MULTI-OBJECTIVE OPTIMIZATION OF INDUSTRIAL STYRENE PRODUCTION USING A PROCESS SIMULATOR AND A GENETIC ALGORITHM

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Abstract

Optimization of the whole plant instead of important individual units is essential for maximizing savings and operational efficiency. Often, there are conflicting objectives for optimizing industrial processes. Many previous studies on multi-objective optimization involved a few critical units (and not complete plants) using models and simulation programs specifically developed for the respective application. Developing rigorous models and a separate code for simulating a complete plant, for the sake of multi-objective optimization is difficult and time consuming. There is potential to make this task easier by employing available process simulators such as Aspen Plus and Hysys. But these simulators do not currently have multi-objective optimization tools. Hence, an interface has been developed between Non-dominated Sorted Genetic Algorithm (NSGA-II) and Hysys. Plant-wide optimization using this interface involves three main steps: (a) development and testing of Hysys model for steady simulation of the process under study; (b) sensitivity analysis and selection of objectives, decision variables and constraints; and (c) optimization of the process for multiple objectives using NSGA-II. This paper describes optimization of a styrene unit/plant for multiple objectives using the interface and compares the obtained results with those obtained using an independently developed simulation program.

Key works: Plant-wide optimization, multi-objective optimization, genetic algorithms, NSGA-II, Hysys

Introduction

Multi-objective problems are important to operate a plant/reactor in an optimized way to have good productivity, yield and/or selectivity with minimal utilization of resources, waste formation and/or pollution. To achieve these goals, optimal operating conditions need to be identified. What is even more important is to formulate and solve an optimization problem based on plant-wide perspective. With the availability of effective methods for multi-objective optimization [2], several studies on multi-objective optimization of important industrial processes and reactors like nylon 6 [6], wiped-film poly (ethylene terephthalate) reactor [1], hydrogen plant [7], epoxy polymerization process [3] and aspergillus niger fermentations for selective product enhancements [5] have been reported. Multi-objective optimization of industrial styrene reactors using non-dominated sorting genetic algorithm

(NSGA-II) was performed by Yee et al. [8]. Two- and three-objectives, namely, production, yield and selectivity of styrene, were considered for adiabatic and steam-injected styrene reactors. Pareto-optimal solutions were obtained due to conflicting effect of either ethyl benzene feed temperature or flow rate. Different variants of NSGA-II were tested for multi-objective optimization of a styrene reactor [11]. The work of [8] was extended to optimizing an industrial styrene manufacture [12].

Practically all the above studies have been performed by writing a simulation program for the reactor/plant in F90 or C++ followed by optimization for multiple objectives. The simulation program was often based on simplified models for units like heat exchanger, partial condenser and distillation column. Obviously developing the simulation program for a whole plant having many units and recycles is time consuming and needs a lot of effort. Also, optimization requires additional effort due to lack of interactive environment. To overcome these problems, an interface has been developed in our research laboratory between NSGA-II in C++ for multi-objective optimization and Hysys that provides a user-friendly environment for process flowsheet development and sensitivity analysis. Development of this interface along with some useful pointers is presented in [13].

This paper briefly describes the using/working of the interface followed by the successful multi-objective optimization of an industrial styrene production unit/plant using Hysys via the interface. Results obtained from the multi-objective optimization by two ways: (1) using F90 code with NSGA-II and (2) using the interface between Hysys and NSGA-II, are compared. The latter not only captures the features and powers of simulators for simulating industrial processes but also makes effective use of genetic algorithms for multi-objective optimization. It also facilitates the employment of new optimization techniques. Design and operating data for an industrial styrene reactor from Elnashaie and Elshishini [4] formed the basis for the complete plant. The results of multi-objective optimization provide an extensive range of optimal operating conditions, from which a suitable operating point can be selected based on the specific requirements in the plant.

Using/Working of the Interface

The interface facilitates the multi-objective optimization of Hysys simulation using NSGA, and involves a number of steps (sketch below). The user supplies the genetic algorithm parameters like crossover & mutation probability, seed for random number generation, population size and maximum number of generations as well as number of (binary/real) decision variables, constraints and objectives through the user interface. When the application is run, these data are used by the optimizer to start simulation followed by initialization of the population of points in the decision variable space by NSGA. The initial population is stored as an array and passed to the visual basic application (VBA), which makes a call to Hysys and supplies decision variables set one by one through the built-in spreadsheet of Hysys. The flowsheet is simulated for the supplied decision variables and the user defined objectives are evaluated in the spreadsheet itself. These objective values are later stored in an array in VBA and ultimately passed to NSGA where individuals are ranked according to there fitness values. After selection, mutation, and crossover operations, next population of points is chosen and submitted to Hysys for simulation and computation of objectives. This carries on till the maximum number of generations is reached.

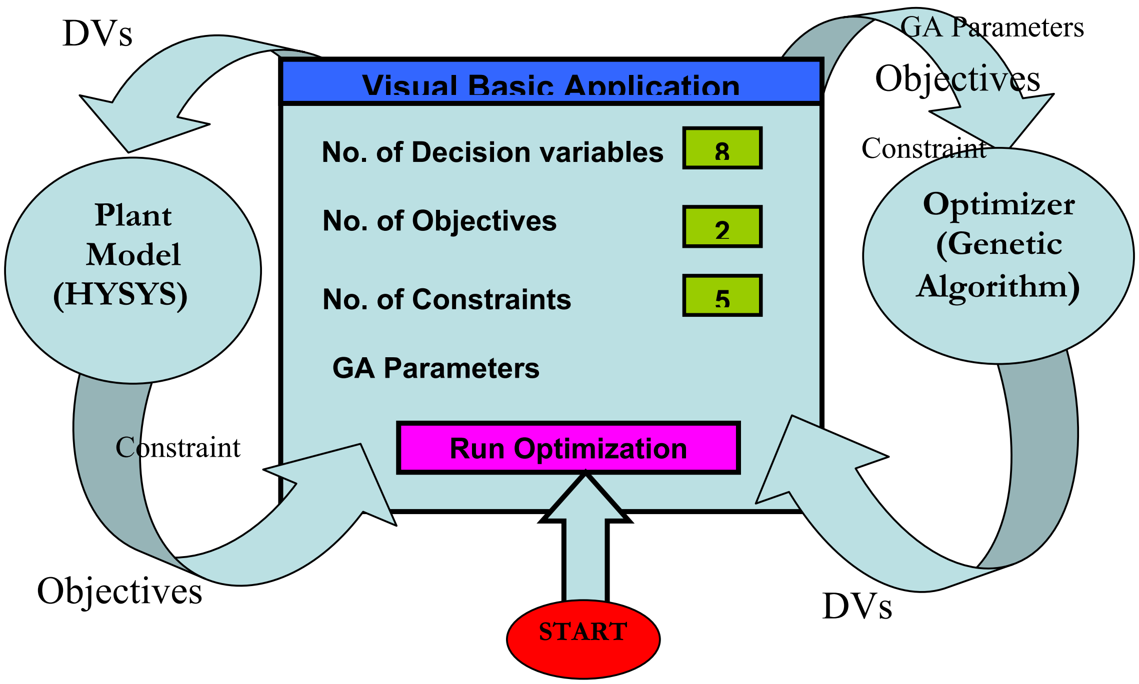


Figure A- Working procedure for Interface.

Modeling and Simulation of the Styrene Reactor Unit

Modeling, simulation and optimization of an industrial styrene reactor unit/plant has been performed by Tarafder et al. [12] using the corrected kinetic model of Sheel and Crowe

[4, 10]. Similar to the study of Tarafder et al. [12], the styrene reactor unit used as Case 1 in the present study, consists of plug flow styrene monomer reactor along with heat-exchanger (HE1) and the superheater for steam (Fig. 1). The overall plant includes all these units and heat exchanger (HE2), partial condenser (PC) and three distillation columns (S1, S2 and S3) as shown in Fig. 1. The model details (mass energy and momentum balance equations), assumptions, rate kinetics data, catalyst information, the six main reactions, including side reactions, occurring in the styrene reactor and operating data for simulation and validation are available in [4, 8]. The same model parameters were used to simulate the flowsheet in Hysys before interfacing with NSGA for optimization. The simulation results obtained using Hysys and F90 program of [12] are very close (Table 1) and the minor differences are due to differences in physical properties. The predicted results are also comparable to the industrial data (Table 1).

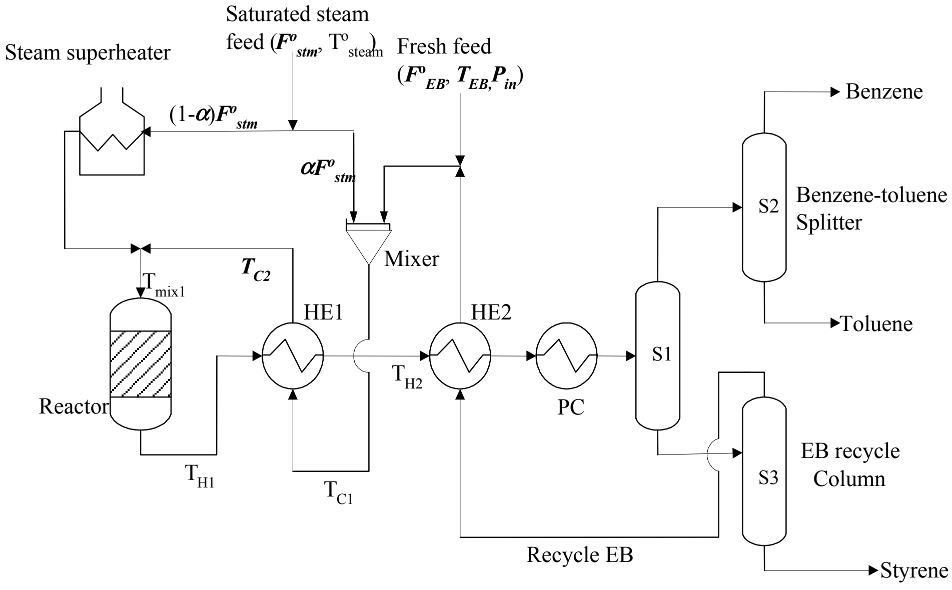


Figure 1: Schematic diagram of Styrene plant. (HE: heat-exchanger, S: Separator, PC: partial condenser). Letters in **bold** & *italics* represent decision variables [12]

Table 1: Comparison of the simulation results obtained by Hysys and F90 with Industrial data

Quantity at reactor exit	Industrial data	Predicted results	
		F90 code	Hysys
Exit Temperature, K	850.00	849.75	850.76
Exit Pressure, bar	2.32	2.33	2.32
Ethyl Benzene Conversion, %	47.25	46.74	46.38
Styrene Flow Rate, kmol/h	15.57	15.4	15.25
Ethyl Benzene Flow, kmol/h	19.45	19.63	19.77
Benzene Flow Rate, kmol/h	1.50	1.44	1.43
Toluene Flow Rate, kmol/h	2.03	2.05	2.08

Case Study 1

The first case study is on two-objective optimization of the single-bed styrene reactor unit and comparison of results for optimization using the two different methodologies: F90 code of Tarafder et al. [12] and Hysys simulation. The objectives are to simultaneously maximize styrene flow rate and styrene selectivity.

$$\text{Maximize: } J_1 = F_{st} \tag{1}$$

$$\text{Maximize: } J_2 = S_{st} = \frac{F_{st} - F^o{}_{st}}{F_{EB,\,total} - F_{EB}} \tag{2}$$

Bounds on decision variables are given as

$$1.4 < P_{in} < 2.63 \text{ bar} \tag{3}$$

$$7 < SOR < 20 \tag{4}$$

$$27.56 < F^o{}_{EB} < 40.56 \text{ kmol/hr} \tag{5}$$

$$1.5 < D < 4.0 \text{ m} \tag{6}$$

$$0.7 < L/D < 1.5 \text{ [-]} \tag{7}$$

$$450 < T_{EB} < 500 \text{ K} \tag{8}$$

$$0.1 < \alpha < 1 \text{ [-]} \tag{9}$$

$$700 < T_{C2} < 900 \text{ K} \tag{10}$$

The optimization problem is subject to the following constraints:

$$650 < T_{inlet} < 950 \text{ K} \quad (11)$$

$$F_{steam} < 459.1 \text{ kmol/hr} \quad (12)$$

$$P_{exit} > 1.4 \text{ bar} \quad (13)$$

$$T_{H1} - T_{C2} \geq 10 \text{ K} \quad (14)$$

$$T_{H2} - T_{C1} \geq 10 \text{ K} \quad (15)$$

Results and Discussion

The Pareto optimal solutions obtained by optimizing the styrene reactor unit using the F90 code and Hysys simulation are shown in Figure 2. They were obtained by NSGA-II after 100 generations with 80 chromosomes in the population. The genetic algorithm parameters used to obtain best Pareto through experimentation with different values are: real coding, seed = 0.557, crossover probability = 0.95, mutation probability = 0.05, distribution index for crossover and mutation are 10 and 20 respectively. To validated the results, optimal decision variables for three chromosomes on the Pareto obtained by F90 program are used in the Hysys simulation, and the objective values calculated by F90 program and Hysys are compared in Table 2. The results are acceptable within 1% difference, which is expected as Hysys employs different solution techniques as compared to F90 code. The F90 model uses IMSL subroutine like DIVPRK which uses Runge-Kutta-Verner fifth-order and sixth-order method.

Values of decision variables and constraints corresponding to the two Paretos in Fig. 2 are shown in Figs. 3 and 4 respectively. Their values by F90 code and Hysys simulation are comparable except that the results for L/D ratio and D (Fig. 3d and 3e) do not match well, probably due to the extra degrees of freedom among the decision variables in the problem. The variable that affects reaction rate is reactor volume which can be achieved through different values of diameter and length. The effect of decision variables and constraints on the objectives has been discussed in detail by Tarafder et al. [12, 13]

Table 2 Comparison of objective values of three chromosomes A, B and C on the Pareto obtained by F90, with those obtained by Hysys simulation with the same decision variable values.

Variables/	Chromosome A		Chromosome B		Chromosome C	
Objectives	F90	Hysys	F90	Hysys	F90	Hysys
T_{c2} (K)	703.20		807.23		700.74	
P_{inlet} (bar)	1.53		1.48		1.48	

SOR [-]	11.20		11.18		11.20	
F^o_{eb}(kmol/h)	39.63		40.43		40.38	
D (m)	2.72		2.67		2.64	
L/D ratio [-]	1.34		1.08		1.06	
Alpha [-]	0.51		0.11		0.10	
T_{eb} (K)	468.66		495.57		453.98	
F_{st} (kmol/h)	10.027	10.062	19.806	19.720	16.295	16.243
S_{st} [-]	0.964	0.963	0.862	0.861	0.918	0.917

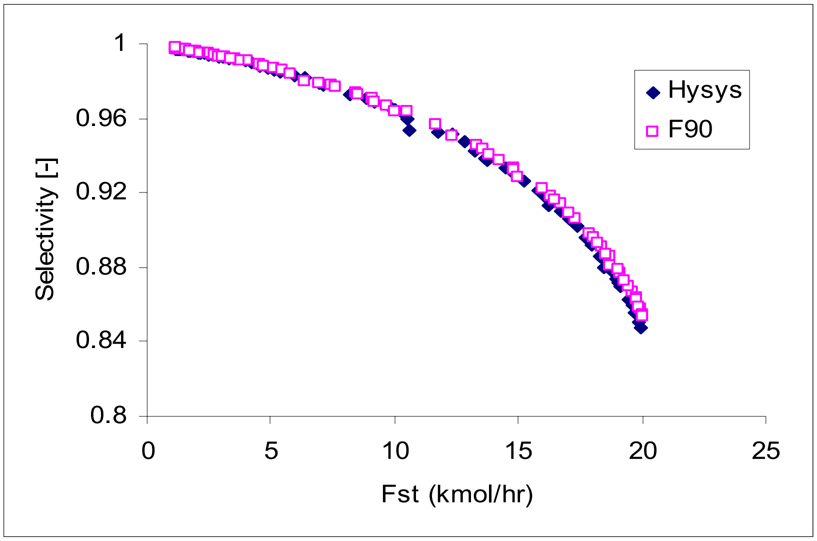
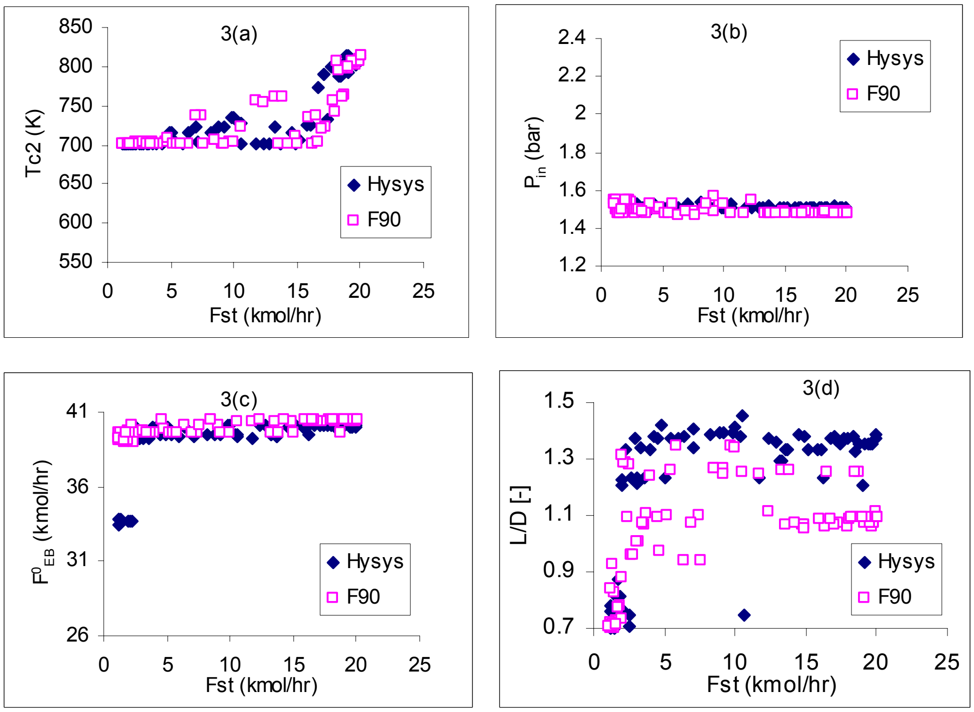


Figure 2 Result of maximizing styrene production and selectivity simultaneously



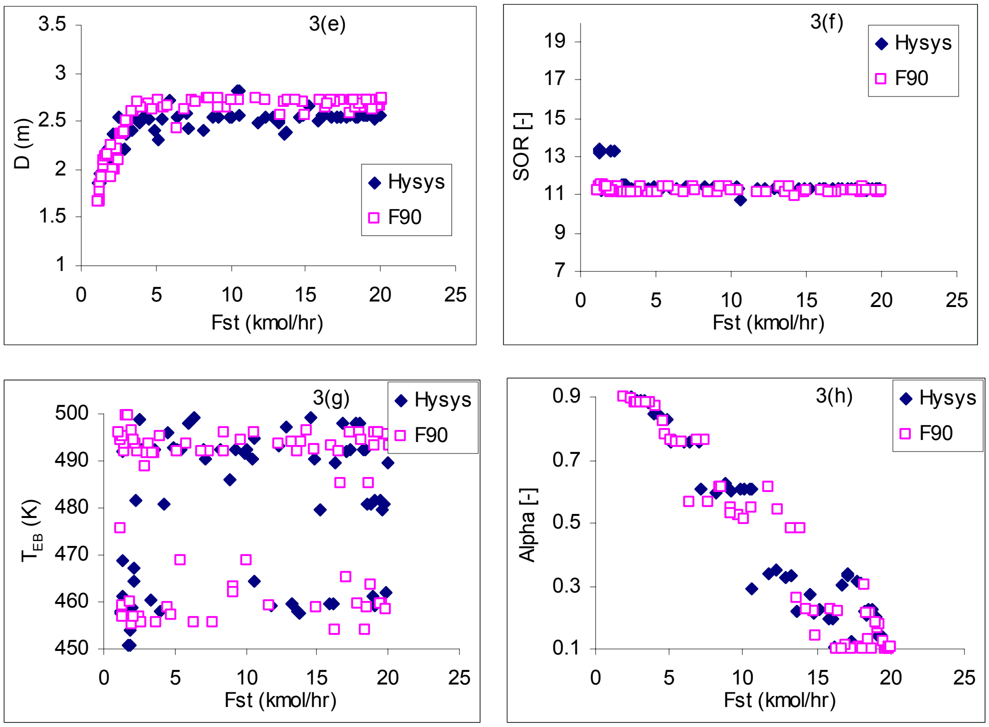
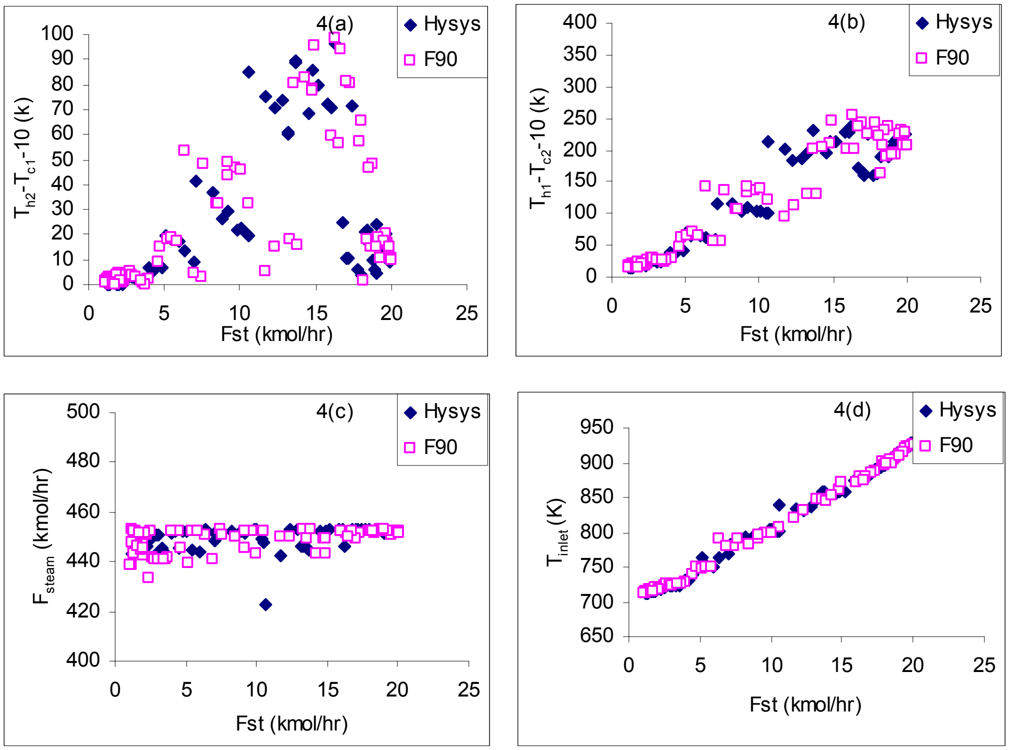


Figure 3 Comparison of plots of decision variables corresponding to the Pareto optimal solutions in Figure 2: (a) inlet temperature before mixing with superheated steam; (b) reactor inlet pressure; (c) flow rate of ethyl benzene; (d) reactor length to diameter ratio; (e) reactor diameter; (f) steam to oil ratio; (g) temperature of fresh ethyl benzene and (h) fraction of total saturated steam mixed with fresh and recycle ethyl benzene (alpha).



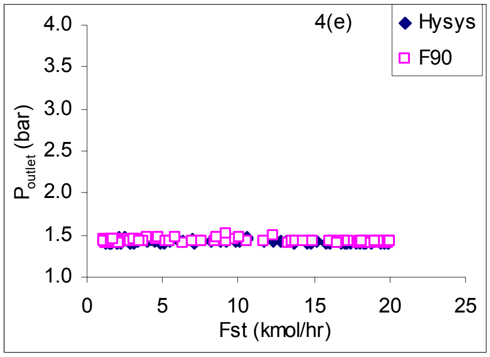


Figure 4 Comparison of plots of constraints corresponding to the Paretos in Figure 2: (a) minimum temperature approach for heat exchanger exit; (b) minimum temperature approach for heat exchanger inlet; (c) flow rate of fresh steam; (d) inlet temperature to reactor after mixing with steam and (e) outlet pressure of the reactor.

Average computational time taken for optimization using F90 model was ~ 6 minutes but using Hysys simulation took ~12 hrs on a 2.4 GHz P4 computer with 512 MB of SDRAM was used. Though building a Hysys simulation model, sensitivity analysis and interfacing it with optimizer is easy for multi-objective optimization, the computational time for optimization is increased exponentially. The computation time for F90 model simulation is around 0.08 second/simulation and the computational time for Hysys model is 6 seconds/simulation run. Hence ~8.4 hour to the total computational time (12 hrs) is taken for simulation of Hysys model when the application is run. Rest of time is taken in data transfer in the form of arrays between applications (NSGA and Hysys) by Visual Basic.

Case Study 2

This case study involves the entire styrene production plant (Fig. 1) including the styrene reactor, heat exchangers, partial condenser and separation columns. The F90 simulation case uses simplified models for partial condenser and three distillation columns**.** The shortcut method, commonly known as Fenske-Underwood-Gilliland (FUG) method [9] is employed for calculation of actual number of theoretical stages, reflux ratio, condenser and reboiler duty in F90. Initially a simplified form of Hysys simulation case is developed to compare the results with F90 code. After comparison and validation of the proposed interface, real distillation unit and partial condenser will be used in Hysys to do multi-objective optimization of the styrene plant. This work is in progress and findings will be presented during the meeting session.

Conclusions

The interface between NSGA and Hysys is employed successfully for styrene unit/plant optimization for multiple objectives. The optimal results are comparable to those obtained using F90 code for simulating the styrene unit/plant. This shows the reliability of the interface developed. The advantages of using the interface for optimization are the ease of rigorous simulation of any process using Hysys. Moreover, the simulation is more realistic and the interactive environment provided by Hysys makes the work simpler. The interface will prove beneficial to industries for designing, operating, debottlenecking and/or retrofitting plants with numerous units. It can be used for multi-objective optimization of any chemical process that can be modeled in Hysys. Business models may be formulated based on market economy and put in VBA to further enhance its applicability to solve industrial problems.

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