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Software Tools Overview: Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction

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The paper provides an overview based on an experience and applications of process integration, modelling and optimisation software tools. The first part reviews the design practice and supporting software tools. General purpose optimisation and modelling tools overviews have been available from conferences and publication (Klemeš, 1977; Friedler, 2009 and 2010; Klemeš et al., 2010; Lam et al., 2010). Those are categorised as (i) Process integration and retrofit analysis tools (ii) Flowsheeting simulation and (iii) General mathematical modelling suites with optimisation libraries. The second part covers assessment of tools which enable the generation of sustainable alternatives. They deal with waste, environment, energy and material depletion and production cost constrains. Emphasis of the sustainable process design tools is on (a) Evaluation of process viability under sustainable economic conditions (b) Synthesis of sustainable processes and supply chains (c) Process maintenance and life cycle analysis. The concluding part provides an overview of software tools development and the potential of the research based tools in solving the problem of sustainable process design.

1. Introduction

Process integration, modelling and optimisation problems in chemical engineering are complex in terms of scale and relationships. The application of IT and computer software are essential to solve these problems, providing fast and as much as possible accurate solutions in user-friendly interface. Software has been widely used for process simulation, integration and optimisation which was able to help process industry companies achieve their operational excellence goals. They have been a variety of efficient tools available. However, each provider mainly stresses their advantages. The main functions of process software (Casavant and Côté, 2004) are to: (1) Model process plants - important for future processes; (2) Design or retrofit complex process facilities; (3) Determine the effects of process changes; (4) Predict capital cost expenditures; (5) Track/predict/minimise emissions; (6) Evaluate optimisation and integration options.

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2. Heat Integration Tools

Process Integration (or Heat and Water Integration/Pinch Technology) has been extensively used in the processing and power generating industry from the late 1980s. Among well established software tools are:

(a) **SPRINT** (2010). A software package used for the design of the energy recovery systems for individual processes. It provides energy targets and optimises the choice of utilities for a process and also designs heat exchanger networks. A grassroots design and retrofit can be carried out automatically, but the designer keeps control over the network complexity.

(b) **STAR** (2010) is applied to the optimisation of site utility and cogeneration systems. The interactions between the processes on the site and the steam system, steam turbines, gas turbines (with auxiliary firing options), boiler house, local fired heaters and cooling systems are all analysed using STAR. The main parts of STAR are (i) Utility system optimisation; (ii) Top Level Analysis; (iii) Process energy targets; (iv) Total Sites; (v) Emissions reduction.

(c) **WORK** (2010) is used mainly for the design of low temperature (sub-ambient) processes. For mixed refrigerants the refrigerant composition can be optimised. It provides: (i) Targeting the minimum shaft work for low temperature cooling duties; (ii) Optimising the number and temperatures of refrigeration levels; (iii) Targeting the minimum shaft work for cascade refrigeration systems; (iv) Determining the optimum composition for mixed refrigeration systems.

(d) **WATER** (2010) for the design of water systems. It targets and designs for minimum water consumption by identification of re-use, regeneration and recycle opportunities.

(e) **HEAT-int** and **SITE-int** (2010) have been developed by the Process Integration Ltd. These are the next generation developments of the SPRINT and STAR software packages by a similar team of developers to a commercial standard.

(e) **SuperTarget®**(2010) is widely used to improve heat integration in new design and retrofit projects reducing operating costs and optimally targeting capital investment. It is a useful tool for users with different levels of expertise. The user interface makes the technology accessible, advanced tools are available to experts and many of the time consuming tasks associated with Pinch Analysis have been fully or partially automated.

3. Flowsheeting Simulation Packages

Balancing reconciliation and flowsheeting simulation tools are frequently used for sustainability design and energy saving analysis. Process data reconciliation has become the main method for monitoring and optimising industrial processes as well as for component diagnosis, condition-based maintenance and online calibration of instrumentation. Some excellent examples of flowsheeting simulation packages are:

(a) **AspenONE** (2010) is an application suite that enables process manufacturers to implement best practices for optimising engineering, manufacturing, and supply chain operations. It addresses inefficiencies end-to-end throughout the plant, which may result in important cost savings. **Aspen Plus** is one of the core elements of AspenONE process engineering application. It is a process modelling tool for conceptual design, optimisation, and performance monitoring for the chemical, polymer, specialty chemical, metals and minerals, and coal power industries.

(b) **HYSYS** (2010) is software for steady state and dynamic simulation of processes created by Hyprotech. It includes tools for (i) Estimation of physical properties and liquid-vapour phase equilibrium, (ii) Heat and material balances, design, optimisation of oil and gas processes and (iii) Process equipment. HYSYS has been acquired and modified by Aspen (2010) and later by Honeywell as **UniSim Design** (2010).
(c) **gPROMS** (2010) is an advanced process modelling environment for the process industries. It provides advanced custom modelling capabilities within a flowsheeting environment. gPROMS's capabilities are used to generate accurate predictive information for decision support in product and process innovation, design and operation. Its modules cater for all phases of the process lifecycle, from laboratory experimentation through process and detailed engineering to online operations.

4. General-Purpose Optimisation Packages

A general process optimisation and synthesis problem can be solved by a mathematical-programming (MP) method. MP aims to find appropriate values for the problem decision variables such that the constraints are satisfied, while a specific objective function is minimised or maximised. The constraints define a search space and the objective function is used to determine the most favourable point in this space. Several general-purpose optimisation tools are to be listed:
(a) **GAMS** (2010) - General Algebraic Modelling System - is a widely used high-level modelling system for mathematical programming and optimisation. It is designed for modelling LP, NLP, MILP and MINLP optimisation problems. The system is tailored for complex, large-scale modelling applications and allows the user to build large maintainable models that can be easily adapted to new situations. GAMS was the first algebraic modelling language and is formally similar to programming languages. Models are described in algebraic statements, which are easy to read.
(b) **LINDO** and **LINGO** (2010) provide an interactive modelling environment to easily build and solve optimisation problems. The latest LINDO version offers a number of enhancements including: (i) Significantly expanded nonlinear capabilities; (ii) Global optimisation tools; (iii) Improved performance on linear and integer problems; (iv) Enhanced interfaces to systems such as MATLAB and Java.
(c) **MATLAB** (2010) - MATrix LABoratory - is an interpreted language for numerical computation. It performs numerical calculations, and visualises the results without the need for complicated and time consuming programming. MATLAB allows users to (i) Accurately solve problems, easily produce graphics and code, (ii) Matrix manipulation, plotting of functions and data, implementation of algorithms, creation of user interfaces, and interfacing with programs in other languages. A popular add-on is **TOMLAB** (2010). Its Optimisation Environment is a powerful platform and modelling language for applied optimisation in MATLAB.

5. Novel tools for energy saving and pollution reduction

5.1 Graph-based Process synthesis

PNS Solutions (2010) is a software package solving Process Network Synthesis (PNS) based on P-graph approach. The P-graph framework has been introduced by Friedler et al. (1992) and further developed for systematic optimal synthesis of industrial

processes. The aim of PNS problem is to examine the feasible structures and select the optimum. The optimal structure can be assessed in terms of cost, profit, etc. To define the optimal structure, both structural information (which and how functional units are connected) and sizing information are needed. The issues addressed by PNS Solutions are: (i) Representation of the building blocks of a process network, (ii) The solution structures of the problem, (iii) Finding the maximal superstructure, (iv) Finding the optimal structure.

5.2 Mixed-Integer process synthesis

MIPSYN - Mixed-Integer Process SYNthesizer (Kravanja and Grossmann, 1994) is a modular computer package for an integrated synthesis of new and innovative retrofit of existing plants at various levels of complexity ranging from a simple NLP to the simultaneous MINLP for optimisation of heat integrated and flexible plants. MIPSYN is based on the advanced modelling and optimisation techniques rooted in disjunctive MINLP. It enables both discrete (selection of process units, their connectivity, ranges of operation) and continuous optimisation (e.g. temperatures, flows, pressure) simultaneously. It can be comprehended and used at different levels of problem abstraction as: (i) An MINLP solver for more general problems; (ii) A tool for the synthesis of process flowsheets; (iii) A synthesiser shell for applications in different engineering domains.

5.3 Ecological evaluation

SPIonExcel introduced by Sandholzer et al. (2005) is a software tool for an easy and quick calculation of the ecological footprint and the Sustainable Process Index (SPI) (Narodoslawsky and Krotscheck, 1995). It is implemented as a Microsoft Excel Macro. SPIonExcel calculates the ecological footprint and the SPI of a product or service through the input that characterizes the process given by an eco-inventory. The eco-inventories used for the overall footprint contain engineering mass and energy flows of processes in terms of input and output flows.

5.4 Decision making tools for waste to energy

W2E (Waste-to-Energy) software is a supporting tool for technological process simulation (Touš et al., 2010). It has been developed in Java and provides a user-friendly environment and intuitive operation. The principle of modelling and simulation is the same as in other similar systems. It creates a flowsheet, setting data and running simulation. W2E uses sequential-modular approach for computations. The main features are (i) Setting input data; (ii) Checking computed values (temperature, enthalpy, and composition); (iii) Easy extension of new blocks and streams is possible. For using it no advanced programming skills are needed. W2E also provides simulation of processes with loops and supports export of data to Excel.

5.5 Integration of renewable energy into various energy systems

The **EMINENT tool** (2010) evaluates the market potential of energy-related Early Stage Technologies (ESTs) in various energy supply chains, and their performance in terms of (Klemeš et al., 2009): (i) CO_2 emissions; (ii) Cost of energy supply; (iii) Use of primary fossil energy; (iv) Cover different subsectors of society. The EMINENT tool uses two databases: (i) National energy infrastructures, which contains information

regarding the number of consumers per sector, type of demand, typical quality of the energy required and the consumption and installed capacity per end-user; (ii) ESTs and other already commercial technologies, which includes key information on new energy technologies currently under development, and proven energy technologies available and in use. As the availability, price, and geographical conditions of primary energy resources differ significantly worldwide, there is a requirement to evaluate the impact of ESTs within a national energy supply system. There are other computer tools to analyse the integration of renewable energy published recently by (Connolly et al., 2009).

6. Conclusions

The reviewed field has been developing very fast together with the continuously accelerating development of the IT. They have been generally several major groups of software tool developers: Universities and academic institutions traditionally have been at the forefront of the development. In many cases their attempts have not been sustained and finished only with completion of a PhD or a cluster of PhDs. Small high tech companies are catching promising directions of the development and delivering fast advanced software tools. Major market players accumulated sufficient market and volume of sales to support an infrastructure for the continuous development and marketing. In most directions they merged or took over small players and currently dominate the market. With respect to software developers, a position of a user is not easy as s/he is bombarded by publicity materials and approached by sales persons, who are demonstrating just advantages of their products. The advisable policy is to use widely offered demonstration and testing versions to form a balanced opinion. This consumes time and money as well. For these reasons the overviews and the papers presenting applications of different case studies are valuable sources of information.

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