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Simulation, control and sensitivity analysis of crude oil distillation unit

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Steady-state and dynamic simulation play important roles in investigation of refinery units. Therefore, simulation can help this investigation and behavior assessment. In this paper, simulation was done by commercial software. In fact, because of solving many state equations simultaneously and using control theory, dynamic simulation has more significant impact than steady-state simulation. Flow, pressure, temperature and level (FPTL) were controlled by Proportional-Integral-Derivative (PID) controllers in the unit. The case study is Kermanshah Refinery. The behavior of the FPTL controllers in dynamic regime were observed after the changing of the crude oil feed flow rate by 3% for 5 h. ASTM D86 boiling points (compositions) of two simulations were compared with experimental data. Finally, system sensitivity to inputs variables was investigated in the MATLAB®/Simulink™ by transferring the dynamic results. Transient responses to changes such as feed temperature, feed flow rates, steam flow rates and the duties of the reboilers of columns in Gasoline unit were plotted. Among of all disturbances, the system is more sensitive to changes in the feed temperature, the duties of the reboilers of columns in gasoline unit and simultaneous combination of above changes.

Key words: Steady-state, dynamic, PID controller, ASTM D86, Sensitivity, MATLAB simulink, transition responses.

INTRODUCTION

Today, distillation of crude oil is an important process in almost all of the refineries. Simulation of the process and analysis of the resulting data in both steady-state and dynamic conditions are fundamental steps in decreasing of the energy costs and controlling the quality of the oil products. The dynamic simulation when adding some Proportional-Integral-Derivative (PID) controllers and setting them to have desired responses, has more significant impacts and challenges than steady-state simulation in crude oil distillation units. A PID controller is a controller that includes three elements (Araki, 2002). PID control systems have exactly the same structure as depicted in Figure 1, where the PID controller is used as

the compensator *C(s)*. The transfer function of a PID controller is:

$$C(s) = K_P\left(1 + \frac{1}{\tau_I s} + \tau_D s\right)$$

(1)

All the three elements are kept in action. Here, K_P, τ_I and τ_D are positive parameters, which are respectively referred to as proportional gain, integral time, and derivative time, and as a whole, as PID parameters. These parameters can be adjusted using some empirical methods. One of them, which is an extension to Ziegler-Nichols method and uses the ultimate gain and frequency for adjustment of the parameters, is Tyreus-Luyben method (Almudena, 2001).

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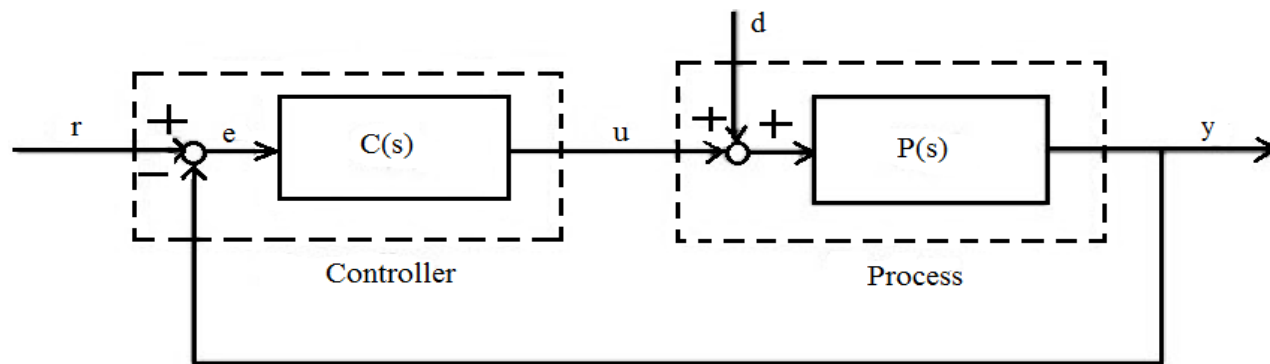*Corresponding author. E-mail: jsadeghi@hamoon.usb.ac.ir. Tel: +989155494265.

Figure 1. Conventional feedback control system.

Crude oil is a mixture of many thousands of components varying from light hydrocarbons such as methane, ethane, propane, etc., to very high molecular weight components. The compositions of crude oil depend also on the location of exploitation. In the present work, the feed flow rate is 0.046 m^3/s (25,000 bbl/day) that is provided by the blending of Crude oils of Ahwaz (60%), Naft-I-Shah (24%) and Maleh-Kuh (16%). Therefore, the feed has very complex compositions. Also the design and optimization of the oil fractionators are very important and complex. In petroleum refining the boiling point ranges are used instead of mass or mole fractions. Four types of boiling point analysis are known: ASTM D86, ASTM D1160, ASTM D158 and TBP (True Boiling Point). Six streams of product were investigated by ASTM D86 from initial boiling point (IBP) to final boiling point (FBP). We studied the system behavior by changing the feed flow rate in the dynamic conditions and MATLAB®/Simulink^{TM}. MATLAB software is very flexible for this work, therefore, it was used.

The aims of this work are to investigate the results in steady-state and dynamic simulations, FPTL control while changing the crude oil feed flow rate and comparison of ASTM D86 boiling points (compositions) in two simulations with the correspondent experimental data. At last, sensitivity analysis of crude oil distillation unit in the MATLAB®/Simulink^{TM} was done by transferring dynamic files to it as the basis aim. Directions of transferring files to sensitivity analysis were:

Steady state files ⟶ Dynamic files ⟶ MATLAB®/Simulink^{TM}

Physical-mathematical model of the distillation column

In the problems of multiple-stage separation for systems in which different phases and different components play a part, we have to resort to the simultaneous or iterative solution of hundreds of equations. This means that it is necessary to specify a sufficient number of design variables so that the number of unknown quantities (output variables) is exactly the same as the number of equations (independent variables). This number of equation can be found and counted in a mathematical model.

The usual method to mathematically model a distillation process in refining columns is the theoretical stage method. To find the number of the theoretical stages of an existing column, the real number of stages might be multiplied by column efficiency. For each theoretical stage, the mass balance of individual components or pseudo components, energy balance, and vapor-liquid equilibrium equation can be written. The set of these equations creates the mathematical model of a theoretical stage. The mathematical model of a column is composed with models of individual theoretical stages. Finally, thermodynamic model Braun K10 "BK10" was used for the unit, because it is a model suitable for mixtures of heavier hydrocarbons at pressures under 700 kPa and temperatures from 170 to 430°C. The values of K10 can then be obtained by the Braun convergence pressure method using tabulated parameters for 70 hydrocarbons and light gases (Aspen Physical Property System, 2009). At low pressures, the Braun K10 model is strictly applicable to predict the properties of heavy hydrocarbon systems. Using the Braun convergence pressure method by the model at, given the normal boiling point of a component, K value is calculated at system temperature and 10 psia. The K10 value is then corrected for pressure using pressure correction charts. Using the modified Antoine equation one can find the K values for any components that are not covered by the charts at 10 psia and corrected to system conditions using the pressure correction charts (Aspen Physical Property System, 2009).
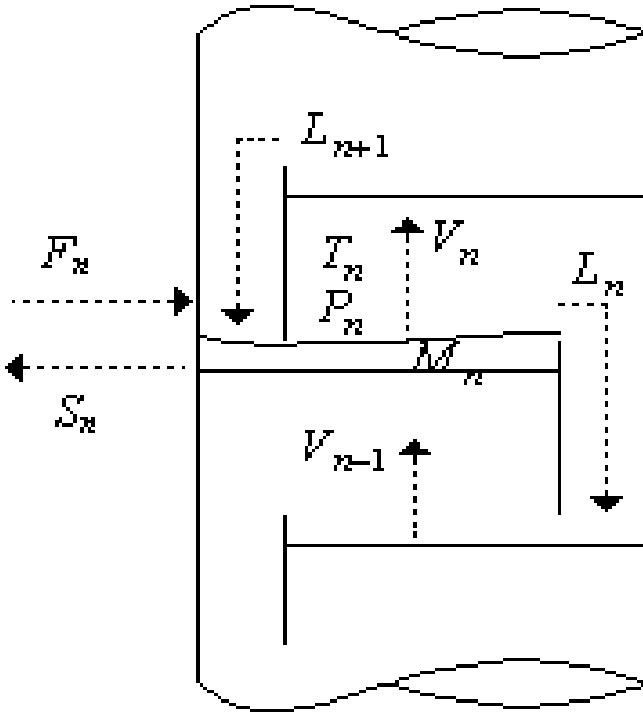
In existence of a large amount of acid gases or light

Figure 2. Scheme of a column stage.

hydrocarbons, the accuracy has encountered some problems with this model. All three phase calculations assume that the aqueous phase is pure H_2O and that H_2O solubility in the hydrocarbon phase can be described using the kerosene solubility equation from the API data book (Aspen Physical Property System, 2009).

The above model was solved by commercial software to select BK10 model in the software space. The obtained model was solved by Newton numerical method that is:

$$X_{n+1} = X_n - \frac{f(X_n)}{f'(X_n)}$$

(2)

Mass balance

The following is a representative sketch of any of these stages (Figure 2):

Dynamic general mass balance of stage *n*:

$$\frac{dM_n}{dt} = L_{n+1} + V_{n-1} + F_n - L_n - V_n - S_n \quad (3)$$

Liquid holdup on stage n can be calculated as:

$$M_n = \rho_{L,n}\left(A_{T,n}h_{T,n} + A_{D,n}h_{D,n}\right)$$

(4)

In the steady-state space, the left side of Equation (3) is equal zero:

$$0 = L_{n+1} + V_{n-1} + F_n - L_n - V_n - S_n$$

(5)

Dynamic component mass balance of stage *n*:

$$\frac{d(M_n x_{n,j})}{dt} = L_{n+1}x_{n+1,j} + V_{n-1}y_{n-1,j} + F_n z_{n,j} - L_n x_{n,j} - V_n y_{n,j} - S_n x_{n,j}$$

(6)

In the steady-state space, the left side of equation (6) is equal zero (Lee et al., 1975):

$$0 = L_{n+1}x_{n+1,j} + V_{n-1}y_{n-1,j} + F_n z_{n,j} - L_n x_{n,j} - V_n y_{n,j} - S_n x_{n,j}$$

(7)

Energy balance

Dynamic general energy balance of stage *n*:

$$\frac{d(M_n h_n)}{dt} = L_{n+1}h_{n+1} + V_{n-1}H_{n-1} + F_n h_f - L_n h_n - V_n H_n - S_n h_n + Q_M - Q_s - Q_{loss}$$

(8)

The changes in the specific enthalpy of the liquid phase are generally very small compared to the total enthalpy of the stage. This means that, normally, the energy balance can be reduced to an algebraic equation which is used as the basis to calculate the flow of vapor from the stage which is made a steady-state space. Finally, the energy balance is as follows (Lee et al., 1975):

$$0 = L_{n+1}h_{n+1} + V_{n-1}H_{n-1} + F_n h_f - L_n h_n - V_n H_n - S_n h_n + Q_M - Q_s - Q_{loss}$$

(9)

Vapor-liquid equilibrium

Vapor-liquid equilibrium of component *j* for theoretical stage *n*:

$$y_{n,j} = \frac{\gamma_{n,j} P_{n,j}^{sat}}{P_n \Phi_{n,j}} x_{n,j}$$

(10)

Table 1. The Mass flows of the atmospheric column products.

Product	Mass flow (Kg/s)
Naphtha	19.43
Blending naphtha	0.25
Kerosene	6.55
Atmosphere gas oil	6.38
Atmospheric residue	15.68

Table 2. The Mass flows of the debutanizer column products.

Product	Mass flow (Kg/s)
To fuel	0.38
To LPG unit	0.72
Bottom product	8.2

Table 3. The Mass flows of the splitter column products.

Product	Mass flow (Kg/s)
To flare	0.01
To LSRG Merox	2.1
HSRG to platforming	6.1

This equation is the equilibrium and in real state. If each of vapor or liquid phase is ideal then $\Phi_{n,j}$ or $\gamma_{n,j}$ is unit, respectively. If both phases are ideal then $\Phi_{n,j}$ and $\gamma_{n,j}$ are unit. Therefore, the above equation is converted to Raoult's equation:

$$y_{n,j} P_n = x_{n,j} P_{n,j}^{sat}$$
(11)

Pressure

$$P_n = P_{n+1} + \Delta P$$
(12)

$$\Delta P = \left(\frac{V_0}{K} \right)^2$$
(13)

Where V_0 the volumetric flow is rate of live stream in m³/h and K is the proportionality constant in m³/bar$^{0.5}$.h. The value of K for each geometry is different and has specific value which is chosen by software (Almudena, 2001; Lee et al., 1975).

Steady-state simulation

In this work, distillation unit of Kermanshah Refinery was simulated. The three assays of crude oil were characterized by the TBP (True Boiling Point) data, API gravity and light components.

The unit consists of 5 heat exchangers, 2 coolers, 2 heaters, atmospheric column, debutanizer column, splitter column, valves and pumps. The atmospheric column as the main part of the unit had three side strippers and two pumparounds. Important parameters for the pumparound specification are the drown off and the return stages, mass flow rate and temperature drop. For the side strippers, beside the product flow rate, the specification of the steam flow and parameters, the drown off and the return stages, and the number of stripper stages were entered. The feed flow rate of 0.046 m³/s (25,000 bbl/day) of crude oil was preheated. Then, it was entered to the 35th stage of the atmospheric column with 38 theoretical stages. Temperature of the feed was 328.11°C (622.6°F). Products of the column are naphtha, blending naphtha, kerosene, atmospheric gas oil and atmospheric residue. Table 1 shows their mass flow rates.

The product of kerosene, atmospheric gas oil and atmospheric residue played an important role in preheating of the feed, because they had high temperatures, hence energy optimization was done.

To purify the naphtha, firstly it was cooled to 26.67°C (80°C). Then the naphtha stream was entered to a two-phase separator and splitter. Fifty percent of the flow was returned as the reflux stream and the other half was preheated and entered to the debutanizer column. The bottom product preheated the feed and entered to splitter column.

Tables 2 and 3 show the mass flow rates of the products (Tables 2 and 3). Also, Figure 3 illustrates the steady-state simulation scheme of the above steps in continuous forms.

Dynamic simulation

After steady-state simulation to observation the effects of changes the crude oil feed in the products of unit and investigation of results in real processes, we exported the stead-state simulation to dynamic simulation.

Before transferring the steady-state files, dynamic simulation requirements should be entered. In addition, the pressure changers (valves, pumps, etc.) are necessary and sensitive to exporting of steady-state simulation to dynamic simulation by "export dynamic (pressure driven)".

For example dynamic requirements of column are column diameter, tray spacing, tray active area, weir
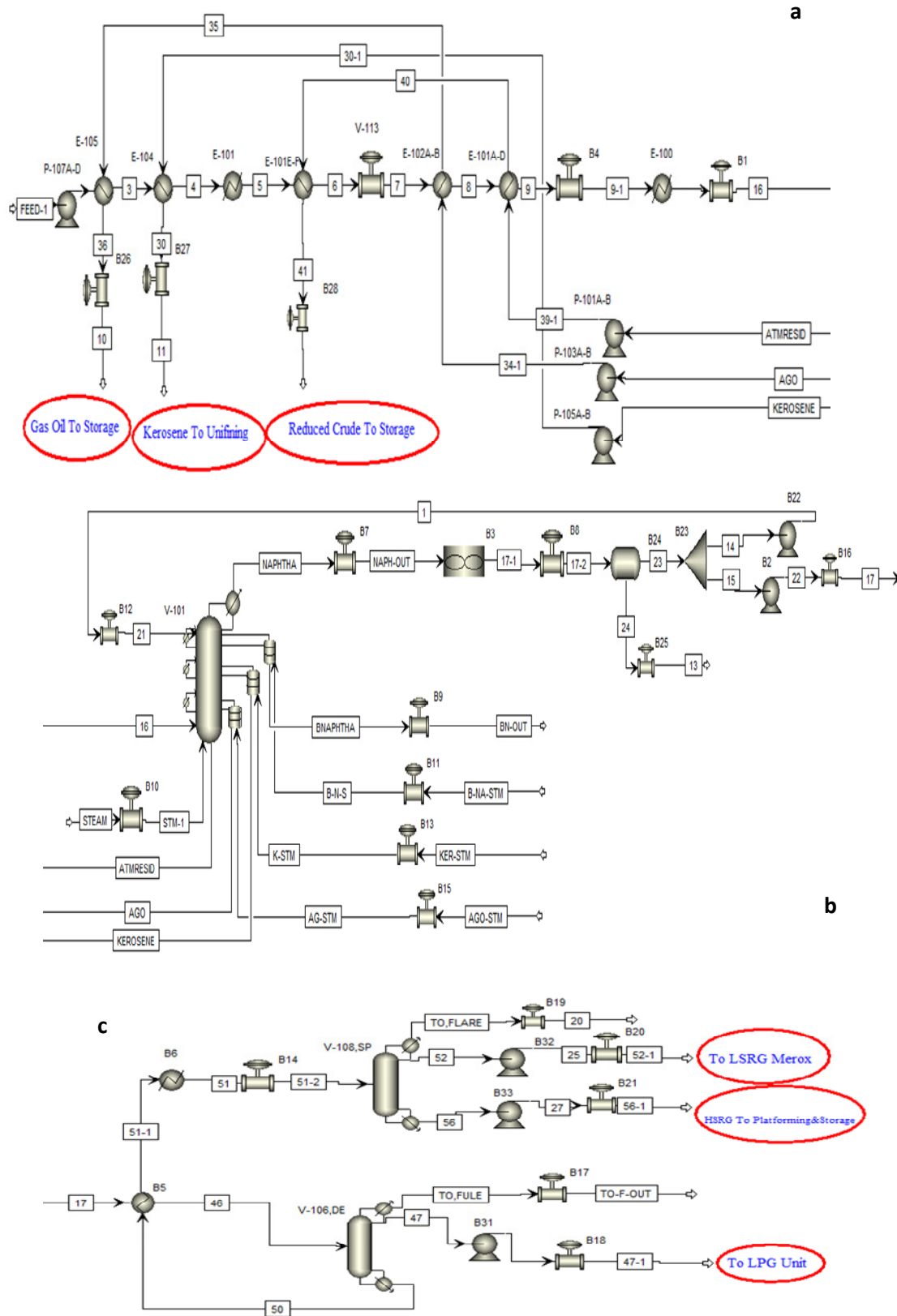
Figure 3. Steady-state simulation scheme of distillation unit; (a) preheating; (b) atmospheric distillation column; (c) Gasoline unit (light and heavy).

length, weir height, reflux drum length and diameter, and sump length and diameter. A "tray sizing" tool can be used to calculate the tray sizes based on flow conditions in the column. Of course, all of dynamic simulation requirements were provided by Research and Development (R&D) Bureau of Kermanshah Refinery.

After entering data and exporting to dynamic simulation in order to control the flow, pressure, temperature and level of streams, especially all products than changing of crude oil feed, controllers should be added in right places in the dynamic space. Dynamic space provides a number of different types of controllers. The PID Incr. model was used for all controllers in the dynamic space. The parameters of each controller (gain, integral time and derivative time) were set to optimal values using the assistance of the "tuning" tool and Tyreus-Luyben method (Luyben, 2006; Juma and Tomáš, 2009). Figure 4 illustrates the dynamic simulation scheme of continuous forms (Figure 4). Streams ID are corresponding to the steady-state simulation scheme.

RESULTS AND DISCUSSION

Distillation temperature ASTM D86

After changing the crude oil feed flow rate, ASTM D86 of six streams (("52-1", light gasoline), ("56-1", heavy gasoline), the feed of debutanizer column (V-106, DE), blending naphtha, kerosene and atmospheric gas oil) in three spaces of experimental, steady-state and dynamic were compared. Experimental data were provided by R&D Bureau of Kermanshah Refinery.

Figures 5 to 10 show a comparison between the experimental ASTM D86 curves with the results of the steady-state and the dynamic simulations. Curves of the feed of debutanizer column (V-106, DE) and atmospheric gas oil stream were in better agreement with the experimental data than the other streams. Of course, maximum difference of other streams was around 12°C. Totally, results of simulations were in good agreement with the experimental data (Kermanshah Refinery, 2009).

2- Sensitivity analysis in the MATLAB simulink

The behaviors of the FPTL controllers in dynamic simulation were observed by increasing the crude oil feed flow rate (+3%). The FPTL were controlled by conventional PID controllers. Set points were set based on Kermanshah Refinery. Twenty-three controllers were applied to control of FPTL of the unit. We tried to set the controller parameters and solved of fluctuations by different control methods to reach a new steady-state. To set the controller parameters, Tyreus-Luyben method

was employed. At last, we investigated of dynamic results by transferring the dynamic files to MATLAB®/Simulink[TM] Figure 11. The first steady-state then system sensitivity was observed by step changes. Input variables were:

1. Feed temperature (+10°C).
2. Feed flow rates: Ahwaz (+1%), Maleh-Kuh (+1%), Naft-I-Shah (+1%)
3. Steam flow rates: STEAM (interring to atmospheric column, +20%), blending naphtha, steam (+50%), kerosene steam (+30%), atmospheric gas oil (AGO) steam (+30%).
4. The duty of Reboilers: debutanizer column (V-106-DE, +3%), splitter column (V-108- SP, +3%).
5. Mixed of above changes simultaneously.

And outputs were: Stream flow rates: "46" (interring to V-106-DE), blending naphtha, kerosene, atmospheric gas oil (AGO), "39-1" (bottom of atmospheric column), "52-1" (light gasoline, up of V-108-SP column), "56-1" (heavy gasoline, bottom of V-108-SP column), "47-1" (to LPG unit).

Because we wanted to increase the products, increasing of inputs were investigated. After performing above changes, we observed that the major sensitivity was related to feed temperature, the duties of the reboilers of columns in gasoline unit and simultaneous combination of above changes (Figures 12-16). Rest of input changes was not significant to steady-state.

Conclusions

Steady-state and dynamic simulations performed a good investigation into the process and discussing the calculated results. Control of variables in dynamic simulation as a flexible simulator like a pilot, was done very well.

Steady-state and dynamic simulations were in agreement with the experimental data. Any Increment of crude oil feed flow rate, made a complex fluctuations in the FPTL controllers that must be rejected by set of controller parameters and different control methods. Because the feed was a mixture of 3 crude oils and many components, control of system was very complex. The dynamic space demonstrated that temperature controllers were faster and more sensitive than the other controllers. Control of temperature can be replaced by control of the product compositions. In this control structure, small control errors in the FPTL controllers were observed. Therefore, some limitations in dynamic simulation were observed. Because of more flexibility of changing the inputs, disturbances and easier handling of graphs, dynamic files results transferred to
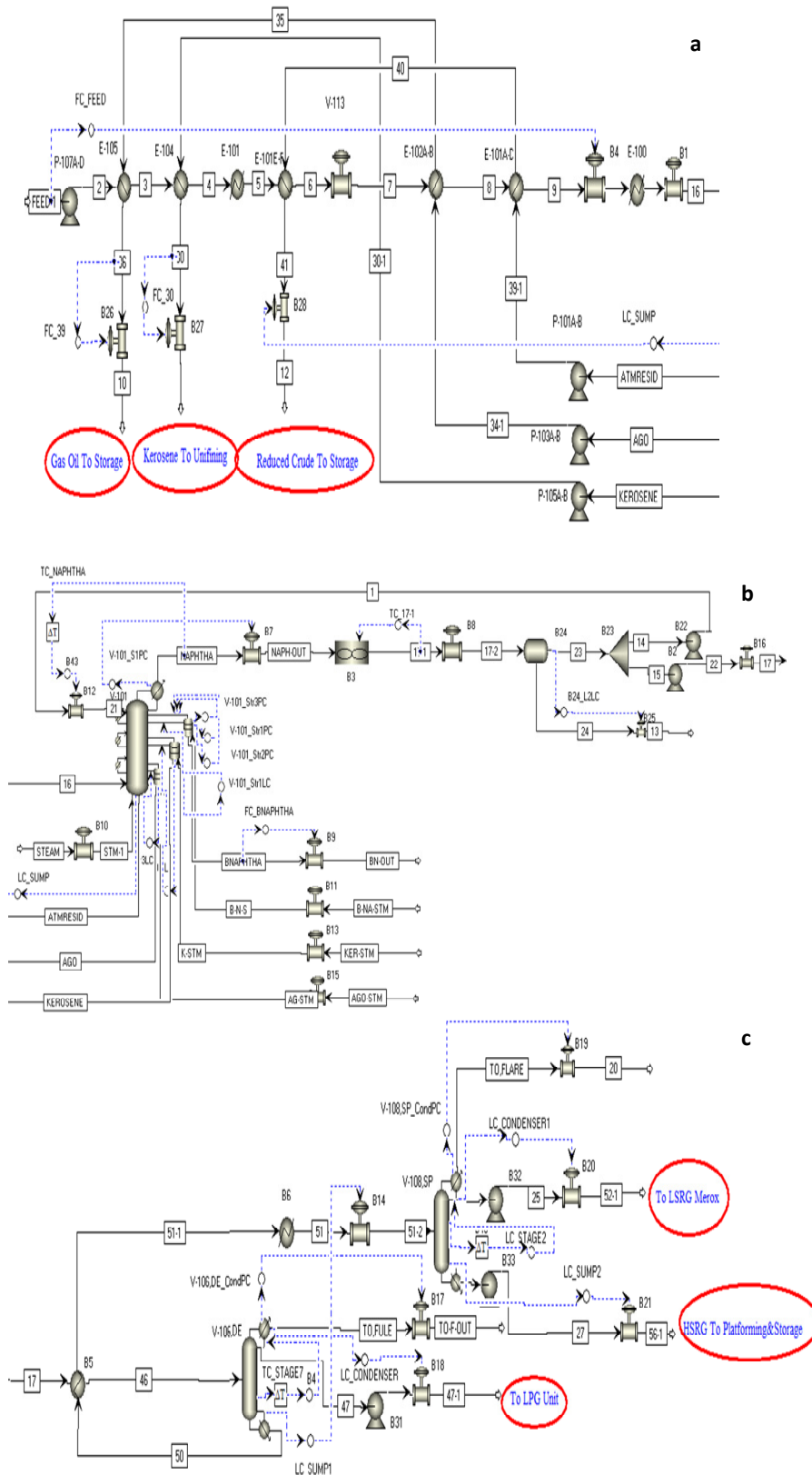
Figure 4. Dynamic simulation scheme of distillation unit; (a) preheating; (b) Atmospheric distillation column; (c) Gasoline unit (light and heavy).
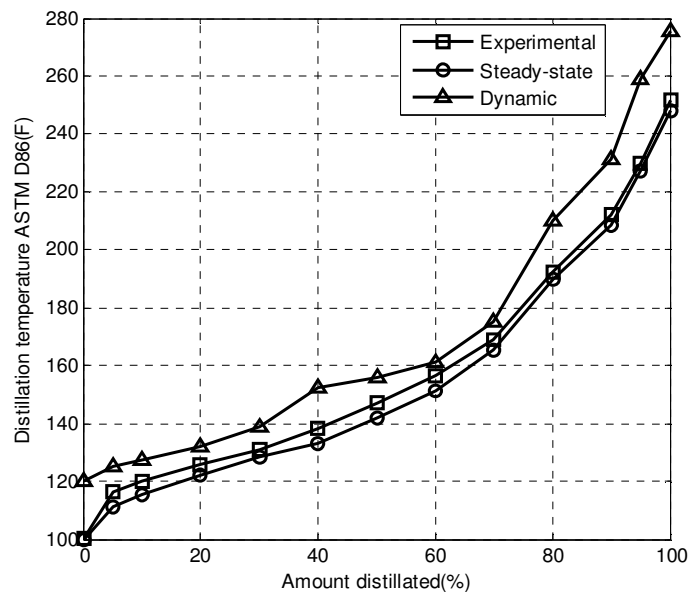
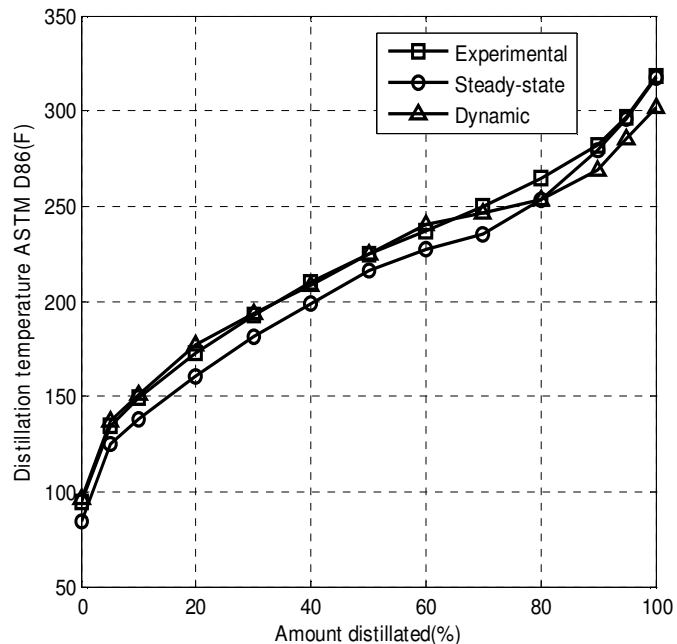**Figure 5**. Steady-state, dynamic and experimental ASTM D86 curves of "52-1" stream.

Figure 6. Steady-state, dynamic and experimental ASTM D86 curves of "56-1" stream.

Figure 7. Steady-state, dynamic and experimental ASTM D86 curves of column feed (V-106, DE).
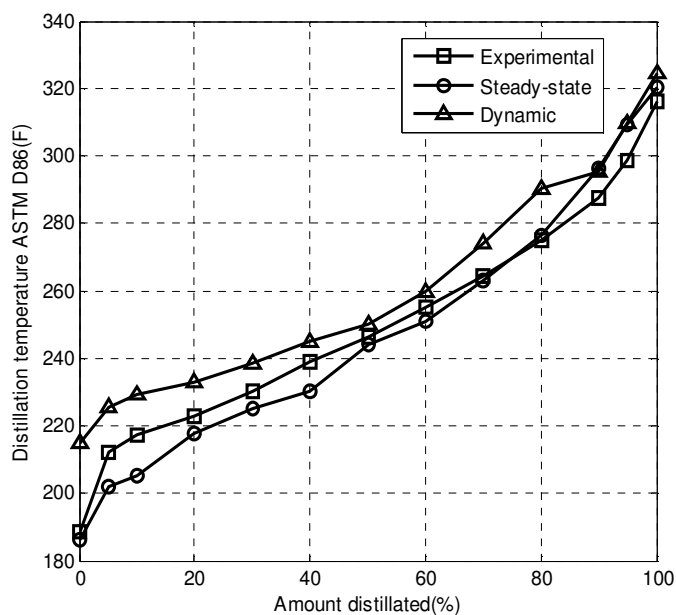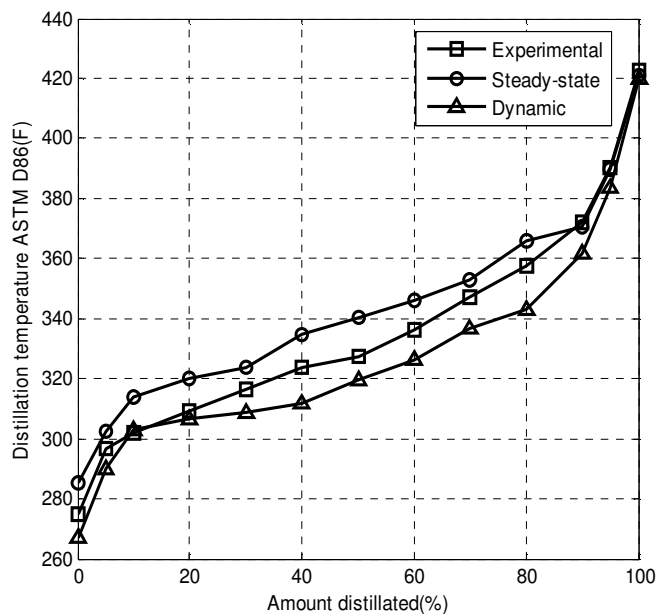

Figure 8. Steady-state, dynamic and experimental ASTM D86 curves of Blending Naphtha (B_NAPHTHA Stream).

MATALB®/Simulink™. Figures 12 to 16 show that more sensitive disturbances were feed temperature, the duties of the reboilers of columns in gasoline unit and simultaneous combination of above changes. Rest of input changes was not significant in transient responses. Therefore, above variables play important roles in the design of distillation units.
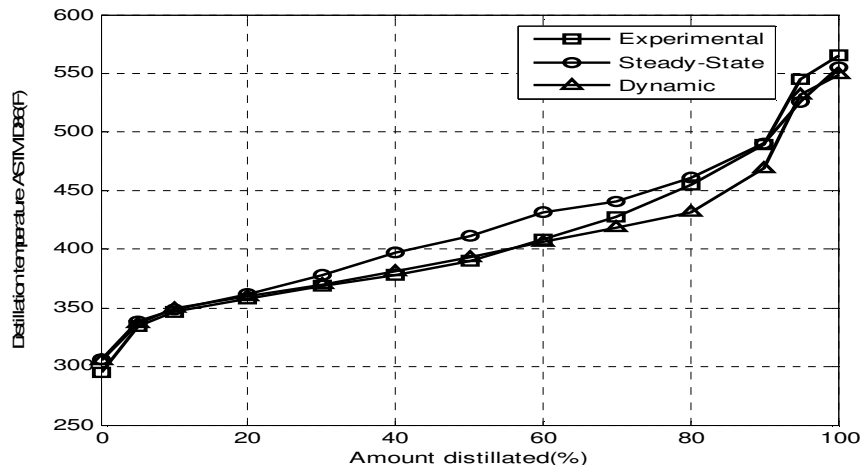
ACKNOWLEDGMENT

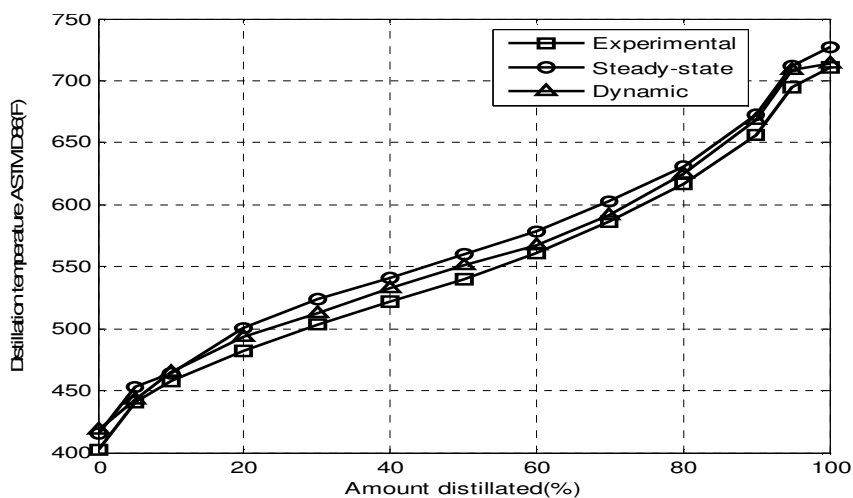**Figure 9.** Steady-state, dynamic and experimental ASTM D86 curves of Kerosene.

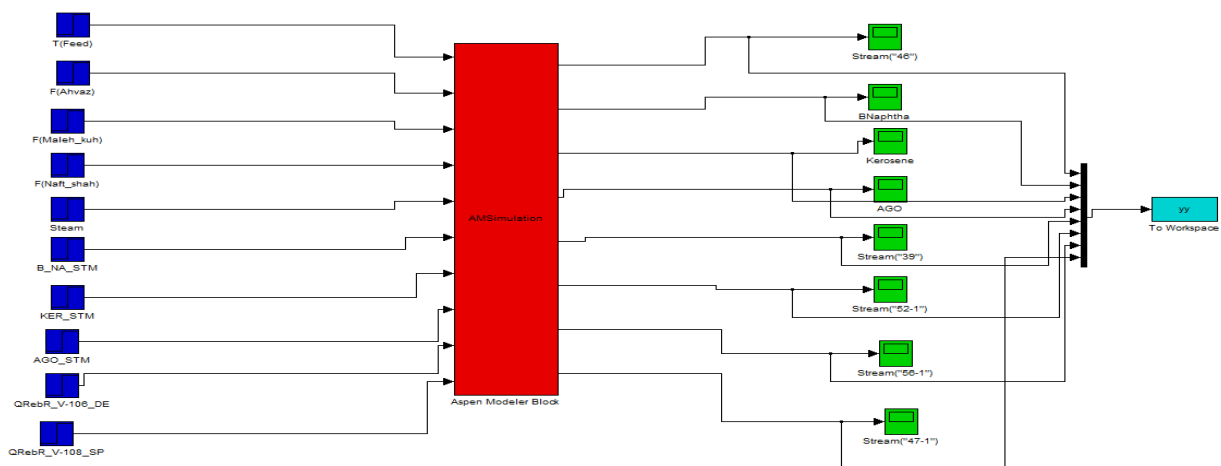**Figure 10.** Steady-state, dynamic and experimental ASTM D86 curves of atmospheric gas oil (AGO stream).

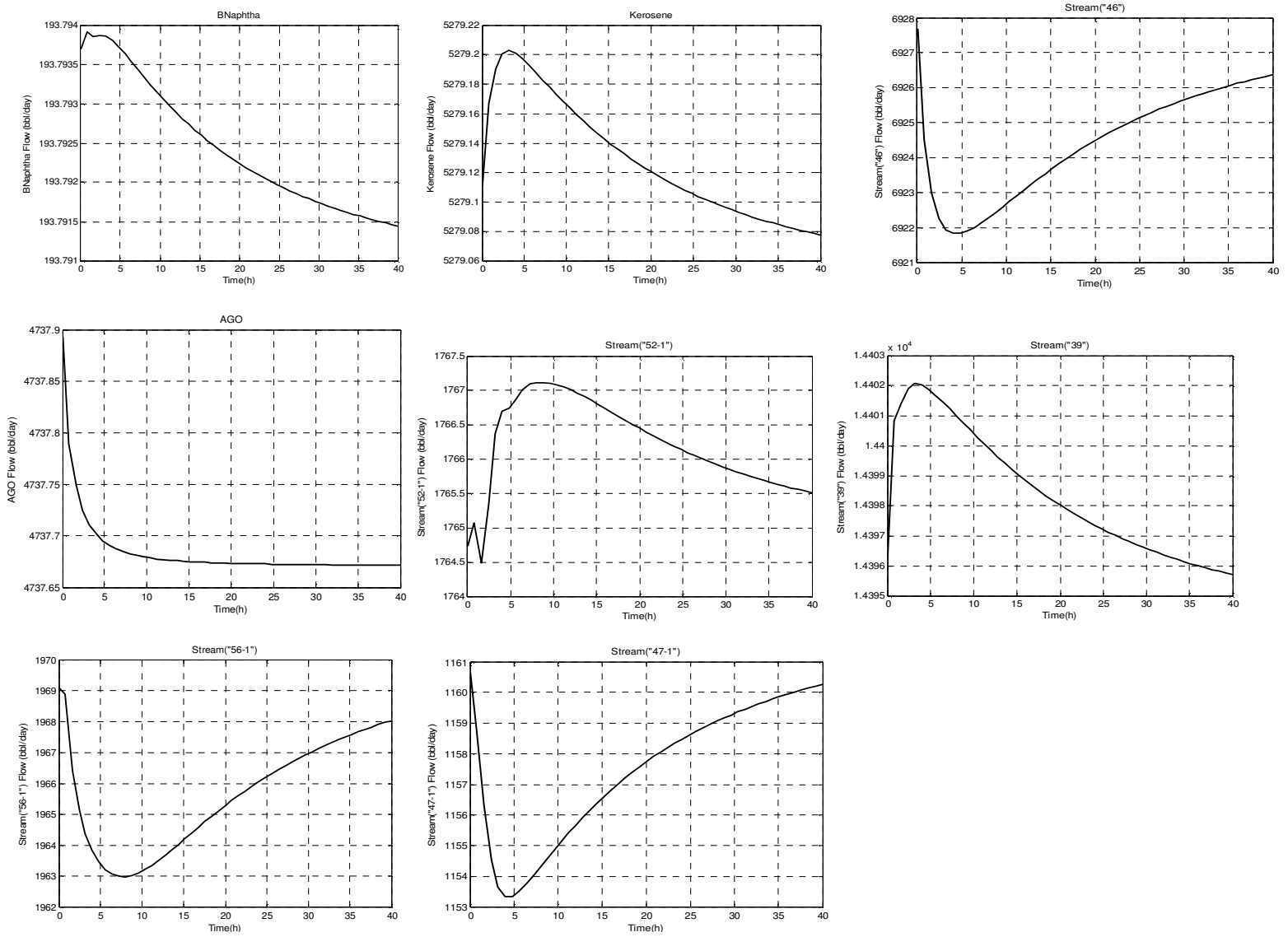**Figure 11.** Scheme of Distillation unit in the MATLAB simulink with inputs and outputs.

Figure 12. Steady-state curves of stream: 46, B_Naphtha, Kerosene, AGO, (39-1), (52-1), (56-1) and (47-1).
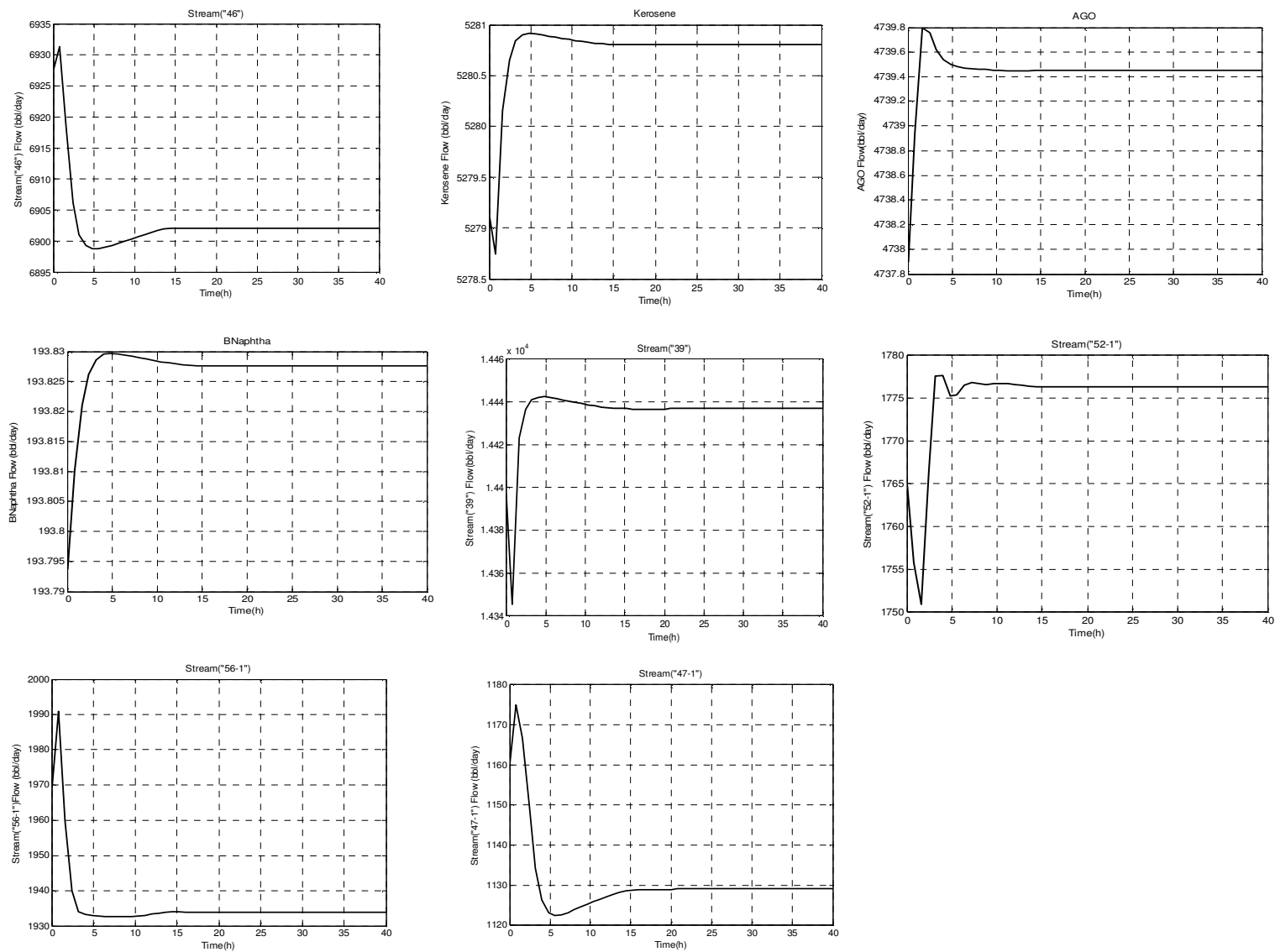
Figure 13. Curves of stream with change of feed temperature (+ 10℃): 46, B_Naphtha, Kerosene, AGO, (39-1), (52-1), (56-1) and (47-1).
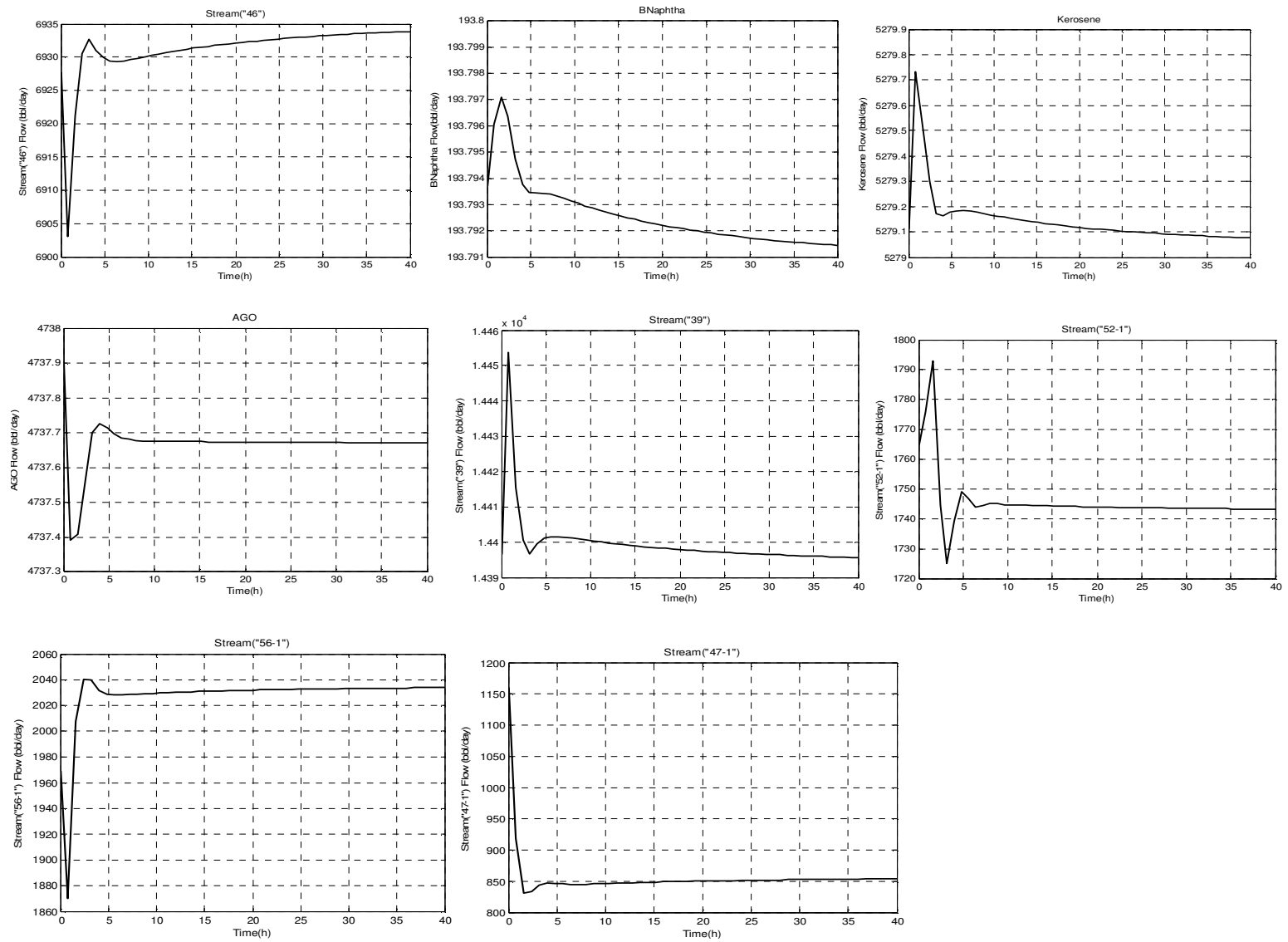
Figure 14. Curves of stream with change of Reboiles duty,V-106-DE (+ 3%): 46, B_Naphtha, Kerosene, AGO, 39, (52-1), (56-1) and (47-1).
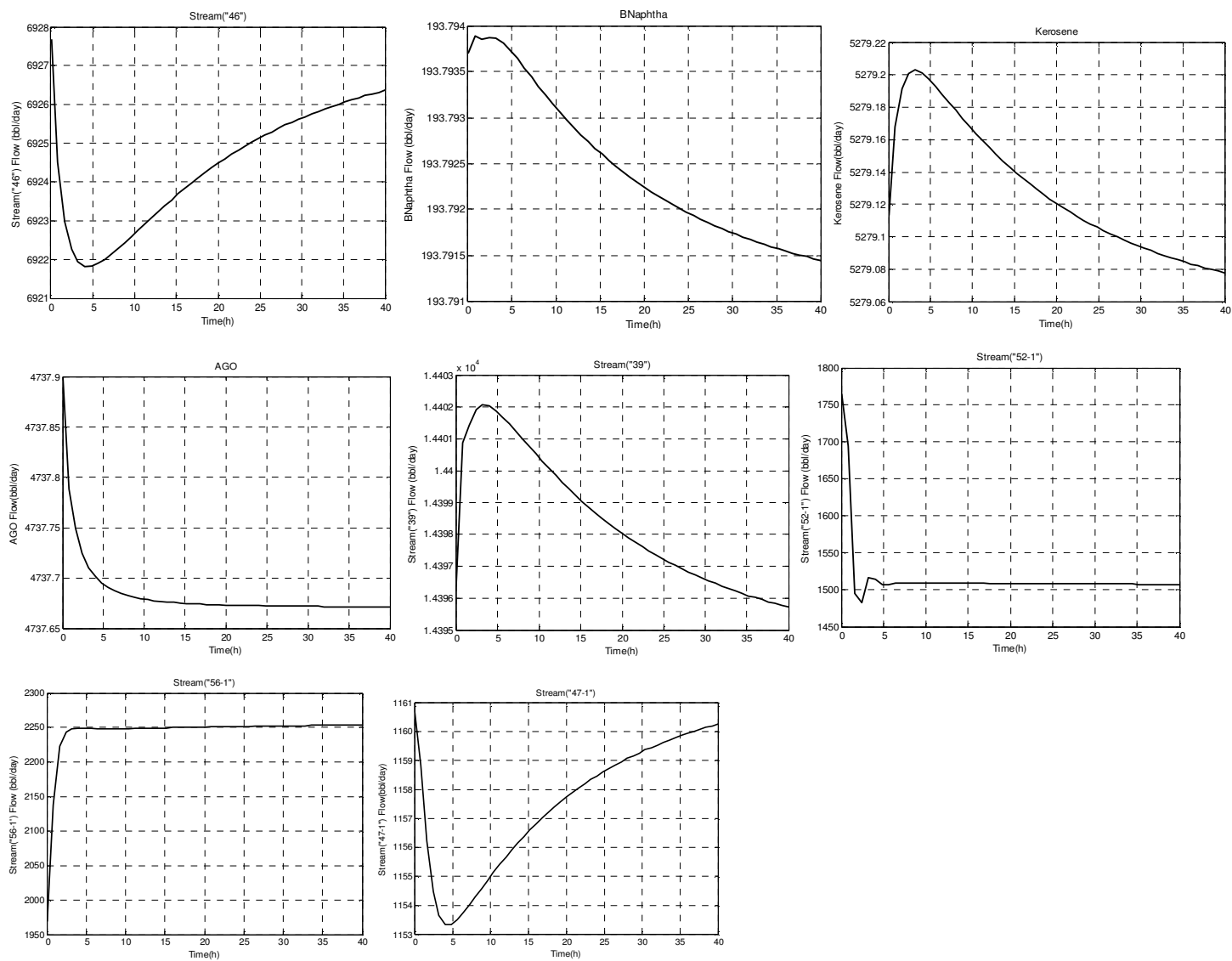
Figure 15. Curves of stream with change of Reboiles duty,V-108-SP (+ 3%): 46, B_Naphtha, Kerosene, AGO, 39 , (52-1), (56-1) and (47-1).
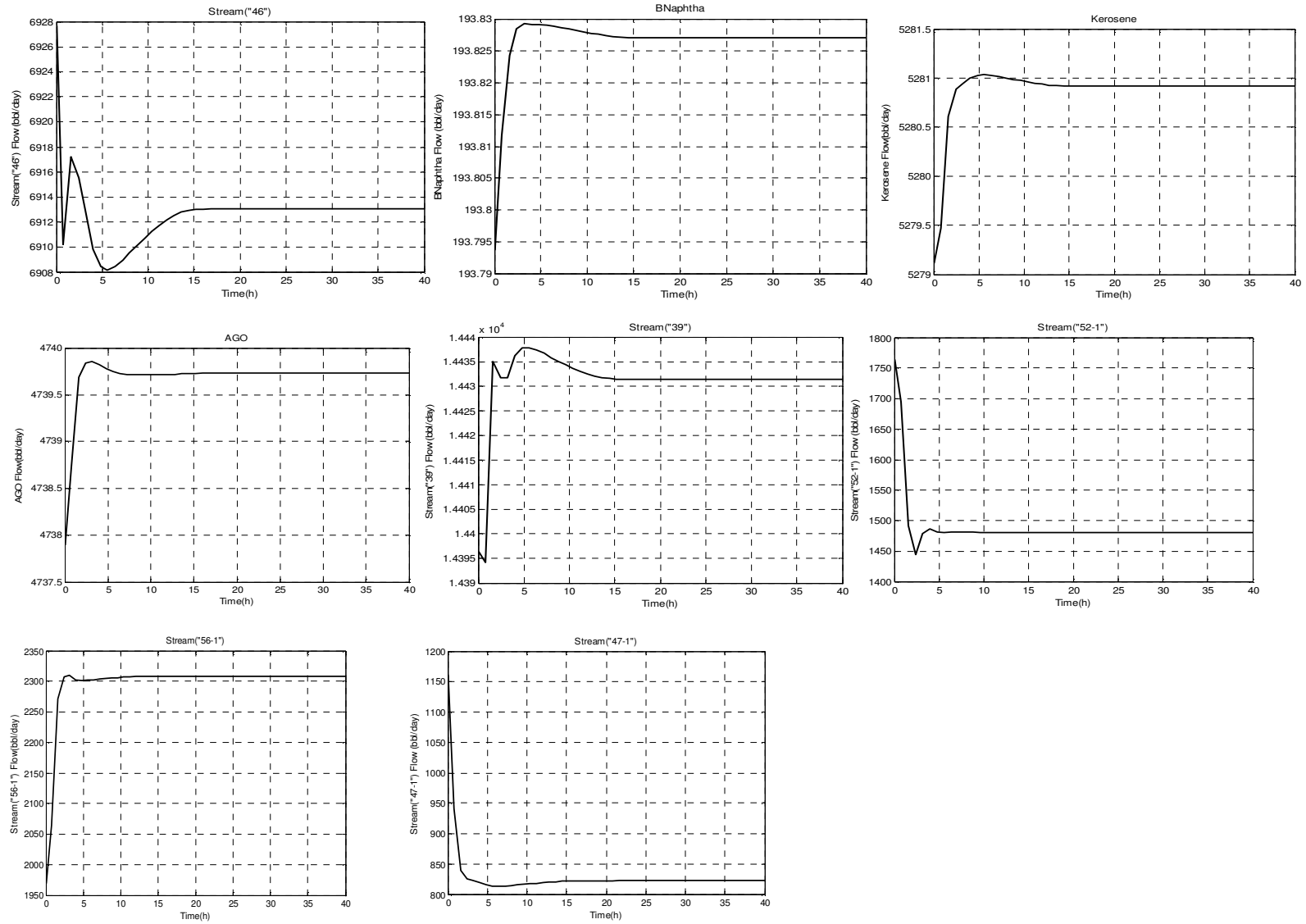
Figure 16. Curves of stream with simultaneous combination of above changes: 46, B_Naphtha, Kerosene, AGO, 39, (52-1), (56-1) and (47-1).

Nomenclature

$A_{D,n}$: surface area of the downcomer [m^2]

$A_{T,n}$: active surface area of the stage n [m^2]

bbl: barrel

C(s): Controller transfer function

D: Load or disturbance

E: Error signal

F_n : molar feed flow onto stage n [$\frac{mol}{s}$]

h_n : molar enthalpy of the liquid on stage n [$\frac{J}{mol}$]

h_{n+1} : molar enthalpy of the liquid from stage $n+1$ [$\frac{J}{mol}$]

H_n : molar enthalpy of the vapor on stage n [$\frac{J}{mol}$]

H_{n-1} : molar enthalpy of the vapor from stage $n-1$ [$\frac{J}{mol}$]

h_f : molar enthalpy of feed [$\frac{J}{mol}$]

$h_{T,n}$: liquid height on the stage n [$\frac{J}{mol}$]

$h_{D,n}$: liquid height on the downcomer [$\frac{J}{mol}$]

K_P : controller gain

L_{n+1} : the molar liquid that overflows onto stage n from stage $n+1$ [$\frac{mol}{s}$]

L_n :   molar liquid flowing from stage n [$\frac{mol}{s}$]

M_n : the liquid mole accumulated on stage n (liquid holdup on stage n) [$\frac{mol}{s}$]

P(s): process transfer function

P_n: pressure on stage n [pa]

Q_M : heat of mixing [$\frac{J}{mol}$]

Q_s : external heat source [$\frac{J}{mol}$]

Q_{loss} : heat losses [$\frac{J}{mol}$]

r: desired value

R&D: Research and Development

S_n : molar side stream from stage n [$\frac{mol}{s}$]

T_n: Temperature on stage n [$^{\circ}C$]

U: Manipulated value

V_{n-1} : the molar vapor flow from stage $n-1$ [$\frac{mol}{s}$]

V_n : molar vapor flow flowing from stage n [$\frac{mol}{s}$]

$x_{n,j}$: molar fraction of component j in the liquid on stage n

$x_{n+1,j}$: molar fraction of component j in the liquid current from stage $n+1$

Y: Output value

$y_{n-1,j}$: molar fraction of component j in the vapor current from stage $n-1$

$y_{n,j}$: molar fraction of component j in the vapor current from stage n

$z_{n,j}$: molar fraction of component j in the feed current on stage n

$\rho_{L,n}$: liquid density at stage n [$\frac{mol}{m^3}$]

τ_D : Controller derivative time [s]

τ_I : Controller integral time [s]

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