Technical University of Denmark



# Computer Aided Flowsheet Synthesis and Design Under Uncertainty In Vegetable Oil Production

Quaglia, Alberto; Sarup, Bent; Sin, Gürkan; Gani, Rafiqul

Publication date: 2011

Document Version Publisher's PDF, also known as Version of record

Link back to DTU Orbit

Citation (APA):

Quaglia, A., Sarup, B., Sin, G., & Gani, R. (2011). Computer Aided Flowsheet Synthesis and Design Under Uncertainty In Vegetable Oil Production. Abstract from 2011 AIChE Annual Meeting, Minneapolis, MN, United States.

### DTU Library Technical Information Center of Denmark

### **General rights**

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

• Users may download and print one copy of any publication from the public portal for the purpose of private study or research.

- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.



### Start | Grid View | Browse by Day OR Group/Topical | Author Index | Keyword Index | Personal Scheduler

## Computer Aided Flowsheet Synthesis and Design Under Uncertainty In Vegetable Oil Production

### Thursday, October 20, 2011: 12:30 PM

### 101 D (Minneapolis Convention Center)

Alberto Quaglia, CAPEC, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Kgs. Lyngby, Denmark, Bent Sarup, Alfa Laval Copenhagen A/S, Soeborg, Denmark, Gürkan Sin, CAPEC, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Kgs. Lyngby, DK-2800, Denmark and Rafiqul Gani, CAPEC, Department of Chemical and Biochemical Engineering, Denmark Technical University (DTU), Kgs. Lyngby, Denmark

Although being a mature and well established industry segment, over the last few decades the vegetable oil industry has been facing many important new challenges due to emerging new products (such as biodiesel and nutraceuticals compounds), as well as new trends and regulations with regards to sustainability, environment and health.

Moreover, since the agricultural commodities market is highly volatile due to seasonal variations in supply and demand as well as intensive trading, the decision making process is complicated by uncertainties in price. These uncertainties in product and feedstock prices, in turn, are propagated to the economical and financial indicators, which are normally used to support and take decisions.

Most of the time the industry responds to these challenges by taking decisions based on heuristic approaches, which arguably are not fit to manage neither the complexity of the entire value chain nor price uncertainties. All these considerations underline the need for Computer-Aided Flowsheet Synthesis and Design tool in vegetable oil industry. Such a tool should be robust, cover all the value chain, ideally be able to handle new product and process development problems as well as retrofitting problem of existing operations and deal with price uncertainties. Moreover, it should be complemented with all data, models and algorithm databases necessary for its use.

In this paper, a systematic framework for Computer-Aided Flowsheet Synthesis and Design(CAFD) and resources allocation under price uncertainties for the vegetable oil sector is presented.

In the framework, the flowsheet synthesis and design problem under uncertainty is cast as a Stochastic Mixed Integer Non Linear Programming (SMINLP) problem, which is then solved using appropriate SMINLP solvers.

The SMINLP problem is formulated and solved in a systematic manner by following a 4 steps procedure: (i) problem definition (ii) data collection and superstructure definition (iii) models selection, development and validation (iv) model solution & analysis.

In the first step, the synthesis/ design problem is defined by stating the purpose (new process, retrofit) and defining the optimality criteria.

The second step deals with the collection and systematization of the existing knowledge (industrial know-how, engineering insights, commercial knowledge...) and data (both scalar value and distribution functions of uncertain parameters) relevant to the problem.

Particular emphasis is given to reconciliation and systematization of this multidisciplinary knowledge, as well as to the development of an appropriate infrastructure for efficient data management, composed by a superstructure representing different flowsheet alternatives, structural constraints list, compounds and unit operations inventory and databases of reconciled data, structured in such a way to be accessible from all project levels [1].

The third step aims at collecting all the submodels needed for the multiscale model formulation. These include physical properties, unit operations, operational and investment cost and sustainability models; a systematic model generation framework is used to ensure consistency among the different models and scales.

### Abstract: Computer Aided Flowsheet Synthesis and Design Under Uncertainty In Vegetable Oil Production (2011 Annual Meeting)

The fourth step deals with the CAFD problem solution, which requires the solution of the SMINLP formulated in the above described steps. Because of the size of the problem and of the combinatorial nature introduced by the binary variables, this task is often not trivial and computational intensive. Therefore particular emphasis is given to the selection of the optimal solution method among the different algorithms [2] [3] [4].

Depending on the nature and size of the problem and on the type and number of uncertain parameters, some of the existing algorithm may not be suitable for the solution of the problem, because (i) the size of the CAFD problem is too large, or (ii) correlation structure of the uncertain parameters cannot be handled or (iii) they don't exploit shortcut calculation to facilitate the convergence to the solution. A rule based method for the selection of the appropriate solver as a function of some key problem characteristic is provided.

The SMINLP solution is the optimal flowsheet and the optimal material flow to each process block, as well as the expected value of the objective function and of all the economical and sustainability metrics calculated at optimality. In addition to the expected value, other conditional value such as value at risk can be also calculated in order to provide additional information for decision making.

In order to test and highlight the features of the methods and tools presented here, a soybean processing case study has been formulated and solved under price uncertainty assumption to determine the optimal processing network for vegetable oil extraction and refining (including various options for byproducts valorization), as well as the optimal material flows to each processing step under the condition of raw material, product and utility price uncertainty.

- 1. R. Singh, K. Gernaey, R. Gani, Computers and Chemical Engineering 33 (2009) 22-42.
- 2. G. E. Paules, C. A. Floudas, Computers and Chemical Engineering 16 (1992) 189-210.
- 3. Z. N. Pintaic, Z. Kravanja, Computers and Chemical Engineering 24 (2000) 195-201.
- 4. V. Duaa, K.P. Papalexandri, E.N. Pistikopoulos, Computers and Chemical Engineering 23 (1999) 19-22.
- 5. G. Sin, R. Gani, Chemical Engineering transactions. In press.

### Extended Abstract: File Not Uploaded

See more of this Session: Model-Based Engineering for Design See more of this Group/Topical: Computing and Systems Technology Division