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Rigorous Dynamic Simulator for Control Study of the Large-scale Benchmark Chemical Plant

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Abstract: A dynamic simulator for the benchmark vinyl acetate (VAc) monomer production process is introduced. Rigorous first-principles dynamic models of the VAc process are implemented on the commercial software package Visual Modeler (Omega Simulation Co.,Ltd.). The simulator employs pressure flow calculations and considers non-idealities in the process equipment, so that more realistic simulations are made possible, compared with the conventional simulators. The simulator's high performance calculation provides an environment where feasibility and performance of designed control systems can be efficiently evaluated without sacrificing high fidelity of the process model. The developed simulator will be made available in the public domain with a free limited license of Visual Modeler.

Keywords: Process simulators, dynamic models, plantwide, process control, benchmark examples

1. INTRODUCTION

The importance of control system design from a plantwide perspective has been well recognized for many years (Buckley, 1964; Foss, 1973; Morari *et al.*, 1980; Stephanopoulos and Ng, 2000). Downs and Vogel (1993) published an industrial plantwide test problem, which has been studied extensively and has served as a realistic check on the industrial and practical relevance of new ideas and technical developments in the fields of process control, optimization, fault detection and diagnosis, and so on. The Tennessee Eastman challenge process was provided as a dynamic simulation, originally in Fortran code, and later in MATLAB code.

Subsequently, Luyben and Tyreus (1998) introduced an industrially relevant larger system having common, real chemical components: a vinyl acetate (VAc) production process. The VAc process contains several standard unit operations, gas and liquid recycle streams, as well as process-to-process heat integration. In the original paper (Luyben and Tyreus, 1998), detailed flowsheet information required to construct rigorous steady state and dynamic mathematical models are given with the control requirements and objectives. So far, several control studies have been reported about this process (Luyben *et al.*, 1997; Chen and McAvoy, 2003b; Olsen *et al.*, 2005; Seki *et al.*, 2010).

While steady state simulations are now routine for much process design work, dynamic simulations based on rigorous first principles models have remained a challenging task to practicing process and control engineers. Although few people would question that dynamic simulations could play a greater role in process engineering, its application has been relatively limited, in most part, to operator training systems. It is only recently that the use of dynamic simulations has grown significantly because of their increased ease of use even for non-simulation engineers. For plantwide control studies, nonlinear rigorous dynamic simulators could be a powerful tool for testing the feasibility and performance of a control strategy under nonlinearities and complexities of chemical plants of industrially relevant scale.

In this paper, a novel dynamic simulator for the benchmark vinyl acetate monomer production process is introduced. Rigorous nonlinear dynamic models of the VAc process are implemented on Visual Modeler (Omega Simulation Co.,Ltd.); Visual Modeler is a commercial simulation package that has found numerous industrial applications as an operator training simulator (OTS). Although dynamic process models based on MATLAB have been provided in the public domain by Chen *et al.* (2003a), their models suffer from some simplifications for the sake of simulation efficiency. In the proposed simulator, flow calculation based on pressure balance is employed and more realistic simulations are made possible without sacrificing high fidelity of the process model.

This paper is organized as follows. In the next section, the VAc process is described with the control objectives and requirements. In section 3, rigorous dynamic model is introduced, which is implemented on Visual Modeler. An example of plantwide control system design is given in section 4, followed by the conclusion.

2. VINYL ACETATE MONOMER PRODUCTION PROCESS

Figure 1 shows the process flow diagram of the vinyl acetate monomer production process. This process involves seven components: ethylene (C_2H_4), oxygen (O_2), acetic acid (HAc), vinyl acetate (VAc), carbon dioxide (CO_2), water (H_2O), and ethane (C_2H_6). Ethylene, oxygen, and acetic acid are provided as fresh feed and converted into VAc with byproducts H_2O and CO_2. Ethane is an inert component entering the process with the fresh ethylene feed stream.

The following gas phase reactions are considered:
Main reaction

$$C_2H_4 + CH_3COOH + \tfrac{1}{2}O_2 \xrightarrow{r_1} CH_2 = CHOCOCH_3 + H_2O$$

Side reaction

$$C_2H_4 + 3O_2 \xrightarrow{r_2} 2CO_2 + 2H_2O$$

The reaction kinetics are given as follows:

$$r_1 = 3.1605 \times 10^{-4} \exp(\frac{-3674}{T}) \cdot p_E \cdot \frac{p_A}{1 + 0.986 p_A} \cdot \frac{p_O(1 + 0.247 p_W)}{1 + 0.0846 p_O(1 + 0.247 p_W)} \quad (1)$$

$$r_2 = 2.8086 \times 10^{4} \exp(\frac{-10,116}{T}) \cdot \frac{p_O(1 + 0.0986 p_W)}{1 + 0.110 p_O(1 + 0.0986 p_W)}, \quad (2)$$

where r_1 (mol/min/g-catalyst) is the rate of vinyl acetate production by the main reaction, r_2 (mol/min/g-catalyst) is the consumption rate of ethylene by the side reaction, T (K) is the reaction temperature, and p_E, p_A, p_O, and p_W (kPa) are the partial pressures of ethylene, acetic acid, oxygen, and water respectively. The reactions are exothermic and occur in a reactor containing tubes packed with catalyst.

The reactor effluent is sent to the gas-liquid separator. The separated gas is recycled back to the reactor through the absorber which recovers liquid carryover in the recycle stream, while the separated liquid is fed to the distillation column, where the product VAc and water are withdrawn and the remaining HAc is recycled. Process-to-process heat integration is done between the reactor effluent and the gas recycle stream (FEHE: feed/effluent heat exchanger).

The original paper (Luyben and Tyreus, 1998) introduces the design requirements for process operation and control objectives that must be achieved for various disturbances. Generally, one should be able to set the VAc production rate while minimizing yield losses to CO_2 and always keep the process close to the economic optimum by reflecting changes in raw material and operating costs. The distillation column must produce an overhead product with essentially very little HAc and a bottoms product with very little VAc.

Specifically, the following requirements have been listed:

- The control system must still function for the changed condition of 20% decrease in the catalyst activity.
- The control system must be able to change the production rate by at least ±20% over the course of 6h.
- The control system needs to accommodate 50% drop of the VAc production rate.
- The control system has to keep safe operation during the course of a 5 min loss of either fresh acetic acid or column feed pump.
- The control system must handle a step change in the ethane composition in the fresh feed stream from 0.001 to 0.003 mol fraction.
- The control system must not shut down the process due to the loss of fresh oxygen feed flow. Instead, this should result in the process going into "hot recycle" mode.

Furthermore, the following constraints have to be respected for safety and other reasons:

- The O_2 concentration should not exceed 8% to avoid explosion.
- The gas loop pressure should not exceed 930kPa.
- The reactor hot spot temperature should be kept below 200 °C to prevent catalyst degradation.
- The feed gas temperature should be kept above 130 °C to avoid condensation.
- The VAc concentration at the distillation column bottom should be kept below 100 mol/million in order to prevent polymerization and fouling in the column reboiler and vaporizer.

3. DYNAMIC SIMULATOR

Based on the information provided by the original paper (Luyben and Tyreus, 1998), a nonlinear dynamic model has been implemented on the commercial software package Visual Modeler (Omega Simulation Co.,Ltd.).

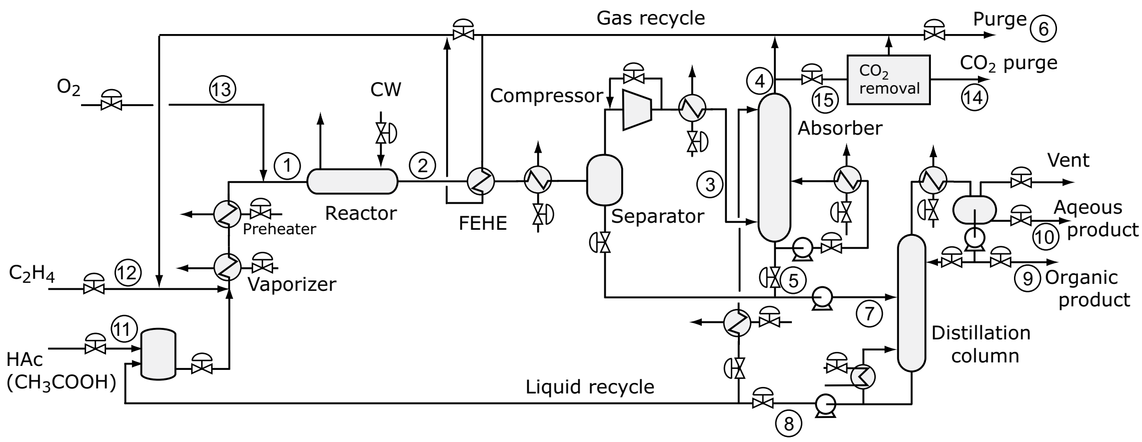

Fig. 1. Process flow diagram of the vinyl acetate monomer production plant. The stream numbers are the same as those of the original paper (Luyben and Tyreus, 1998).

3.1 Software package: Visual Modeler

Visual Modeler is intended to provide a virtual plant as a replica of a real plant for such objectives as operator training, operation assistance, operation optimization, design and verification of control systems, and education of chemical processes.

In particular, the modeling tool is designed to support simulations of very large-scale models which cover an entire plant. Experience with modeling large-scale plants such as ethylene plants has shown that the tool is capable of handling plant models with more than 10,000 units. In fact, Visual Modeler is used in 13 out of the 15 ethylene plants in Japan.

Visual Modeler has the following general features:

F1) Easy construction of rigorous dynamic simulation models by selecting process models from the unit operation library with ready-to-use physical properties.
F2) Customization and creation of process instruments models. Addition of user-defined components and user-supplied data to the physical property library.
F3) Steady state calculation by using the model prepared for dynamic simulation.
F4) Calculation of (sub-)optimal operation points by solving a minimization/maximization problem posed as a linear or quadratic program.
F5) Data reconciliation through the least square minimization problem.
F6) Incorporation of such non-idealities as dead band and stick band into the valve models. Additional consideration of noise or offset in the valve and measurement instrument models.
F7) Various types of PID controller models to account for miscellaneous functions of industrial controllers, including action modes (I-PD, PI-D, I, PID, cf. Fig. 2), modes (AUT, MAN, CAS), types (velocity, position), anti-reset windup, input signal filter (PV filter), measurement tracking, gap gain, incomplete differential gain, feed forward factor) and so on.
F8) Open-loop identification of process dynamics using the data collected in the dynamic simulation. Graphical user interface for selecting the scope of the target instruments.
F9) Very fast execution of dynamic as well as steady state calculations even on a low performance PC with a single-core CPU.

3.2 VAc *plant model implementation*

The VAc process consists of many kinds of process instruments such as the reactor, distillation column, absorber, separator, decanter, CO_2 remover, heat exchangers, compressor, pumps, valves, PID controllers, and measurement instruments. For the most part, standard unit operations provided by the software package have been utilized except for the reactor. To represent the complex kinetic behavior of the reactions given in (1) and (2), the standard plug flow reactor model provided by Visual Modeler has been customized.

Some of the differences in this implementation from the original paper are:

- Heat removal at the reactor is done through the jacket cooling water instead of the steam drum vapor system.
- The Antoine constants of $C_2H_4, C_2H_6, CO_2, O_2$ for vapor pressure calculations are tuned so that these components are not included in the separated liquid in the gas/liquid separator. As a result, the ideal com-

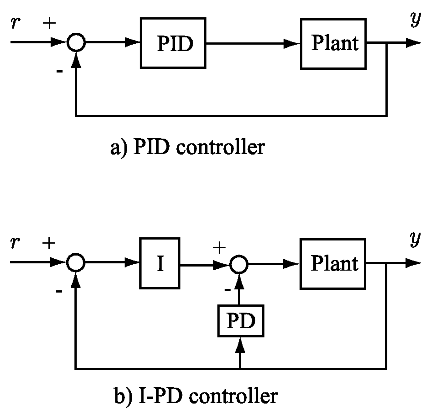

Fig. 2. Two different implementations of PID controller. a) standard PID controller, b) I-PD controller.

ponent separator, which was assumed in the original model, no longer needs to be considered.

Table 1 compares some of the major stream data provided by the Visual Modeler model and the original model (Luyben and Tyreus, 1998). In Fig. 3, the temperature profiles in the reactor and the distillation column are shown, which apparently coincide well with those provided by Luyben and Tyreus (1998).

By exploiting the features of Visual Modeler listed in the previous subsection, the developed simulator has achieved improvements from the simplified MATLAB version (Chen *et al.*, 2003a). Some of them are:

- The pressure flow calculation makes it possible to express the dynamic behavior of the gas loop pressure, which may affect designed controller performance. For example, as shown in the next section, the optimal operating point lies on the upper limit of the gas loop pressure, so that its dynamic behavior should be carefully observed under constraint control. Also, coupling between the gas loop pressure and the reactor temperature dynamics may be present to make regulatory controller tuning for these variables more realistic and challenging.
- More realistic disturbances are generated by incorporating such non-idealities as actuator dead band, stick band, sensor noises, sensor resolution limits, etc., which are almost always present in actual chemical plants. This feature allows the simulator to serve as a more appropriate test bed for technical developments (Seki and Shigemasa, 2010).
- Simulations of start-up and shut-down procedures are possible.
- Despite the higher fidelity of the models, simulations are executable at a speed between 100 and 400 times real time even on a single core CPU.

4. CONTROL SYSTEM DESIGN EXAMPLE

4.1 Optimal steady state operation policy

As a preliminary study, a steady state optimal operating condition has been derived using a simplified reactor/separator model. The model assumes the detailed model for the reactor but ideal separation for the separators (Seki *et al.*, 2010). The optimization problem is posed as maximization of the product yield, equivalently, minimization of the fresh ethylene feed rate $F_{\mathrm{C_2H_4}}$ for a prescribed VAc production rate F^P_{VAc}:

$$\min_{x,u} \ F_{\mathrm{C_2H_4}} \tag{3}$$

subject to

$$\begin{aligned} &f(x,u) = 0 && (4)\\ &F^P_{\mathrm{VAc}} = 47.4 \text{ kmol/h} \\ &u^{LL} \le u \le u^{UL} \\ &y^{LL} \le y \le y^{UL}, \end{aligned}$$

where equation (4) denotes the process model describing the mass and heat balances, x is the state variable, u is the operational degree of freedom, u^{LL} and u^{UL} are the lower and upper limits for the decision variable u, y is the variable other than the decision variable for which process constraints have to be considered, for example, reactor temperatures.

Table 2 shows the optimal operating condition compared with the nominal one provided by Luyben and Tyreus (1998). The derived optimal operating condition achieves around 3% increase in the product yield (94.4% → 97.5%) for a nominal VAc production rate of 47.4kmol/h.

The increased yield is realized by lowering the reaction temperature to suppress the side reaction, while increasing the ethylene partial pressure to secure the production rate. For this purpose, the gas-loop pressure is maximized and the partial pressures of the acetic acid, ethane, and water at the reactor inlet are reduced by appropriately adjusting the related flows.

4.2 Control loop configuration

A multi-loop controller configuration which realizes the optimal operation is designed. The loop configurations described in the previous studies (Luyben *et al.*, 1997; Chen and McAvoy, 2003b; Olsen *et al.*, 2005) should be applicable, but the configuration shown in Fig. 4 is considered here as an alternative.

The characteristics of the configuration in Fig. 4 is that the fresh acetic acid feed stream is on flow control to set the production rate. Although this configuration violates Luyben's rule (Luyben, 1994) and the positive feedback effect in the liquid recycle loop may be anticipated (Morud and Skogestad, 1996), such dynamic effects could be made negligible because the liquid recycle flow rate is minimized (almost zero) with the optimal operation.

However, this configuration is not self-regulatory under the gas-loop pressure control by the fresh ethylene feed, unless the additional loop, which adjusts the reactor temperature set point by looking at the liquid recycle flow rate, is applied. Inspection of the reaction kinetics (1) reveals that if the recycle HAc feed stream increases for some reason, the gas-loop pressure controller decreases the ethylene partial pressure to keep the total pressure constant. This decreases the VAc production, resulting in the further increase of HAc recycle, so that the system is not self-regulatory. The additional loop will make the reaction temperature higher as the HAc recycle increases, which then promotes the reaction and reduces the amount of recycled HAc, thus realizing regulation of the HAc mass balance.

It was easy to verify whether or not the above intuition is correct by using the dynamic simulator. Indeed, the control loop configuration without the liquid recycle/reactor temperature loop was found to be infeasible: the liquid recycle grows infinitely. On the other hand, the control system with the additional loop was certainly found to work to realize the optimal operation. Figure 5 shows responses of the designed control system around the optimal operating condition for ±20% changes in the production rate: the fresh HAc feed rate is changed stepwise.

Table 1. Comparisons of some of the stream data: Visual Modeler/Luyben and Tyreus (1998)

	Reactor outlet	Absorber vapor in	Column feed	Column bottom	Organic product
Stream number	2	3	7	8	9
Flow kmol/h	1128.5/1131.4	974.4/974.4	228.8/229.2	129.2/129.6	49.3/ 49.7
Temperature °C	159.0/158.9	71.7/80.0	48.6/42.5	136.8/137.2	47.8/45.8
Pressure kPa	619.2/620.7	900.5/882.8	147.8/579.3	207.6/206.8	101.3/124.1
O_2 (mol.frac)	0.049/0.049	0.057/0.057	0/0	0/0	0/0
CO_2	0.012/0.011	0.013/0.013	0/0	0/0	0/0
C_2H_4	0.552/0.551	0.639/0.642	0/0	0/0	0/0
C_2H_6	0.220/0.221	0.255/0.256	0/0	0/0	0/0
VAc	0.044/0.043	0.023/0.021	0.205/0.206	0.0/0.0	0.9505/0.9498
H_2O	0.054/0.055	0.009/0.007	0.277/0.281	0.083/0.093	0.0490/0.0498
HAc	0.070/0.070	0.005/0.004	0.518/0.513	0.917/0.907	0.0005/0.0004

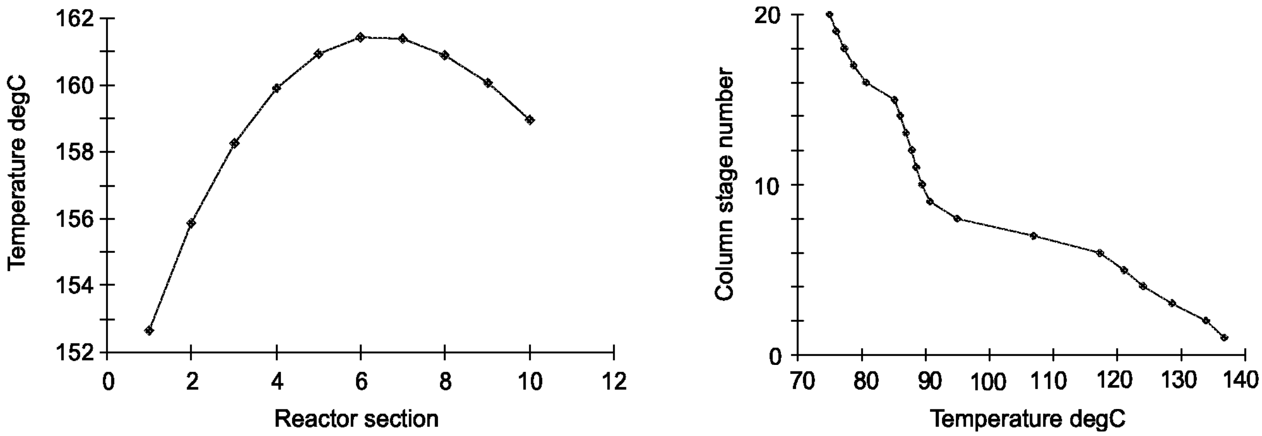

Fig. 3. Temperature profiles in the reactor (left) and the distillation column (right).

Table 2. Optimal operating conditions.

		Nominal	Optimized
VAc production rate	kmol/h	47.4	47.4
Gas-loop pressure*	kPa	883	930
Reactor inlet temp.	°C	150	137
O_2 conc. at the reactor inlet	mol frac	0.075	0.048
C_2H_6 conc. in the recycle gas	mol frac	0.249	0.163
CO_2 conc. in the recycle gas	mol frac	0.0073	0.0000
Gas recycle flow rate	kmol/h	990	516
H_2O conc. in the liquid recycle	mol frac	0.107	0.002
Liquid recycle flow rate	kmol/h	106.2	8.4
Reactor outlet temp.	°C	159.2	138
Fresh ethylene feed rate	kmol/h	50.22	48.60

* The upper limit is set at 930kPa

The calculation time for the 80 h simulation in this example was only around 16 min (single-core use of AMD Opteron 3.2 GHz).

5. CONCLUSION

A rigorous nonlinear dynamic simulator of the benchmark vinyl acetate production plant has been introduced. It can serve as a test bed for new technical developments in the fields of process control, fault detection and diagnosis, etc.

The VAc plant models with a free limited license of Visual Modeler will be made available by Omega Simulation Co.,Ltd. through the company's web site:
`http://www.omegasim.co.jp/index_e.htm` .

ACKNOWLEDGEMENTS

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[1] The task force "Workshop No.27 Process Control Technology" was launched in 2007 to sift through problems regarding process control and investigate solutions. It consists of 32 engineers from industry and 12 researchers from universities.

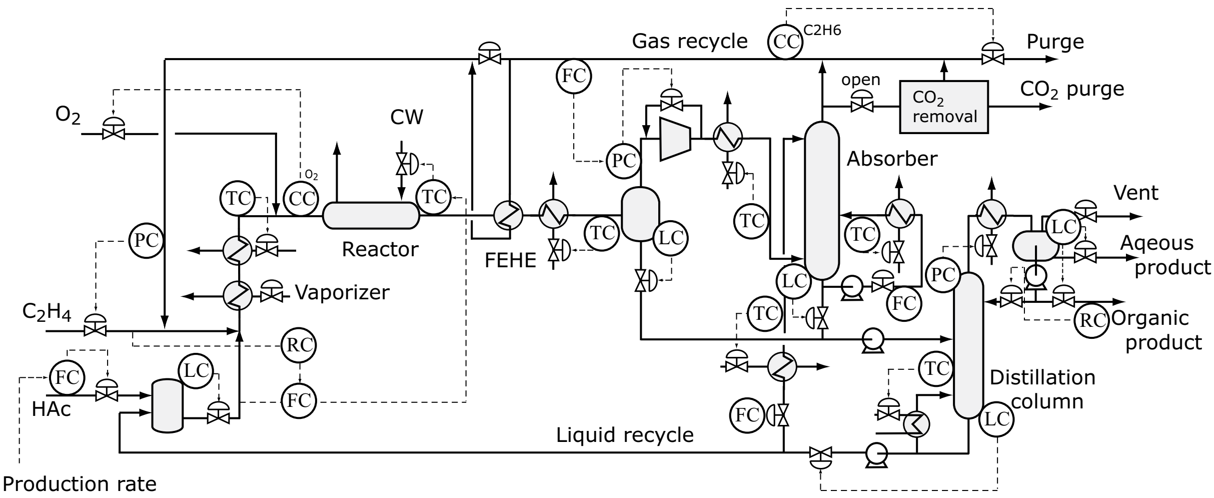

Fig. 4. An alternative control loop configuration. The fresh acetic acid feed is on flow control to set the production rate. A cascade loop from the liquid reactor feed flow to the reactor temperature setpoint is incorporated to ensure regulation of the acetic acid inventory.

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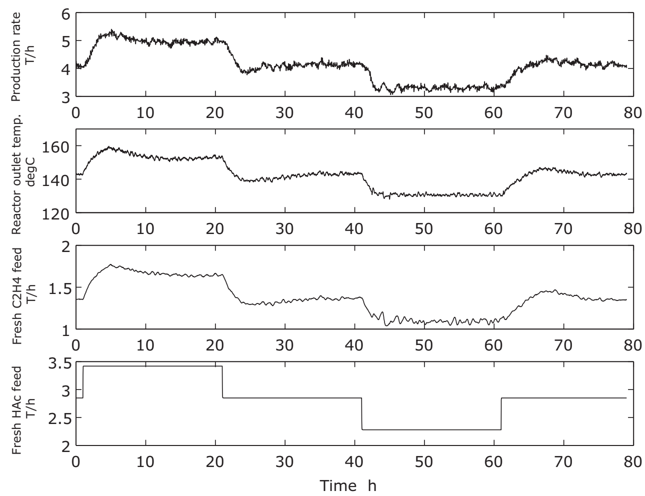

Fig. 5. Simulation results for ±20% step changes in the fresh HAc feed rate.

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