Modeling and Simulation of the Oil/Water Quench System in an Olefin Unit

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A mathematical model is developed for the simulation of a general oil/water quench system in an olefin unit. The quench system involves a series of towers in which pyrolysis products, containing a wide boiling range of hydrocarbons and water vapor, are cooled by direct contact with quench oil and water and are separated into major fractions. The system is modeled as a single distillation column with multiple feeds and side stream drawoffs, in which parts of the condensed water and heavier hydrocarbons are recirculated to the column as cooling media. The model is based on the assumption that water and hydrocarbons are completely immiscible in the liquid phase. A computational scheme is developed which requires estimates of column temperatures, hydrocarbon vapor rates, and circulating quench rates. An example problem is given to illustrate the applicability of the proposed model. It is shown that the calculated results are in good agreement with the data obtained in a typical industrial olefin plant.

Introduction

The purpose of this paper is to present a mathematical model for the simulation of a general oil/water quench system in an industrial olefin unit. The model may be used in the evaluation of plant performance and in the design of new plants.

Thermal cracking of hydrocarbons to produce ethylene and higher olefins is one of the main processes in the petrochemical industry. Faced with variations in feedstock availability, a modern olefin plant in the United States may be designed with flexibility to use gaseous and/or liquid hydrocarbon feeds. The feedstocks are cracked in the pyrolysis furnaces at relatively high temperature and low pressure in the presence of dilution steam. The furnace effluent is rapidly cooled in a quench system for heat recovery and for separation of the gasoline and fuel fractions. The remaining gas is then compressed to the pressure required for entering the downstream fractionation sections.

The rapid cooling of the furnace effluent is essential to prevent the loss of valuable products by secondary reactions and to minimize the formation of heavy tars. The cooling is accomplished by a sequence of direct and indirect methods. The direct method cools the furnace effluent either by injection of quench oil which is recirculated through exchangers to remove the absorbed heat, or by injection of water which is vaporized through intimate contact with hot gases to condense heavier hydrocarbons and dilution steam. The indirect method cools the furnace effluent by the utilization of transfer line heat exchangers, where heat is recovered to generate high pressure steam. Depending upon the feedstock being pyrolyzed and the cracking conditions, the cooling of the furnace effluent may be accomplished by transfer line heat exchangers followed by the oil- and/or water-quench towers.

While general information is available on the design and operation of olefin plants (Zdonik et al., 1969ab; Baba and Kennedy, 1976), no thorough theoretical analysis has been made on the quench system in a large industrial olefins unit. This paper presents a mathematical model for a general olefin quench system and the results obtained with it. The quench system involves a series of fractionation towers in which pyrolysis products, containing a wide boiling range of hydrocarbons and water vapor, are cooled by direct contact with quench oil and water and separated into major fractions. Depending upon the operating conditions of the pyrolysis furnaces and the compression section, the tower temperature can vary from 800 °F to less than 80 °F, and the flow rate from several thousand mol/h to less than 100 mol/h. A novel approach is taken to treat the quench system as a single continuous distillation column with multiple feeds and side stream drawoffs. Other pieces of auxiliary equipment, such as a quench-oil fitting, an oil–water separator, and quench-water and quench-oil coolers, are also incorporated into the model, in which parts of the condensed water and heavier hydrocarbons are recirculated to the column as cooling media. The model is based on the assumption that water and hydrocarbons are completely immiscible in the liquid phase. A method of solution is presented for the model equations of three-phase distillation with internal recycle cooling. The computational scheme requires the estimates of only column temperatures, hydrocarbon vapor rates, and circulating quench rates. A numerical example for a 13-stage and 22-component water–hydrocarbon system is used to illustrate the applicability of the model for the simulation of an olefin oil/water quench system. Within the limitations of the equilibrium data and feed characterization, the calculated results agree well with the data obtained in an industrial plant. Thus in addition to providing a practical technique for treating the three-phase distillation problem, the model presented may be used to advantage for analyzing the operating conditions of quench systems generally encountered in the petrochemical industry.

Description of the Quench Process

The following simplified process description makes reference to Figure 1, covering a general oil/water quench system in an olefin unit typically encountered in the industry.

For the purpose of maintaining generality, the system model assumes multiple entries of feeds to the quench system. Feeds may enter through the normal route of oil quenching followed by water quenching or they may enter water quenching directly. Recycle streams to the quench system can also be handled in a similar manner.

The oil-quench tower is normally operated with an overhead temperature high enough to prevent condensation of gasoline fractions and water vapor. The circulating quench oil rejects heat to a group of exchangers and coolers. The cooled quench oil flow then splits, a portion flowing to the quench-oil fitting to cool the furnace effluent, while the remainder flows to the middle section of the oil-quench tower. A slip stream of the circulating quench oil is routed to a fuel

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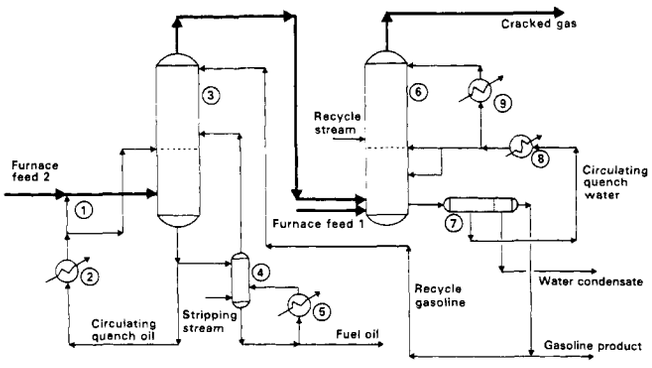

Figure 1. Process flow diagram of a general oil/water quench system in an olefin unit: 1, quench-oil fitting; 2, quench-oil heat recovery system; 3, oil-quench tower; 4, fuel oil stripper; 5, fuel oil stripper reboiler; 6, water-quench tower; 7, oil–water separator; 8, quench-water primary cooler; 9, quench-water secondary cooler.

oil stripper, where the light ends are stripped from the net fuel oil make.

The overhead from the oil-quench tower, together with other furnace effluents and recycle streams, flows directly to the bottom of the water-quench tower. The tower is usually designed to provide the final cooling of the cracked gas before its compression, resulting in condensation of gasoline fractions and most of the water vapor. Cooling is accomplished by a circulating quench water system which rejects heat to the quench-water coolers. Circulating quench water, together with the condensed water vapor and hydrocarbon, flows to the oil–water separator. The quench water is then cooled and recirculated to the various stages of the water-quench tower, while a portion equivalent to the condensed dilution steam is withdrawn and recycled to a dilution steam generator. The condensed hydrocarbon is pumped as reflux to the oil-quench tower and as net gasoline product to storage. The overhead gas from the water-quench tower flows to the cracked gas compression section for further processing.

Description of the Model

In order to simulate the quench towers, it is desirable to have a model which realistically describes their operation and interactions. Figure 2 shows the model selected, giving all feeds, products, and circulating quench streams based on the oil/water quench system shown in Figure 1. The general model combines the water-quench tower, the oil-quench tower, the fuel oil stripper, and other pieces of auxiliary equipment into one distillation column. The column consists of a total of N theoretical stages, assuming N_W stages for the water-quench tower, N_O for the oil-quench tower, and N_F for the fuel oil stripper. Vapor and liquid flows between the quench towers resemble those in a steady-state distillation column, except for the fuel oil stripper overhead which actually enters into the middle stage of the oil-quench tower. For simplicity and because it is usually a relatively small stream, this vapor stream is instead assumed to enter directly into the bottom of the oil-quench tower.

The major feed streams entering the quench system are the recycle stream F_{N_D} and the furnace effluent 1 F_{N_W} to the water-quench tower, the furnace effluent 2 F_{N_L} to the oil-quench tower, and the stripping stream F_N to the fuel oil stripper. The circulating quench oil is taken from the bottom of the oil-quencher tower as a side-draw S_Q, which is then cooled, split, and reintroduced into the column as the feed streams $F_{Q_{N_G}}$ and $F_{Q_{N_L}}$. These circulating quench oil streams are a simplification of the actual flows on the process flow diagram Figure 1. Essentially, the model incorporates the line-quenched process in the quench-oil fitting, where the

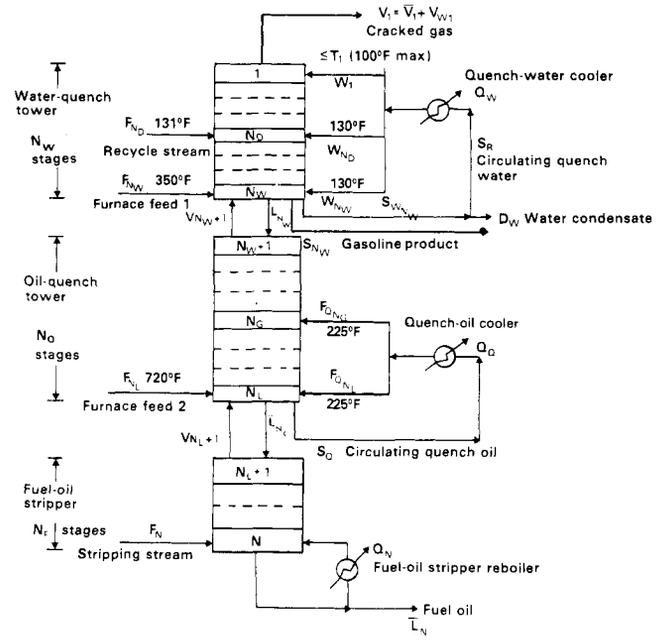

Figure 2. General model of an olefin oil/water quench system.

quench oil stream $F_{Q_{N_L}}$ is sprayed into the furnace effluent 2 F_{N_L} before it enters into the bottom of the oil-quench tower.

The major product streams leaving the quench system are the cracked gas V_1 that goes overhead, the gasoline product S_{N_W}, the water condensate D_W, and the fuel oil bottoms product $\bar{L}_N$. The oil–water separator is incorporated into the bottom of the water-quench tower, giving rise to a hydrocarbon side stream S_{N_W}, an aqueous side stream $S_{W_{N_W}}$, and an internal hydrocarbon reflux stream $\bar{L}_{N_W}$. The aqueous side stream includes the circulating quench water stream S_R, which is cooled and separated into three quench water streams W_1, W_{N_D}, and W_{N_W}, as well as an aqueous stream D_W, which may be regenerated as dilution steam.

Heat can be added or withdrawn at each stage and around the circulating quench stream loops. The reboiler duty for the fuel oil stripper is given as Q_N. For convenience, the exchangers in the circulating quench stream loops are lumped into a single quench-oil cooler with a total cooling duty Q_Q and a single quench-water cooler with a total cooling duty Q_W. However, it should be noticed that the quench water temperature at stage 1 is different from those at stages N_D and N_W as shown in Figure 2.

Mathematical Formulation of the Model

A mathematical model of the quench system can be developed from a consideration of the physical and interactive processes which occur within the towers. To make it completely general, the distillation column shown in Figure 2 is considered to have an arbitrary number of feeds, side stream drawoffs, and quench-water and quench-oil streams. Equilibrium stage concept is assumed in the towers. Water is assumed to be completely immiscible with hydrocarbons in the liquid phase. The oil-quench tower and the fuel oil stripper normally operate well above the dew point of water. Under these conditions, water only serves to reduce the hydrocarbon partial pressure in the vapor phase, permitting the vapor–liquid equilibrium constants K_{ji} to be evaluated at the temperature and hydrocarbon partial pressure of each stage. It should be noticed that the above assumption of idealized phase behavior for water–hydrocarbon systems is not strictly correct but should be reasonably accurate since the total

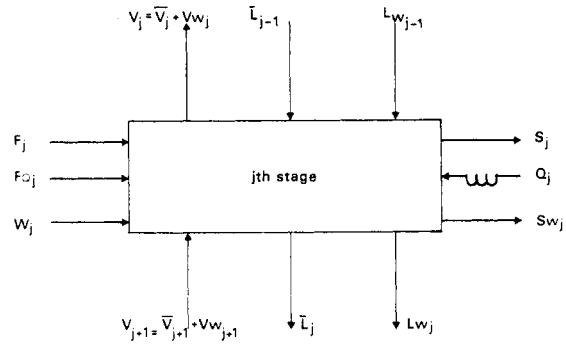

Figure 3. Schematic diagram of stage j of the model column.

pressure in these towers is usually slightly above atmospheric. A more rigorous analysis of the distillation problem involving three coexisting phases (two partially miscible liquid phases and a vapor phase) has been presented recently by Block and Hegner (1976).

Referring to Figure 3, the following model equations apply to stage 1 with $L_0 = \bar{L}_0 = L_{W_0} = 0$ and to stage N with $V_{N+1} = \bar{V}_{N+1} = V_{W_{N+1}} = 0$. Notice that the variables L_j (or $\bar{L}_j$) and V_j (or $\bar{V}_j$) are respectively the molar flow rates of liquid and vapor streams at stage j. The variables without superscript bars refer to the water–hydrocarbon phase, while the ones with bars refer to the hydrocarbon phase only. The subscript W refers to the streams containing water only.

Hydrocarbon Mass Balance Equations for the *i*th Component.

$$F_{Q_j}x_{Q_{ji}} + \bar{L}_{j-1}\bar{x}_{j-1,i} - (\bar{L}_J + S_j)\bar{x}_{ji} - \bar{V}_j\bar{y}_{ji} + \bar{V}_{j+1}\bar{y}_{j+1,i} = -F_jx_{F_{ji}} \quad (2 \le i \le m,\ 1 \le j \le N) \tag{1}$$

Enthalpy Balance Equations.

$$G_j = Q_j + F_jH_{Fj} + F_{Q_j}h_{FQ} + W_jH_{W_j} - S_j\bar{h}_j - S_{W_j}h_{W_j} \tag{2}$$

$$= L_jh_j - L_{j-1}h_{j-1} + V_jH_j - V_{j+1}H_{j+1} \quad (\text{for } 1 \le j \le N_W) \tag{3}$$

$$= \bar{L}_j\bar{h}_j - \bar{L}_{j-1}\bar{h}_{j-1} + \bar{V}_j\bar{H}_j + V_{W_j}\bar{H}_{W_j} - \bar{V}_{j+1}\bar{H}_{j+1} - V_{W_{j+1}}\bar{H}_{W_{j+1}} \quad (\text{for } N_W + 1 \le j \le N) \tag{4}$$

Phase Equilibrium Equations.

$$\bar{y}_{ji} = K_{ji}\bar{x}_{ji} \quad (\text{for } 2 \le i \le m;\ 1 \le j \le N) \tag{5}$$

Stoichiometric Equations.

$$\sum_{i=1}^{m} y_{ji} = \sum_{i=2}^{m} \bar{y}_{ji} = 1 \quad (\text{for } 1 \le j \le N) \tag{6}$$

$$\sum_{i=1}^{m} x_{ji} = \sum_{i=2}^{m} \bar{x}_{ji} = 1 \quad (\text{for } 1 \le j \le N) \tag{7}$$

The vapor–liquid equilibrium constant K_{ji} of component i at stage j is evaluated at the stage temperature and hydrocarbon partial pressure. The y_{j1} and x_{j1} are the vapor and the liquid mole fractions of water, respectively.

The vapor flow from stage j is

$$V_j = \bar{V}_j + V_{W_j} \tag{8}$$

The amount of water in the vapor phase, V_{W_j}, is calculated either from the water mass balance or from the stage temperature and water vapor pressure.

$$V_{W_j} = V_jy_{j1} = V_jP^*_{W_j}(T_j)/P_j \tag{9}$$

It should be noticed that $L_j = \bar{L}_j$ and $h_j = \bar{h}_j (N_W + 1 \le j \le N)$ in the oil-quench tower and the fuel oil stripper, since water is not condensed in these towers within the temperature range of interest.

The solution procedure for eq 1 to 7 can be facilitated by the introduction of the following variables

$$Z_j = \sum_{k=1}^{j} (F_k + F_{Q_k} + W_k - S_k - S_{W_k}) \tag{10}$$

$$\bar{Z}_j = \sum_{k=1}^{j} (F_k(1 - x_{F_{k1}}) + F_{Q_k} - S_k) \tag{11}$$

where $S_k = S_Q$ for $k = N_L$. Then the following equations are obtained with $Z_0 = -V_1$ and $\bar{Z}_0 = -\bar{V}_1$ for stage 0, and $Z_N = L_N$ and $\bar{Z}_N = \bar{L}_N$ for stage N

$$L_j = Z_j + V_{j+1} \quad (\text{for } 1 \le j \le N - 1) \tag{12}$$

$$\bar{L}_j = \bar{Z}_j + \bar{V}_{j+1} \quad (\text{for } 1 \le j \le N - 1) \tag{13}$$

Substituting eq 5, 12, and 13 into eq 1 to 4 to eliminate the variables $\bar{y}_{ji}$, $\bar{L}_j$, and L_j, one obtains the following equations expressed in vector notation.

$$\mathbf{M}_i\bar{\mathbf{x}}_i = -\mathbf{F}_i \quad (\text{for } 2 \le i \le m) \tag{14}$$

$$\mathbf{HV} = \mathbf{G} \tag{15}$$

where

$$\bar{\mathbf{x}}_i = (\bar{\mathbf{x}}_{1i}, \bar{\mathbf{x}}_{2i}, \ldots, \bar{\mathbf{x}}_{Ni})^T \tag{16}$$

$$\mathbf{F}_i = (\mathbf{F}_1x_{F1i}, F_2x_{F2i}, \ldots, F_Nx_{FNi})^T \tag{17}$$

$$\mathbf{V} = (V_1, V_2, \ldots, V_{N_W}, \bar{V}_{N_W+1}, \ldots, \bar{V}_N)^T \tag{18}$$

The elements of the vector $\mathbf{G}$ are

$$g_j = -G_j - Z_{j-1}h_{j-1} + Z_jh_j \quad (\text{for } 1 \le j \le N_W) \tag{19}$$

$$= -G_j - \bar{Z}_{j-1}\bar{h}_{j-1} + \bar{Z}_j\bar{h}_j + V_{W_j}\bar{H}_{W_j} - V_{W_{j+1}}\bar{H}_{W_{j+1}} \quad (\text{for } N_W + 1 \le j \le N) \tag{20}$$

The matrix $\mathbf{M}$ is $N \times N$ matrix with the elements

$$a_{j,j-1} = \bar{Z}_{j-1} + \bar{V}_j \tag{21}$$

$$a_{jj} = -(\bar{Z}_j + \bar{V}_{j+1} + K_{ji}\bar{V}_j + S_j) \quad (\text{for } 1 \le j \le N) \tag{22}$$

$$a_{j,j+1} = K_{j+1,i}\bar{V}_{j+1} \tag{23}$$

and

$$a_{kj} = 0 \quad (\text{for } j < k - 1 \text{ or } j > k + 1) \tag{24}$$

except at the stage where the circulating quench oil is introduced. In this case, $x_{Q_{ji}} = \bar{x}_{N_{L,i}}$, and

$$a_{kj} = F_{Q_j}x_{N_{L,i}} \tag{25}$$

for $k = N_G$ or N_L as shown in Figure 2. Notice that, because of the introduction of circulating quench streams at various stages of the towers, the matrix $\mathbf{M}$ is no longer a tridiagonal one that is normally encountered in multicomponent distillation problems. The elements in the matrix $\mathbf{H}$ are

$$b_{jj} = \begin{cases} h_{j-1} - H_j & (\text{for } 1 \le j \le N_W) \\ \bar{h}_{j-1} - \bar{H}_j & (\text{for } N_W + 1 \le j \le N) \end{cases} \tag{26}$$

$$b_{j,j+1} = \begin{cases} H_{j+1} - h_j & (\text{for } 1 \le j \le N_W) \\ \bar{H}_{j+1} - \bar{h}_j & (\text{for } N_W + 1 \le j \le N) \end{cases} \tag{27}$$

with all other elements being zero.

Hence, the problem of the oil/water quenching processes is reduced to the one of three-phase distillation, which is characterized by m matrix equations of order N, $(m - 1)$ of which are determined by the equilibrium properties of the hydrocarbon mixture and the other by the enthalpy of the water–hydrocarbon mixture. In addition, the water vapor flows in the water-quench tower ($1 \le j \le N_W$) are determined by eq 9. The solution of these equations is obtained by finding

Table I. Data for the Example Problem

Number of stage in the water-quench tower = 6
Number of stage in the oil-quench tower = 5
Number of stages in the fuel oil stripper = 2
Feed rates, temperatures, and compositions to stages 5, 6, 11, and 13 are shown in Table II
Column pressure = 18.5 psia
Gasoline draw-off rate = 31 mol/h from stage 6
Fuel-oil draw-off rate = 36 mol/h from stage 13
Water condensate draw-off from stage 6
Quench water recirculated to stages 1, 5, and 6
Quench oil recirculated to stages 10 and 11
Quench temperatures shown in Figure 2
Recirculating ratio of quench water = 34% to stage 1, 53% to stage 5, remaining to stage 6
Recirculating ratio of quench oil = 71% to stage 10, remaining to stage 11
Stream to fuel oil stripper = superheated steam at 200 psia and 570 °F
Reboiler duty = 50 000 Btu/h

a set of temperatures, phase flow rates, and compositions which satisfies all the equations of the tower model. For multicomponent systems, the enthalpies and vapor–liquid equilibrium constants may be expressed by the following functions.

Enthalpy Function of the Vapor Phase.

$$H_j = H_j(y_{ji's}, P_j, T_j) \tag{28}$$

Enthalpy Function of the Liquid Phase.

$$h_j = h_j(x_{ji's}, T_j) \tag{29}$$

Vapor–Liquid Equilibrium Constants.

$$K_{ji} = K_{ji}(\bar{x}_{ji's}, \bar{y}_{ji's}, \bar{P}_j, T_j) \tag{30}$$

In addition, the enthalpies $\bar{H}_j$ and $\bar{h}_j$ are evaluated by the same functions as eq 28 but on a water-free ($\bar{y}_{ji's}$ and $\bar{x}_{ji's}$) basis.

The overall hydrocarbon material balance is obtained by the summation of eq 1 with eq 6 and 7.

$$\sum_{j=1}^{N} [F_j(1 - x_{F_{j1}}) + F_{Q_j} - S_j] = \bar{V}_1 + \bar{L}_N \tag{31}$$

The overall material balance is given by the expression

$$\sum_{j=1}^{N} (F_j + F_{Q_j} + W_j - S_j - S_{W_j}) = V_1 + \bar{L}_N \tag{32}$$

A complete heat balance around the column, including the reboiler and the quench coolers is

$$\sum_{j=1}^{N} Q_j + \sum_{j=1}^{N} F_j H_{F_j} - Q_w - Q_Q - V_1 H_1 - \bar{L}_N \bar{h}_N - D_W h_{W_{Nw}} - S_{N_w} \bar{h}_{N_w} = 0 \tag{33}$$

where

$$D_W = S_{W_{Nw}} - S_R \tag{34}$$

and Q_w and Q_Q are the respective duties of the quench-water and quench-oil coolers

$$Q_w = S_R h_{W_{Nw}} - W_1 H_{W1} - W_{N_D} H_{W_{ND}} - W_{Nw} H_{W_{Nw}} \tag{35}$$

$$Q_Q = S_Q(\bar{h}_{N_L} - h_{FQ}) + S_{Nw} \bar{h}_{Nw} \tag{36}$$

In the analysis of distillation column models, enough specifications must be made to define a unique set of operating conditions. For the present system, it is convenient to specify in advance the conditions of feed streams (rates, temperatures, and compositions), the hydrocarbon product stream drawoff rates, the quench temperatures, the column pressures, the number of stages, the locations of feed and side streams, and the rates and locations of the circulating quench streams. The reboiler duty is also specified, since its value is usually very small compared to the heat of other streams. Figure 2 and Table I illustrate the multicomponent distillation column with such specifications.

Method of Computation

A number of workers (Amundson et al., 1959; Friday and Smith, 1964; Wang and Henke, 1966; Naphtali and Sandholm, 1971; Ishii and Otto, 1973) have proposed general computational procedures for the solution of the distillation model equations (eq 14 and 15) by use of successive approximation techniques. The success of these iterative methods generally depends on the selection of appropriate convergence schemes, as was shown by experience in the solution of the present problem. Therefore, the general computational procedure is modified in order to improve the rate of convergence. The procedure to be used is summarized as follows.

(i) Assume initial column temperature profiles, hydrocarbon vapor rates, circulating quench-water and quench-oil rates. (ii) Adjust the overhead vapor and water condensate rates from the overall material balance equations (eq 31 and 32). (iii) Calculate the vapor–liquid equilibrium constant of each component except water at each stage. (iv) Solve the mass balance equation (eq 14) for the composition of each component at each stage on a water-free basis. (v) Correct the stage temperatures by the Newton–Raphson convergence scheme such that the sums of hydrocarbon vapor and liquid mole fractions at each stage equal unity. (vi) Calculate the vapor pressure and mole fraction of water vapor at the new stage temperature and convert mole fractions to the water–hydrocarbon basis. (vii) Calculate the total vapor and liquid flows at each stage from eq 8, 9, and 12. (viii) Adjust the circulating quench rates from the overall energy balance equation (eq 33) in which the new rates are simply determined by the ratio of new and old combined quench cooler duties, Q_w and Q_Q. (ix) Compute the vapor rates from a stage-by-stage enthalpy balance, starting from the bottom, where the reboiler duty is fixed. (x) Repeat steps (ii) through (ix) in order until the desired degree of accuracy in the vapor rates is reached.

Thus, an iterative procedure on the model equations is instituted, as eq 14 and 15 may be used alternately to calculate compositions, new temperatures, new circulating quench rates, new vapor rates, new compositions, etc., until convergence by the preceding criteria results. The method can be recognized as a modified bubble point iterative procedure. The convergence characteristics of the solution procedure generally depend on the initial estimates of the independent variables. A little experience with the system and the method would provide reasonable estimates of these variables. The proposed computational procedure has been applied successively to the following numerical example with satisfactory convergence stability.

Numerical Example

A numerical example is now presented to illustrate the applicability of the model for the simulation of the oil/water quench system shown in Figure 1, which is typical of those encountered in industrial olefin units. The model column is assumed to consist of 13 stages, six for the water-quench tower, five for the oil-quench tower, and two for the fuel oil stripper. Referring to Figure 2, four feed streams, including the stripping stream, are introduced respectively at stages 5, 6, 11, and 13, while four product streams, including gasoline and water condensate, are respectively withdrawn from stages 1, 6, and 13. The column operates at constant pressure. The circulating quench streams are introduced at stages 1, 5, and 6 for the

Table II

Feed Conditions					
Feed stage	Feed rate, lb-mol/h		Feed temp, °F		
5	200		131		
6	12 000		350		
11	14 300		720		
13	15		570		
Component Mole Percent (%) in the Feed					
Comp. no.	Comp. name	$F(5)$	$F(6)$	$F(11)$	$F(13)$
1	Water	0.66	25.28	53.59	100.0
2	H_2	0.18	21.93	6.13	0.0
3	CH_4	0.97	11.22	11.87	0.0
4	C_2H_4	6.05	23.28	12.39	0.0
5	C_2H_6	3.87	13.25	2.05	0.0
6	C_3H_6	7.74	2.34	6.20	0.0
7	C_3H_8	1.51	1.37	0.17	0.0
8	C_4H_6	7.07	0.33	1.31	0.0
9	C_4H_8	9.31	0.23	1.98	0.0
10	nC_5	26.36	0.31	1.75	0.0
11	Benzene	14.33	0.17	0.95	0.0
12	nC_6	4.59	0.05	0.30	0.0
13	Toluene	6.35	0.07	0.42	0.0
14	nC_7	2.01	0.02	0.14	0.0
15	Styrene	1.93	0.02	0.13	0.0
16	Xylene	2.77	0.03	0.19	0.0
17	nC_8	0.42	0.01	0.03	0.0
18	Pseudocum.	3.88	0.05	0.26	0.0
19	450 Cut	0.00	0.01	0.04	0.0
20	500 Cut	0.00	0.01	0.02	0.0
21	550 Cut	0.00	0.01	0.05	0.0
22	700 Cut	0.00	0.01	0.03	0.0

Table III. Comparison of Results between Model Prediction and Plant Operating Data (Heat Duty in mm Btu/hr; Flow Rate in mol/h)

	Calcd	Actual
Water-Quench Tower		
Quench-water cooler duty	240.6	235.6
Overhead vapor rate	6 350	16 850
Upper quench flow rate	64 638	65 556
Middle quench flow rate	115 018	116 666
Lower quench flow rate	19 475	19 750
Oil—Quench Tower		
Quench-oil cooler duty	81.6	78.9
Overhead vapor rate	15 460	15 150
Lower reflux flow rate	7 668	7 778
Quench oil to fillings	3 967	4 022

quench water, and at stages 10 and 11 for the quench oil. The temperature of the quench water entering the top stage is initially set equal to 100 °F but is not allowed to exceed the overhead vapor temperature. The feed streams consist of a wide boiling range of hydrocarbons and water vapor to be cooled by direct contact with quench oil and water within the column. For demonstration purposes, the number of components including water in the feed is set to 22, with the gasoline and fuel-oil fractions being represented by nine and four different components, respectively. Normal tower operating variables range in temperature from 80 to 750 °F and in flow rate from less than 100 to more than 20 000 mol/h. The data are summarized in Table I, with the feed description given in Table II.

The calculation of thermodynamic properties generally follows standard correlation and prediction procedures (Prausnitz et al., 1967). The vapor pressures are computed with the Antoine equation. For computational convenience, the enthalpy constants are approximated by polynominal

Table IV. Comparison of Overhead Vapor Composition (Mol %) between Model Prediction and Plant Data on the Hydrocarbon Basis

	Water-quench tower (Stage 1)		Oil-quench tower (Stage 7)	
Component name	Plant	Prediction	Plant	Prediction
H_2	22.22	22.22	11.74	12.33
CH_4	19.27	19.28	22.73	23.88
C_2H_4	28.97	28.97	23.74	24.93
C_2H_6	11.98	11.97	3.94	4.13
C_3H_6	7.48	7.48	11.90	12.49
C_3H_8	1.20	1.21	0.33	0.34
C_4H_6	1.50	1.51	2.52	2.64
C_4H_8	2.07	2.06	3.82	3.99
Gasoline[a] fraction	5.31	5.30	19.28	14.32
Fuel oil[a] fraction	0.0	0.0	0.0	0.95

[a] Referring to Table II, component gasoline is represented by nine components (components 10 to 18) and component fuel oil is represented by four components (components 19 to 22) in the model.

functions of the temperature. To account for the nonideal situation occurring in the system, a semiempirical approach has been taken to obtain a set of implicitly composition-dependent K values. Four streams, including the two major furnace effluents as well as the overhead vapors from the water-quench and oil-quench towers, are used for the calculations of the phase equilibria over the temperature range of interest. These equilibrium data are then fitted to a polynomial function of the temperature with pressure-dependent coefficients. It should be noticed that this approach does not result in rigorous answers, but it has practical application here as the equilibrium data for the hydrocarbon system in the presence of water are not known with precision. This simplification is also justified by the complex nature of the furnace effluents which contain a spectrum of hydrocarbon components that are not readily identifiable. In any event, the equilibrium constants can be calculated without much difficulty from more fundamental thermodynamic relationships.

The example problem is solved by applying the computational procedure described earlier. The calculated results for overhead vapor rates, compositions, and quench cooler duties are given in Tables III and IV. The predicted temperatures and vapor rates throughout the column are plotted against stage number in Figure 4. Plant operating data are also compared with the calculated results in Tables III and IV and Figure 4. The comparisons are made, although the feed compositions may not be exactly the same due to the variability in day-to-day operation at the plant. As can be seen, the agreement between the respective vapor rates and composition profiles is quite good, while the temperature profiles qualitatively agree. Notice that there is a drastic change of the vapor rates from 16 000 mol/h at stage 11 (quench-oil tower bottoms) to 20 mol/h at stage 12 (fuel-oil stripper top) as most of the hydrocarbon feed is vaporized in the quench-oil tower. It is also noticed that the predicted temperature at the bottom (stage 11) of the oil-quench tower is approximately 20 °F lower than the operating temperature of the plant. This may be due to the approximations made on the feed component distribution of high-boiling hydrocarbons as well as in the model, which assumes that the overhead from the fuel-oil stripper enters directly into the bottom of the oil-quench tower, while in reality it enters into the middle stage of that tower. In view of the difficulties involved in the identification of heavier hydrocarbon components for furnace effluents and in the

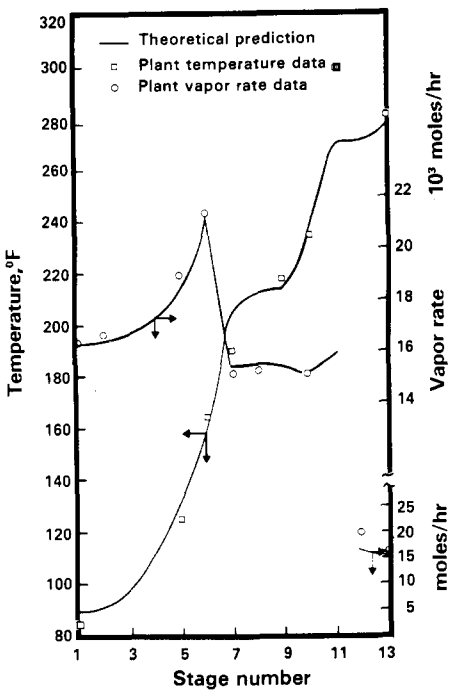

Figure 4. Comparison of predicted temperature and vapor profiles with plant data.

evaluation of equilibrium data for water–hydrocarbon systems, the model prediction of the operating conditions of the oil/water quench system is considered reasonable and satisfactory.

Conclusions

A mathematical model for a general oil/water quench system in an olefin unit has been developed. The approach is novel in that a series of distillation columns is treated as a single tower with internal recycle quench streams. The model has been applied to the simulation of an olefin unit typically encountered in the petrochemical industry. The adequacy of the model has been demonstrated by direct comparison of calculated results of the quench cooler duties, the vapor rates, the product distributions, and the temperature profiles with the data obtained in an industrial plant. The model may be used in evaluation of plant performance and in design of new plants.

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Nomenclature

a, b, g = elements of matrix or vector
D_W = water condensate drawn from the oil–water separator
F = feed stream molar flow rate
G = variable defined by eq 2
h = enthalpy of liquid stream
h_{FQ} = enthalpy of circulating quench oil stream
H = enthalpy of vapor stream
H_W = enthalpy of circulating quench water stream
K = equilibrium constant of hydrocarbons
L = liquid stream molar flow rate
m = total number of components with water named as component 1
N = total number of stages = $N_F + N_O + N_W$
N_F, N_O, N_W = number of stages for the fuel oil stripper, the oil-quench tower, and the water-quench tower, respectively
N_D, N_G = stage number where the circulating quench water or quench oil enters
N_L = stage number for the bottom of the oil-quench tower = $N_W + N_O$
P = stage pressure
Q = heat input to a stage
S = side stream molar flow rate
S_Q = total circulating quench oil molar flow rate = $\Sigma_j F_{Q_j}$
S_R = total circulating quench water molar flow rate = $\Sigma_j W_j$
T = temperature
V = vapor stream molar flow rate
W = circulating quench water molar flow rate
x = liquid mole fraction
y = vapor mole fraction
Z = variable defined by eq 10 or 11

Superscripts

overbar = hydrocarbon phase
* = vapor pressure

Subscripts

F = feed
i = component index
j, k = stage index
Q = quench oil
w = water

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