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Integrated Knowledge Based System for Process Synthesis

Abdullah Alqahtani,[a] Klaus Hellgardt,[b] Richard Holdich [a], Iain Cumming [a]

[a]*Department of Chemical Engineering, Loughborough University, Loughborough, Leicestershire, LE11 3TU, UK, a.alqahtani@lboro.ac.uk*
[b]*Department of Chemical Engineering and Chemical Technology, Imperial College London, London, SW7 2AZ, UK.*

Abstract

The combined use of heuristics such as expert systems, databases, mathematical process simulators, equipment sizing and cost estimation is a potential way of exploring improved chemical process synthesis. We report on the development of a software that integrates knowledge based system with HYSYS process simulator and Icarus economic evaluator utilising knowledge from existing processes to obtain heuristic rules. The structure and the systematic procedure of the proposed Integrated Knowledge Based System (IKBS) have been discussed. The prototype IKBS has been applied for the selection of reactor systems for the ethylene oxide and ethylene glycol manufacturing processes. Analysis by the software suggests the use of two reactor systems and a list of suitable reactors. The list contained new and currently used reactors in addition to the recommended reactors by industrial research.

Keywords: Chemical process synthesis, chemical reactor system selection, knowledge based system.

1. Introduction

Process synthesis is one of the most important areas of chemical process design as it deals with the problem of how to develop and integrate flowsheets for a chemical product manufacturing processes. Since Rudd [1] proposed the first method for process synthesis, several works have been published based on the systematic generation of a flowsheet, evolutionary modification, and superstructure optimization. Due to the fact that process synthesis problems are by nature combinatorial and open ended, a number of different approaches have been proposed. The two main approaches for process synthesis are heuristic methods which consist of a series of heuristic rules to screen process alternatives and the mathematical methods which rely on optimization techniques. When only heuristics are used, optimal design is not guaranteed and the method is limited to the state of knowledge. The mathematical programming methods restrict design considerations to the proposed superstructure and only limited size problems can be handled [2]. Based on the previous research efforts on process synthesis, existing approaches mostly use heuristics based on the study of reactors and separation systems in isolation. Therefore, the synthesis of a total process flowsheet using a practical method has not yet been fully investigated.

2. Problem Statement and Background

The objective of this research is to develop an Integrated Knowledge Based System (IKBS) for the synthesis of a complete chemical process flowsheet. This work has been structured around two themes, the structure of a hierarchical knowledge base, and the development of software that can provide an automation of the synthesis procedure to exploit interactions between reaction and separation. This research differs from the previous research work in the following aspects:

- It integrates knowledge based systems with third-party process simulators and economic evaluators,
- The developed flowsheet includes alternative advanced unit operations,
- The capability to synthesis multiple reactor-separator-recycle systems,
- The use of databases to obtain physical properties, safety and environmental impacts, and prices instead of relying on the user to provide them,
- The knowledge base uses existing processes to obtain heuristic rules,
- A wide range of petrochemical processes is used to validate the software decision.

3. Process Synthesis Approach

A Knowledge Based System (KBS) is essentially a computer program that has a specialised knowledge about a specific area and solves a specific class of problems using that knowledge [3]. The structure of the proposed IKBS is illustrated in Figure 1. Excel Visual Basic for Application (VBA) is being used as a tool to provide the basic elements of the knowledge based system. IKBS makes use of available internal and external databases. Aspen open simulation environment (OSE) is being used as a tool for interfacing Aspen HYSYS with Excel worksheets. Aspen Icarus Process Evaluator (IPE) is a tool to extend the results of HYSYS to generate rigorous size and cost estimates for processing equipment, and to estimate operating costs [4]. This structured method allows systematic identification of the most economical process flowsheet.

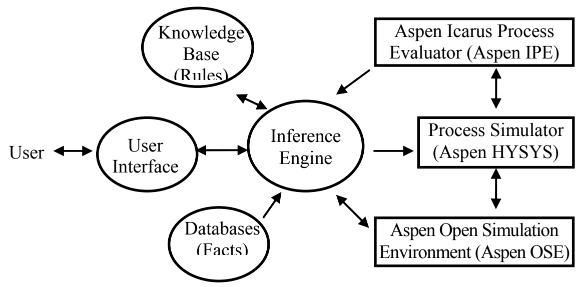

Figure 1: Structure of the Integrated Knowledge Based System (IKBS) for process synthesis

3.1. Total flowsheet Synthesis Systematic Procedure

The proposed strategy integrates heuristics with process simulation and economic evaluation in a set of synthesis levels as illustrated in Figure 2. The user starts to specify some process data required by IKBS to build a knowledge base for the process in a form of input/output information. Economic potential is used to eliminate some of the alternatives that are not economically viable.

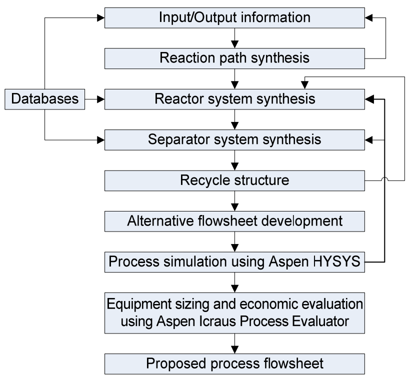

Figure 2: Flowchart of IKBS steps

The main task of the separation system synthesis consists of selecting the type, location, sequences and operating conditions of the separation system. The design of recycle from separators to reactor involves recycle component classifications, number of recycle streams determination, and the specifications and locations of liquid/vapour recycle and purge. These alternative flowsheets can be simulated using Aspen HYSYS to solve the mass and energy balances, calculate the thermodynamic properties, and determine operating conditions. Simulated flowsheets are loaded into Aspen IPE for sizing and economic evaluation. A limited number of process flowsheets are proposed based on meeting the design requirements at low investment cost and high profit.

3.2. Reactor System Synthesis Strategy

Reactor system synthesis is an important part of an overall chemical process flowsheet development. In a chemical process, feed preparation, product recovery and recycles steps are directly influenced by the reactor system. Reactor system synthesis illustrated in Figure 3, starts with providing process chemistry information by selecting reactants and products chemical name from a database where chemical prices and other physical properties are exported automatically. If there is any safety and environmental concern about the economically viable paths, warning will be given to the user. Conversion, selectivity and recycle of unreacted material are considered.

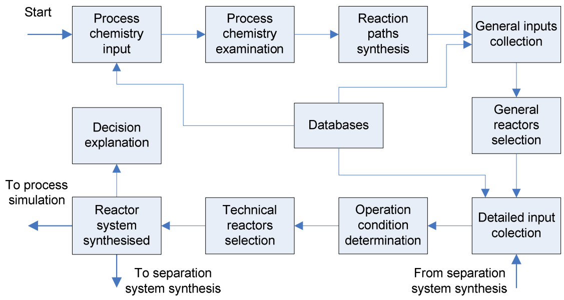

Figure 3: Reactor system synthesis strategy

General input information such as reaction phase, temperature and pressure, the use of catalyst and its life time etc. are provided to start the general reactor selection process. Further details on the reaction exotherm, residence time and kinetics lead to suggested operating conditions and a list of technical reactors. The scoring system used in the selection process ranges from "not suitable" to "highly recommended". Multiple reactor systems can be synthesised and decisions are explained. Results from reactor and separator systems are linked for total flowsheet synthesis.

3.3. Ethylene Glycol Reactor Systems Synthesis Case Study

Ethylene glycol is an important industrial petrochemical in many countries. It is a feedstock for the production of polyester, and is used as antifreeze and solvent. There are many different reaction routes to synthesis ethylene glycol such as (1) hydration of ethylene oxide, (2) ethylene oxide via ethylene carbonate, (3) synthesis gas, (4) formaldehyde via glycolaldehyde, (5) directly from ethylene etc. [5]. Some of these reaction routes are being evaluated and this case study illustrates the reactor system synthesis for the ethylene oxidation to ethylene oxide and the subsequent hydration to ethylene glycol.

3.4. Results and Discussions

Analysis by the software of different alternative reaction route to the synthesis of ethylene glycol shows that the route via ethylene oxidation and ethylene oxide hydration is economically viable as long as the other production costs are sufficiently lower than the gross profit. By-product of a reaction is not taken into account but can have a significant impact on the economics of the process. Figure 4, is a screenshot of the user interface showing input process chemistry information for ethylene oxidation primary and secondary reactions.

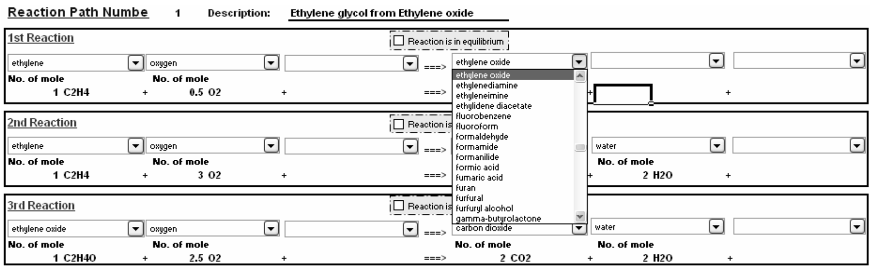

Figure 4: Process chemistry input screen

Selection results in Table 1, illustrate that two reactor systems are required. The user will not be required to specify the number of reaction systems required. The IKBS will make this decision based on the information provided, such as reaction conditions and phase, and the use of catalyst. For the ethylene oxide reactor system, the multi-tubular fixed bed reactor has the highest scores among the alternative reactors. This reactor is currently used in commercial processes because of the special requirements on temperature control throughout the catalyst bed.

Reactors Type	Ethylene oxide reactor system scores	Ethylene glycol reactor system scores
Continuous Stirred Tank Reactor (CSTR) with Jacket	Not Suitable	11
CSTR with Jacket and internal coil	Not Suitable	12
CSTR with external heat exchanger on circulation loop	Not Suitable	13
Sparged CSTR	Not Suitable	Not Suitable
Simple tubular reactor	Not Suitable	12
Simple tubular reactor with circulation of heat transfer fluid	Not Suitable	13
Simple tubular reactor placed in a furnace	Not Suitable	Not Suitable
Adiabatic fixed bed reactor	Not Suitable	Not Suitable
Fixed bed with intermediate cooling/heating	12	Not Suitable
Fixed bed with cold/hot shot	13	Not Suitable
Multitubular fixed bed reactor with indirect cooling/heating	14	Not Suitable
Trickle-bed reactor	Not Suitable	Not Suitable
Fluidized bed reactor	13	Not Suitable
Moving bed reactor	13	Not Suitable
Riser reactor	13	Not Suitable
Bubble column	Not Suitable	Not Suitable
Spray column reactor	Not Suitable	Not Suitable
Falling thin-film reactor	Not Suitable	Not Suitable
Agitated thin-film reactor	Not Suitable	Not Suitable
Monolith reactor	12	Not Suitable
Gauze reactor	12	Not Suitable
Reactive distillation	Not Suitable	Not Suitable

Table 1: List of proposed reactors for ethylene oxide and ethylene glycol process

The next highest scores were given to fluidized bed, riser and moving bed reactors. The use of these reactors can improve the heat removal from such highly exothermic reactions. These three reactors may have two drawbacks, possible catalyst attrition and the back mixing of ethylene oxide may result in a long residence time; hence more oxidation of ethylene oxide. Fixed bed reactors with intermediate cooling or cold shot are alternatives currently under consideration in industrial research [6]. Monolith and gauze reactors are low pressure drop alternatives that can be recommended for this highly exothermic and fast gas catalytic reaction. The software carried out a heat balance which suggests that the reactors should be operated isothermally. Heat carrier such as methane can be used to increase the heat capacity flowrate. This temperature control will reduce the loss of selectivity and catalyst performance.
Results for the ethylene glycol reactor system show CSTR and tubular reactors can be used. As the reactions are mixed parallel and series excess of one reactant can be used to improve the selectivity and plug flow reactors are preferred to back mixed reactors (CSTR) to minimize the formation of higher glycols. Based on the heat balance carried out by the software, reaction can take place adiabatically. Therefore, adiabatic tubular reactor can be the best choice for such liquid phase reaction. This type of reactor is currently implemented.

4. Conclusions and Future Work

This paper represents the proposed integrated knowledge based system procedure and structure for the synthesis of a total process flowsheet. The synthesis system integrates the knowledge base with third party software and databases. The prototype software has been successfully applied for the selection of chemical reactors for the manufacture of ethylene glycol via different reaction routes. The synthesis of ethylene oxide and ethylene glycol reactor systems proves that the developed software is able to suggest alternative reactors that are validated based on existing commercial processes or recommendations by industrial research.
The ongoing work on the synthesis of reactor-separator-recycle systems will lead to linking the developed alternative flowsheets to the simulator, equipment sizing and economic evaluator.

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