrated Approach to Computer Aided Process Synthesis

This paper presents an integrated approach to the solution of process synthesis, design and analysis problems. Integration is achieved by combining two different process synthesis techniques, one based on thermodynamic insights and the other based on structural optimisation, together with a simulation engine and a properties prediction package. Process flowsheets with or without reaction blocks are considered in this paper. Results from three illustrative case studies, highlighting different features of the integrated approach, are presented. (C) 2001 Elsevier Science Ltd. All rights reserved.

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Contributors: Gani, R., Hostrup, M., Kravanja, Z., Grossmann, I., Sorsak, A.
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Tools for Reactive Distillation Column Design: Graphical and Stage-to-Stage Computation Methods

Based on the element mass balance concept, a graphical design method and a stage-to-stage multicomponent design method for reactive distillation columns have been developed. For distillation columns comprising reactive and non-reactive stages, a simple design strategy based on reactive and non-reactive bubble point calculations is proposed. This strategy tracks the conversion and temperature between the feed and the end stages of the column. An illustrative example highlights the verification of the design strategy through rigorous simulation.

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Using Driving Force Based Separation Efficiency curves within an Integrated System for Process Synthesis/Design

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Solvent Based Separation: Solvent Selection

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Systematic methodologies for chemical reaction analysis

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A new integrated framework for synthesis and design of process flowsheets

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An integrated computer aided system (ICAS) for educational purposes

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Design of environmentally benign processes: Integration of solvent design and separation process synthesis

This paper presents a hybrid method for design of environmentally benign processes. The hybrid method integrates mathematical modelling with heuristic approaches to solving the optimisation problems related to separation process synthesis and solvent design and selection. A structured method of solution, which employs thermodynamic insights to reduce the complexity and size of the mathematical problem by eliminating redundant alternatives, has been developed for the hybrid method. Separation process synthesis and design problems related to the removal of a chemical species from process streams because of environmental constraints are particularly suited for solution with the hybrid method. Application of the hybrid method is highlighted through two illustrative examples. The first example involves the determination of an optimal flowsheet for the removal of a chemical species from an azeotropic mixture and the second example involves the determination of environmentally benign substitute solvents for removal of a chemical species from wastewater. (C) 1999 Elsevier Science Ltd. All rights reserved.

Integration of thermodynamic insights and MINLP optimisation for the synthesis, design and analysis of process flowsheets

This paper presents an integrated approach to the solution of process synthesis, design and analysis problems. Integration is achieved by combining two different techniques, synthesis based on thermodynamic insights and structural optimization together with a simulation engine and a properties prediction package. Results from three case studies, highlighting different features of the integrated approach, are presented.

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Integration of thermodynamic insights and MINLP optimization for the synthesis of process flow sheets

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An Integrated Computer Aided Approach for Environmental Studies

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An Integrated Computer-Aided Approach for Environmental Studies
A general framework for an integrated computer-aided approach to solve process design, control, and environmental problems simultaneously is presented. Physicochemical properties and their relationships to the molecular structure play an important role in the proposed integrated approach. The scope and applicability of the integrated approach is highlighted through examples involving estimation of properties and environmental pollution prevention. The importance of mixture effects on some environmentally important properties is also demonstrated.

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