Iranian Journal of Chemical Engineering
Vol. 1, No. 2, summer & autumn 2004, IACHE

SHAHAB-A PC-Based Software for Simulation of Steam Cracking Furnaces (Ethane and Naphtha)

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Abstract
SHAHAB is a PC- based simulator developed by Olefin Research Group (ORG), with the simultaneous simulation of the reactor, the firebox, the convection section and the transfer line exchanger in steam Cracking units. The reaction mechanism of thermal cracking of hydrocarbons is generally accepted as free-radical chain reactions. Using a rigorous kinetic model, a complete reaction network for representing the decomposition of hydrocarbon feedstocks has been developed and used for simulation of thermal hydrocarbon crackers. Taking into account the kinetics of coke formation, SHAHAB provides a detailed understanding of product, temperature and pressure distribution, coke thickness profile, reactor run length, fuel consumption and the amount of steam generated.

Keywords: *SHAHAB, PC- Based software, Cracking Furnace, Steam Cracking, Olefins*

Introduction

Pyrolysis of hydrocarbons such as ethane, naphtha and gas oil is an important commercial process for the production of ethylene, propylene and 1,3-butadiene. These low-molecular-weight olefins are among the most important base chemicals for the petrochemical industries. Modern steam cracking plants are the main part of petrochemical complexes, producing 500,000 to 1,000,000 tpy of ethylene, the main petrochemical building block. These plants consist of furnaces and a separation train. As shown in Figure 1 schematically, the furnace has a radiant section, a convection section and a so- called transfer line exchanger (TLE). In the convection section, feed and steam are preheated up to approximately 600 °C in order to recover the sensible heat contained in the flue gases leaving the radiant section. The radiant section consists of a set of coils typically with an internal diameter of 50-150 mm and a length of 20-100 m where they are heated by gas-fired burners. The residence time of the mixture of hydrocarbons and steam in the radiant coils is between 0.2-0.6 sec. The range of steam- to-hydrocarbon ratio varies from 0.3 for ethane feed to 0.7 for naphtha. The cracking reactions inside the coils are endothermic and the temperature is increased from about 600 °C at the inlet of the cracking coil to 820-870 °C at the outlet. Under these conditions, the feed-stock is converted through a free-radical

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mechanism to the products. Ethylene yield is typically 30 % on weight basis with naphtha and goes down to 25% for gas oil feedstock. The inner surface of a cracking coil is gradually covered with coke, which is deposited during the furnace on- stream time. The coke layer reduces the heat transfer to the process gas and, in order to maintain the performance of the reactor, the external tube metal temperature has to be raised. The operation of the reactor has to be interrupted when the skin temperature reaches the limit imposed by coil metallurgy, which is typically in the range of 1050-1150 °C.

This paper describes SHAHAB simulation software, which has been developed in the Olefin Research Group (ORG) of Tarbiat Modares University, for the prediction of product yields and run length of thermal cracking furnaces. For this purpose, the reactor, the firebox, the convection section and the TLE are simulated simultaneously. This PC-based software has a convenient graphical user interface and it can easily be used for the training of ethylene plant operators. A schematic block diagram of this simulator is shown in Figure 2.

T*he* R*eactor* M*od*el

T*he* K*inetic* M*od*el

The mechanism of thermal cracking of hydrocarbons is generally accepted as free-radical chain reactions. Ethane cracking represents the simplest application of the free-radical mechanism. The reaction scheme with heavier feeds such as naphtha is much more complex than that of gaseous feedstocks, due to the fact that hundreds of reactants react in parallel and some of those reactants are formed as reaction products during the reaction. As the reaction conversion and hence, concentrations of olefins and other products increase, secondary reactions become more significant. Partial pressure of olefins and diolefins increases, favoring condensation reactions, which produce cyclodiolefins and aromatics.

In this software, a complete reaction network, for decomposition of hydrocarbon feeds is developed, using a rigorous kinetic model. The detailed mechanistic kinetic scheme in this simulation network, developed by Towfighi, *et al*. [1,2], involves 1230 reactions and 122 molecular and radical species. As usual, this chain radical mechanism consists of several radical and molecular elementary reactions, such as initiation reactions, H-abstractions, radical additions, decompositions, isomerization reactions, termination reactions, and Diels-Alder cyclizations. To obtain reliable results, the reaction network should be verified and tuned using experimental data. For this purpose, large amounts of experiments were carried out, using a pilot plant reactor. Details of this system are presented in ORG documents [4]. Some kinetic extensions had to be made and the parameters were tuned and verified with large amounts of pilot plant and industrial data [3,4]. This rigorous kinetic model can be briefly summarized with examples of different types of reactions, as shown in Table 1.

M*od*el E*q*uations

A one-dimensional plug-flow model is used to simulate the thermal cracking reactor. The set of continuity equations for the various process gas species is solved simultaneously with the energy, momentum and the coking rate equations [5]. These equations are as follows:

Mass balance:

$$\frac{dF_j}{dz} = (\sum_i n_{ij} r_{ri}) \frac{\pi d_t^2}{4} \qquad (1)$$

Energy balance:

$$\sum_j F_j c_{pj} \frac{dT}{dZ} \equiv Q(z)\pi d_t + \frac{\pi d_t^2}{4} \sum_i r_{ri} (-\Delta H)_i \qquad (2)$$

Momentum balance:

$$\left(\frac{1}{M_m P_t} - \frac{P_t}{\beta G^2 RT}\right)\frac{dp_t}{dz} = \frac{d}{dz}\left(\frac{1}{M_m}\right) + \frac{1}{M_m}\left(\frac{1}{T}\frac{dT}{dz} + Fr\right) \quad (3)$$

where β is the conversion factor.
Friction factor for the straight part of the reactor coils is:

$$Fr = 0.092\frac{Re^{-0.2}}{d_t} \quad (4)$$

and for the tube bends:

$$Fr = 0.092\frac{Re^{-0.2}}{d_t} + \frac{\zeta}{\pi R_b} \quad (5)$$

where R_b and Λ represent the radius of the tube bend and angle of bend, respectively.

$$\zeta = (o.7 + 0.35\frac{\Lambda}{90^\circ})(0.051 + 0.19\frac{d_1}{R_b}) \quad (6)$$

Since coking is slow, quasi steady state conditions may be assumed. The thickness of coke deposited on the inner walls of coils is obtained by:

$$\Delta t_c = \frac{\alpha . r_c}{\rho_c}\Delta t \quad (7)$$

Therefore, the new diameter of coil will be:

$$d_{t\,new} = d_{t\,old} - 2\,t_c \quad (8)$$

The governing mass, energy, and momentum balance equations for the cracking coil constitute a boundary value problem which has a significant stiffness in the numerical solution due to the large differences in concentration gradient between radicals and molecules. This problem can be tackled through the application of the Gear method.

T*he Co***k***ing* **M***o***d***el*

Coke formation in the pyrolysis of hydrocarbons is a complex phenomenon, due to the various free-radical reactions involved. A number of coke precursors were found to contribute to the formation of coke. Unsaturates and aromatics are a very important class of coke precursors. They are products of the pyrolysis reactions so that their concentration in the high-temperature zone of the reactor is higher. Unsaturates are reactive components. Therefore, they are good candidates for the radical addition. Since aromatic ring structure is close to the structure of the coke matrix, branched aromatics are also considered as reactive components contributing to coke formation, especially at high temperatures prevailing in thermal cracking coils. Literature survey and plant data led to a coking model considering also a number of coke precursors, the relative coking rates of which had been obtained experimentally [6-8]. The precursors are classified into groups, such as olefinics, dienes, acetylenic, naphthenics and aromatics [3, 4, 9].
In the present work, the residual sum of squares between the calculated values and asymptotic coking rates were used as the objective function and the kinetic parameters of coking were estimated by using the Marquardt algorithm. The rate of coke formation from contributed precursors is expressed by:

$$r_{ci} = k_i C_i^{\,n} \quad (9)$$

where:

$$k_i = A\exp(-E/RT) \quad (10)$$

Total coking rate is calculated as:

$$r_c = \sum_i r_{ci} \quad (11)$$

The temperature of coking rate is calculated at gas/coke interface.

T*he mo***d***el of the* **R***a***d***iation* **S***ection*

The geometry of the reactor coil inside the furnace and the configuration and type of the burners require special attention. The multi-

zone mathematical model has been used for the simulation of the cracking furnaces [10,11]. The furnace refractory walls, the surface of reactor coils and the flue gas volume were discretized into a number of isothermal surface and volume zones with uniform properties. The energy balance, containing contribution of radiative, convective and/or conductive heat exchange, is constructed for each of these elements, resulting in a set of non-linear algebraic equations in the form:

$$+\frac{\partial}{\partial z}\left[\mathbf{k}\frac{\partial \mathbf{T}}{\partial z}\right]=\rho Cp\frac{\partial \mathbf{T}}{\partial t} \tag{13}$$

Assuming that the temperature in each small element is constant, equation 13 can be simplified as:

$$\nabla^2\mathbf{T}=\frac{\partial^2\mathbf{T}}{\partial r^2}+\frac{1}{r}\frac{\partial \mathbf{T}}{\partial r}+\frac{1}{r^2}\frac{\partial^2\mathbf{T}}{\partial \theta^2}=0 \tag{14}$$

$$\begin{bmatrix} Z_1Z_1-\sum Z_iZ_j \text{.....} \text{....} Z_2Z_1 \text{.....} \text{.....} \text{.....} Z_nZ_1 \\ \text{.....} Z_1Z_2 \text{.....} \text{.....} Z_2Z_2-\sum Z_2Z_2 \text{.....} \text{.....} Z_nZ_2 \\ \text{.....} \\ \text{.....} \\ \text{.....} \\ \text{.....} Z_1Z_n \text{.....} \text{.....} \text{...} Z_2Z_n \text{.....} \text{.....} Z_nZ_n-\sum Z_nZ_j \end{bmatrix}\begin{bmatrix} E_1 \\ E_2 \\ .. \\ \\ \\ .. \\ E_n \end{bmatrix}=\begin{bmatrix} Q_1A_1 \\ Q_2A_2 \\ \\ \\ \\ \\ Q_nA_n \end{bmatrix} \tag{12}$$

The matrix element ZiZ j represents the total exchange area between zones Zi and Zj. This is the amount of radiative energy emitted by zone Zi and absorbed, both directly and after reflection on other zones, by zone Zj, divided by the black body emissive power Ei. The non-radiative heat flux emitted by zone Zi is represented by Qi. Solving the set of energy balances yields the heat flux and temperature distribution in the furnace [12]. When the reactor tubes are discretized in axial direction only, heat flux profiles q(z) and external tube skin temperature profiles $T_{ext}(z)$ are obtained. When the tubes are also discretized along the perimeter, heat flux profiles T(r, θ, z) are obtained. The conduction equations for each axial tube zone with the appropriate boundary conditions are:

$$\frac{1}{r}\frac{\partial}{\partial r}\left[\mathbf{k}r\frac{\partial \mathbf{T}}{\partial r}\right]+\frac{1}{r^2}\frac{\partial}{\partial \theta}\left[\mathbf{k}\frac{\partial \mathbf{T}}{\partial \theta}\right]$$

The boundary conditions for equation 14 are now defined in the internal and external surfaces of the coils as:

$$\text{at} \quad r=r_{ext} \quad k\frac{\partial T}{\partial r}(r,\theta)=q(r,\theta) \tag{15}$$

$$\text{at} \quad r=r_{int} \quad k\frac{\partial T}{\partial r}(r,\theta)=h_p\left[T(r,\theta)-T_p\right] \tag{16}$$

$$T(r,\theta)=T(r,\theta+\pi) \tag{17}$$

and

$$\frac{1}{r}\frac{\partial T(r,\theta)}{\partial \theta}=\frac{1}{r}\frac{\partial T(r,\theta+\pi)}{\partial \theta} \tag{18}$$

The calculation module for the circumferential temperature profiles is coupled to the furnace and reactor simulation model.

T*a*b*le 1.* Typical radical and molecular reactions

A. **R*a*d*ical reactions***

1. Initiation reactions

Unimolecular: $CH_3-(CH_2)_4-CH_3 \rightarrow C_2H_5\bullet + CH_3-CH_2-CH_2-CH_2\bullet$

Bimolecular: $CH_3-CH_3+CH_2=CH_2 \rightarrow C_2H_5\bullet + C_2H_5\bullet$

2. Propagation reactions

Radical decomposition is one of the most important reaction types and is directly producing ethylene according to the following scheme .

Radical decomposition: $\bullet CH_2-CH_2-CH_3 \rightarrow C_2H_4+CH_3\bullet$

Radical lsomerization: $\bullet CH_2-(CH_2)_3-CH_2-CH_3 \rightarrow CH_3-(CH_2)_3-\dot{C}H-CH_3$

H- abstraction on molecules:

$$CH_3\bullet \; + \; CH_3-CH_2-CH_3 \rightarrow CH_4+CH_3-CH_2-CH_2\bullet$$

Addition of radicals on unsaturated molecules:

$$CH_3\bullet \; + \; CH_2=CH-CH_3 \rightarrow CH_3-CH_2-CH_2-CH_2\bullet$$

3. Termination reactions

Recombination of radicals to form one molecule:

$$C_2H_5\bullet + C_2H_5\bullet \rightarrow CH_3-CH_2-CH_2-CH_3$$

Recombination of radicals forming two molecules:

$$C_2H_5\bullet + C_2H_5\bullet \rightarrow CH_3-CH_3+CH_2=CH_2$$

B. **M*olecular reactions***

Olefin isomerization:

$$CH_3-CH=CH-CH_3 \rightarrow CH_2=CH-CH_2-CH_3$$

Olefin dehydrogenation:

$$CH_2=CH-CH_2-CH_3 \rightarrow CH_2=CH-CH=CH_2+H_2$$

Olefin decomposition:

$$CH_2=CH-CH_2-CH_2-CH_3 \rightarrow CH_2=CH-CH_3+CH_2=CH_2$$

Diels- Alder reaction:

$$CH_2=CH-CH=CH_2+CH_2=CH_2 \rightarrow CycloC_6H_{10}$$

T*he* M*o*d*el of the Con*v*ection S*ection an*d TL*E*

Flue gases leaving the firebox transfer a considerable amount of energy that can best be recovered in the convection section of a thermal cracking furnace. Usually, this energy is used to preheat the reactor feed and BFW required for TLEs and to produce superheated steam. The convection section can be divided into several banks, depending on the type of hydrocarbon feed. Each bank in turn is divided into several rows of bare and/or finned tubes.

The cracked gas, which is the product of the pyrolysis reactor, is led to separation section through transfer line exchangers (TLEs). In order to retain ethylene and propylene yields, the cracked gas, which is usually at 820-860 ºC, must be rapidly cooled down to 340 - 400 ºC.

This is done by means of BFW. Because of the relation between TLE and BFW

preheater, convection section and TLE are solved simultaneously.

Starting from the first bank of convection section, which is the closest one to the fire box for each bank, we have the following energy balance equations:

$$\int_{T_n}^{T_{n+1}} (mc_p)_{fg}\, dT = (UA\,\Delta T_{Ln})_{Bank-i} \qquad (19)$$

$$\int_{T_n}^{T_{n+1}} (mc_p)_{fg}\, dT = \int_{T_{pg,in}}^{T_{pg,out}} (mc_p)_{pg}\, dT + \dot{m}_{pg}\,\lambda \qquad (20)$$

The first term at the right hand of the above equation will be zero if there is no change of phase.

Having solved the radiation section, the temperature of the flue gas at the entrance of the convection section is known. Therefore, for each bank we will have two equations and two unknowns.

For BFW preheater and TLE we can write:

$$\int_{T_n}^{T_{n+1}} (mc_p)_{fg}\, dT = (UA\,\Delta T_{Ln})_{BFWPH} \qquad (21)$$

$$\int_{T_n}^{T_{n+1}} (mc_p)_{fg}\, dT = \int_{T_{B,in}}^{T_{B,out}} (mc_p)_{BFW}\, dT \qquad (22)$$

$$\int_{T_{B,out}}^{T_{sat}} (mc_p)_{BFW}\, dT + m_{BFW}\lambda = \int_{T_{cg,in}}^{T_{cg,out}} (mc_p)_{cg}\, dT \qquad (23)$$

$$\int_{T_{cg,in}}^{T_{cg,out}} (mc_p)_{cg}\, dT = (UA\,\Delta T_{Ln})_{TLE} \qquad (24)$$

M_{BFW}, $T_{cg,out}$, $T_{B,out}$ and T_{n+1} are unknowns of this section.

Energy balance equations are solved by the generalized form of Newton-Raphson method. For calculation of Jacobian for n equations and n unknowns, the Gaussian elimination method was used.

Calculation of the **Ov***erall Heat* **T***ransfer Coefficient*

Mathematical modeling is different for bare and finned tubes. Therefore, different equations are used for calculating the overall heat transfer coefficient in these tubes.

For bare tubes:

$$\frac{1}{u} = \frac{1}{hi} + etc.$$

$$\frac{1}{u} = \left(\frac{1}{h_i} + \frac{1}{F_i} + \frac{\delta_{ir}}{k_w} + \frac{1}{F_0} + \frac{1}{h_0}\right) \qquad (25)$$

F_i and F_o are inside and outside fouling factors, and d_w and k_w are wall thickness and wall conductivity, respectively.

Although convective heat transfer is predominant in this section, the effects of radiation from radiating walls and radiating media on the heat transfer coefficient shall be taken into account. This is especially important for the first few rows of the first bank, which are exposed to radiation effects. Therefore:

$$H_o = h_{conv} + h_{rad} + h_{shock} \qquad (26)$$

$$h_{conv} = (k_{fg} / d_o)\, Nu_o \qquad (27)$$

For finned tubes:

$$Nu_o = 0.257 \times Re_o^{.635} \times Pr_o^{.34} \qquad (28)$$

For bare tubes:

$$Nu_o = 0.211 \times Re_o^{.635} \times Pr_o^{.34} \qquad (29)$$

For radiation heat transfer, we have:

$$h_{rad} = \sigma\left(\frac{\varepsilon_w + 1}{2}\right)\left[\varepsilon_g\left(\frac{T_{fg}}{100}\right)^4 - \alpha_{abs}\left(\frac{T'_{Fg}}{100}\right)^4\right] \qquad (30)$$

T'_{Fg} = average cold plane temperature

e_w = tube emissivity at T'_{Fg}

$\mathbf{e}_g$ = gas emissivity at T'_{Fg}
$\mathbf{a}_{abs}$ = gas absortivity

The heat transfer coefficient due to radiating walls is obtained by:

$$h_{shock} = \frac{F_{shock}}{S_{row}(T_{Fg} - T'_{Fg})} \quad (31)$$

$\mathbf{f}_{shock}$ = shock duty
S_{row} = total outside surface (bare)

The inside heat transfer coefficient is written in terms of Nusselt number:

$$h_i = \frac{Nu_i \mathbf{k}_{pg}}{(\mathbf{d}_o + 2\mathbf{T}_F)} \quad (32)$$

$$Nui = 0.0237 \times Re^{0.8} \times Pr^{0.33} \quad (33)$$

For finned tubes:

$$\frac{1}{u} = \left(\frac{1}{A_{\mathbf{b}}^{*} \alpha_i} + \frac{1}{A_{\mathbf{b}.eff} \times \alpha_o} \right) \quad (34)$$

where:

$$\frac{1}{\alpha_i} = \left(\frac{1}{h_i} + \frac{1}{F_i} + \frac{1}{\mathbf{K}_w} + \frac{1}{\mathbf{K}_F} \right) \quad (35)$$

T_F and k_F are fin thickness and conductivity, respectively.

$$\frac{1}{\alpha_o} \left(\frac{1}{h_o} + \frac{1}{F_o} \right) \quad (36)$$

Areas are calculated by the following formulas:

$$A_{\mathbf{b}} = \pi \times \mathbf{d}_o \quad (37)$$

$$A_{\mathbf{b}}^{*} = n(\mathbf{d}_o + 2\mathbf{T}_f) \quad (38)$$

$$A_{tot} = A_{\mathbf{b}}^{*} + E.A_{ext} \quad (39)$$

where E is fin efficiency and A_{ext} is calculated by the following formula:

$$A_{ext} = 2(H_f - \mathbf{T}_f)\left(1 + \frac{\mathbf{T}_f}{H_f}\right)\sqrt{1 + (\pi N_f \mathbf{d}_o)^2} \quad (40)$$

Fin efficiency is also an important parameter.

$$Eff = \frac{\tanh(EF)}{EF} \quad (41)$$

$$EF = H_f \sqrt{\frac{2h_o}{\mathbf{k}_f}} \left(\frac{1}{\mathbf{T}_f} - \frac{1}{W_f} \right) \quad (42)$$

S*imulation Proce***d***ure*

The procedure for simultaneous simulation of thermal cracking furnace including the reactor, the fire box, the convection section and the TLE as programmed into the software, can be described in the following steps:

1. The set points of program are defined by the user.
2. Simulation of reactor starts by an initial guess for heat flux profile, gas inlet temperature (cross temperature) and inlet pressure.
3. Mass, energy and momentum balance equations are solved along the length of the reactor.
4. Coil outlet temperature (COT) obtained in step 3, is compared with the set value. Heat flux profile is modified and calculations are repeated until the obtained value equals the set value.
5. The recycle rate is adjusted for steady-state conditions.
6. The amount of fuel gas needed to provide the necessary energy for reactions is determined.
7. Flue gas flow rate and flue gas temperature, leaving the radiation section are calculated.
8. Mass, energy and momentum balance equations for convection section and TLE are solved simultaneously.

9. Cross temperature, obtained in step 8, is compared to the initial guess. In case of any discrepancies observed, calculations will be repeated from step 2 on, using the obtained value as the initial guess.
10. If TLE outlet pressure, obtained in step 8, is not equal to pressure set value, the initial guess for reactor inlet pressure shall be modified using following equation and calculations shall be repeated from step 2 on.

    Pnew = Pin + Error

    Error = Obtained value – Set value
11. After the results are obtained for start of run (time = 0.0), the time element is increased by a time increment and calculations are repeated from step 2 on.

    time = time + dtime
12. The amount of coke deposited in the reactor will cause an increase in coil inlet pressure and also in tube skin temperature. These two factors are the main constraints imposed on the program and eventually determine reactor run length.

Case Studies

Simulation of two industrial olefin furnaces are explained below as case studies.

Naphtha Cracker

The first case study is simulation of the naphtha cracking furnace in the olefin plant of Arak Petrochemical Complex, Arak, Iran. Table 2 shows input data, including furnace dimensions, reactor geometry, TLE geometry, feed specifications, fuel specifications and operating conditions. The results of this simulation are summarized in Table 3.

Figures 3 and 4 show part of the results obtained from simulating the naphtha thermal cracking reactor using SHAHAB. The yield profile of the main products along the length of the reactor under start of run (SOR) condition is shown in Figure 3. Reactor surface is clean in the beginning. But the thickness of the coke deposited on the inner surface of reactor increases with time. Coke thickness profiles along the length of the reactor under middle of run (MOR) and end of run (EOR) conditions are shown in figure 4. The coke thickness is high in the second part of the reactor because the concentration of coke precursors in the high- temperature zone of the reactor is high. As a consequence, the coke layer grows fast there, creates an additional resistance to heat transfer and causes a decrease of the tube cross- sectional area. Increasing the heat flux increases the gas/coke interface temperatures and the coking rates.

Figure 5 shows the heat flux profiles obtained from simulation of the naphtha cracking reactor as a function of run time. The high heat flux in the first part of the reactor results from the requirement of achieving a higher conversion, therefore, the ethylene yield remains constant, despite an increase in inlet pressure. The resistance against heat transfer caused by the coke layer causes the external tube skin temperature to rise, especially in the second part of the reactor. Figure 6 shows the evolution with time of the external tube skin temperature. The temperature profile shows a significant increase in the first part of the reactor, but this is mainly due to the higher heat flux. The maximum value is reached at the end of the second part. The run-time of cracking furnace is usually limited by external tube skin temperature. In present case, the maximum allowable temperature at the second part of the coil is 1100 °C. Therefore, in our case, the run length was predicted to be 62 days.

Ethane Cracker

The second case study is simulation of the ethane cracking furnace at Bander Imam Petrochemical Complex (BIPC), Mahshahr, Iran. Input data for this furnace are shown in Table 4 and simulation results of ethane furnace are shown in Table 5.

The results of the simulation are shown in Figures 7 and 8. Ethylene, propylene, hydrogen, methane and C_5^+ yields along the length of the reactor at SOR are shown in Figure 7 and variation of the coke thickness on reactor surface along the length of reactor at MOR and EOR is shown in Figure 8.

Table 2. Input data of naphtha cracker furnace simulator (Arak Olefin Plant Furnace)

Furnace Specifications			
Fire Box		Reactor Configuration	
Height (m) Length (m) Depth (m) Number of Burners	11.5 10.5 2.1 108	Total Length (m) Length of Coil 1 (m) Internal/External diameter (mm) Length of Coil 1 (m) Internal/External diameter (mm)	45 22.5 85/92 22.5 121/130
Transfer Line Exchanger (TLE)			
No. of TLE No. of Tubes in TLE	1 152	Tube Diameter ID/OD (mm) Tube Length (m)	24/32 4.96
Feed and Operating Condition			
Naphtha Composition (wt%)			
n-Butane	4.53	2,2,3-trimethylbutane	7.20
iso-Butane	0.12	Benzene	2.17
n-Pentane	22.52	Toluene	0.37
iso-Pentane	16.48	P-& m-Xylene	0.44
2,2-dimethylbutane	0.30	Cyclohexane	7.13
2,3-dimethylbutane	1.18	n-Heptane	1.69
Cyclopentane	7.38	2,3-dimethylpentane	1.10
2-Methylpentane	12.17	n-Octane	0.63
n-Hexane	12.02	iso-Octane	0.20
2,4-diMethylpentane	2.30	n-Nonane	0.07
Naphtha Flow Rate (kg/h)	11600	Boiler Feed Water (BFW) Temp. (^oC)	155
Naphtha Inlet Temp. (^oC)		BFW Pressure (bar)	120
Steam to Naphtha Ratio (g/g)	0.7	Coil Outlet Temp. (^oC)	866
Dilution Steam Temp. (^oC)	190	Maximum Skin Temp. (^oC)	1100
Fuel Composition (mol%)			
H_2 CH_4	14.0 86.0	Excess Air (%)	15

T*a*b*le* 3. Output results of naphtha cracker furnace simulator (Arak Olefin Plant Furnace)

Run Length (days)		62		
Y*iel*d *of Pro*d*ucts (*d*r*y w*t*%)**				
	Start of Run		End of Run	
Components	Simulation	Plant	Simulation	Plant
Hydrogen	1.00	1.20	0.95	1.12
Methane	17.07	17.74	16.95	17.43
Acetylene	1.16	0.93	1.03	0.80
Ethylene	35.14	35.42	34.05	34.22
Ethane	6.07	5.67	6.57	6.42
Methylacetylene +Allene	0.95	1.15	0.93	1.10
Propylene	12.53	12.07	13.67	13.04
Propane	0.43	0.48	0.44	0.57
1,3- Butadiene	4.52	4.23	4.7	4.14
Butene	2.56	2.52	2.87	3.01
Butane	0.36	0.24	0.48	0.31
C_5 Fraction	2.1	2.34	2.4	2.70
Benzene	6.86	7.11	6.34	6.84
Toluene	2.61	2.12	2.35	2.13
Xylene + Ethylbenzene	0.46	0.45	0.47	0.49
Styrene	1.10	1.30	0.94	1.20
C^+_6	5.01	4.60	4.8	4.42
Carbon Oxides	0.07	0.07	0.06	0.06
BFW Fow Rate (kg/h)	24700	26300	19800	22400
Fuel Flow rate(kmol/h)	135	142	139	146
Temp. of Cracked Gas at TLE Outlet (ºC)	367	371	407	410

Conclusion

SHAHAB is a PC-based simulator developed by ORG, with the simultaneous simulation of the reactor, the firebox, the convection section and the transfer line exchanger. A complete reaction network, using a rigorous kinetic model, for the decomposition of the hydrocarbon feedstocks has been developed and used for simulation of thermal hydrocarbon crackers. A coking model considering 24 coke precursors is used. Taking into account the kinetics of coke formation, SHAHAB provides a detailed understanding of product yields, temperature and pressure distribution, coke thickness profiles, tube skin and refractory temperature profiles, furnace conditions, reactor run length, fuel consumption and the amount of steam generated.

The simulation results and plant observations agree very well. Simulations of this type can be used to optimize furnace operation for various feedstocks and operating conditions. They can be used as a guide for the adaptation of the operating variables aiming at prolonging the run length of the furnace. It can also be used for determining the optimal operating strategy for different hydrocarbon feeds, controling fuel flow rate or, hydrocarbon feed load, and so on. Farther, it can be used for the design purpose and can be expected to help to maximize the plant efficiency and profit.

***Acknowledgment*:** The authors acknowledge the support of the process data for this work by NPC, ARPC, TPC, AMPC, BIPC petrochemi-cal companies of Iran.

T*able* 4. Input data of ethane cracker furnace simulator (Bandar Imam Olefin Plant Furnace)

Furnace **S***pecifications*			
Fire Box		Reactor Configuration	
Height (m) Length (m) Depth (m) Number of Burners	13.3 11.7 3.0 112	Total Length (m) Internal/External diameter (mm)	98.0 128/141
T*ransfer* **L***ine Exchanger (***TL***E)*			
No. of TLE No. of Tubes in TLE	2 85	Tube Diameter (mm) Tube Length (m)	25 4.46
*Fee***d** *an***d** **O***perating Con***d***ition*			
*Fee***d** *Composition (***w***t***%***)*			
Ethane Propane	98.07 1.93		
Feed Flow Rate (kg/h)	11600	Boiler Feed Water (BFW) Temp. (^oC)	145
Feed Inlet Temp. (^oC)	60	BFW Pressure (bar)	52
Steam to Feed Ratio (g/g)	0.4	Coil Outlet Temp. (^oC)	828
Dilution Steam Temp. (^oC)	180	Maximum Skin Temp. (^oC)	1100
*Fuel Composition (mol***%***)*			
H_2 CH_4 C_2H_6	3.6 95.4 1.0	Excess Air (%)	15

T*a*b*le* 5. Output results of ethane cracker furnace simulator (Bandar Imam Olefin Plant Furnace)

Run Length (days)	60			
Y*iel*d *of Pro*d*ucts (*d*r*y w*t*%*)*				
	Start of Run		End of Run	
Components	Simulation	Plant	Simulation	Plant
Hydrogen	2.93	2.88	2.77	2.72
Methane	3.32	3.59	3.53	3.80
Acetylene	0.26	0.241	0.23	0.20
Ethylene	39.31	40.50	36.83	38.50
Ethane	50.22	49.21	52.29	51.08
Methylacetylene +Allene	0.07	0.02	0.07	0.03
Propylene	1.37	1.39	1.56	1.70
Propane	0.22	0.15	0.20	0.20
1,3- Butadiene	0.57	0.88	0.49	0.65
Butene	0.09	0.31	0.09	0.30
Butane	0.32	0.74	0.32	0.70
C^{+}_{5}	1.47	0.05	1.47	0.05
Carbon Oxides	0.13	0.08	0.14	0.07
BFW Flow Rate (kg/h)	15757	16852	15359	16253
Fuel Flow rate(kmol/h)	96.83	100.17	98.36	102.21
Temp. of Cracked gas at TLE outlet (ºC)	359	360	383	385
Hot and Cold Flows Temperatures in the Convection Section (^{o}C)				
Bank No. 1				
BFW Temp., In/Out	117/655	117/649	117/655	117/668
Fobt Flue Gas Temp., In/Out (Stack)	461/206	460/240	468/210	520/260
Bank No. 2				
Feed Temp., In/Out	146/256	146/265	146/256	146/256
Flue Gas Temp., In/Out	1135/461	1100/460	1134/468	1135/520

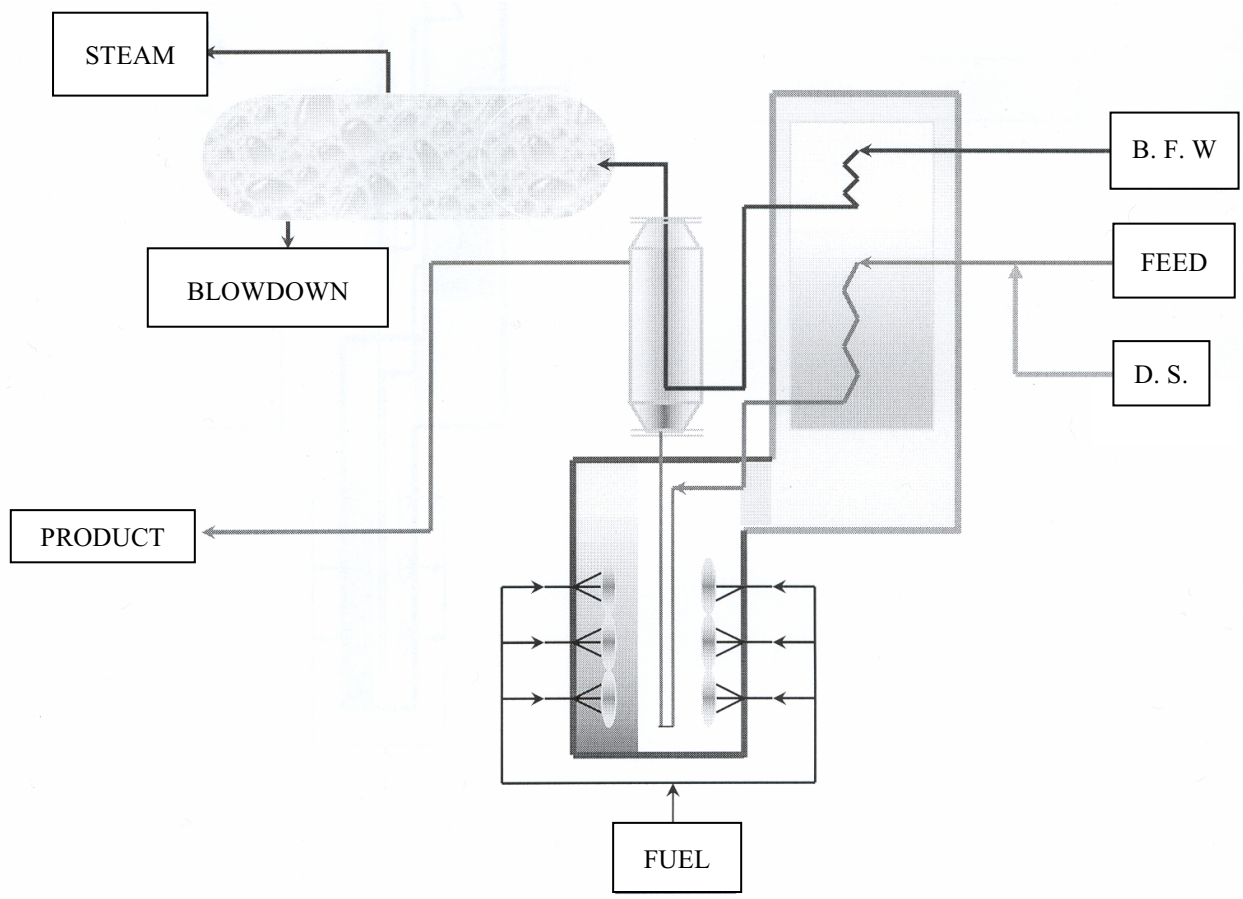

Figure 1. Schematic diagram of a cracking furnace

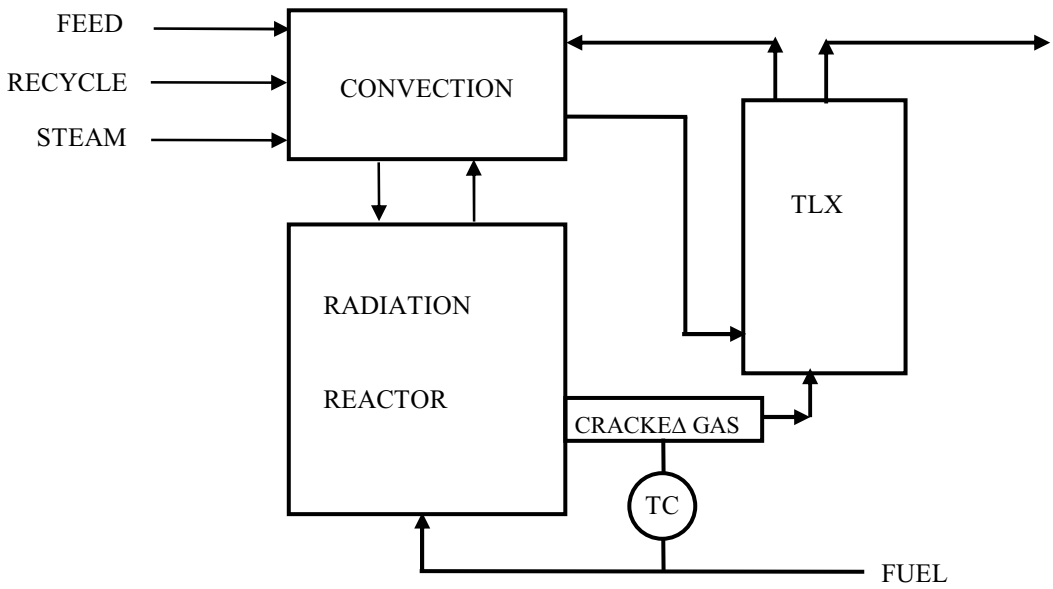

Figure 2. Block diagram of SHAHAB Simulator

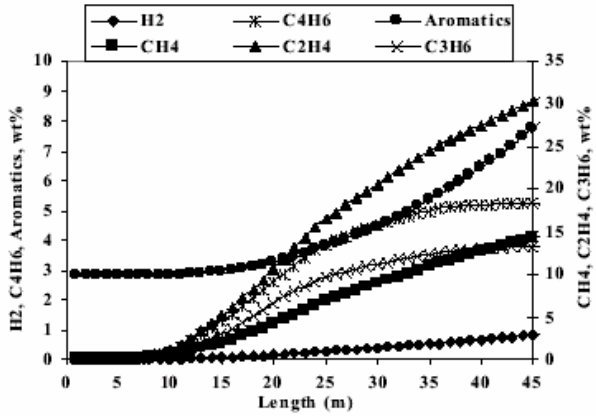

Figure **3**. Product yields of steam cracking of naphtha.

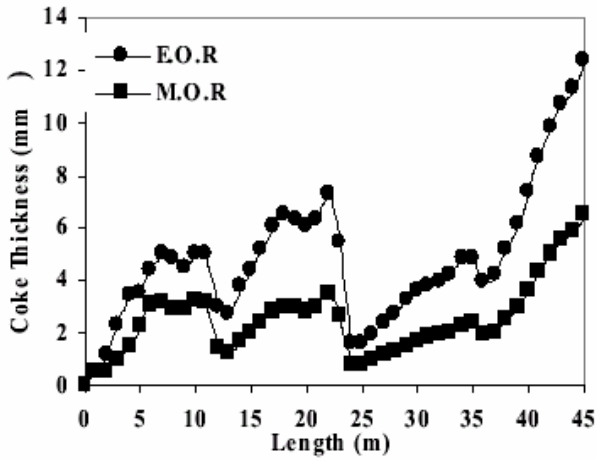

Figure 4. Profile of coke thickness in steam cracking of naphtha.

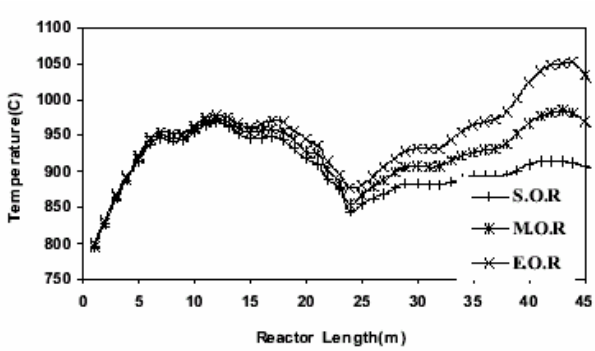

Figure **5**. Profile of Tube Skin Temperature in steam cracking of naphtha at Different Run Time.

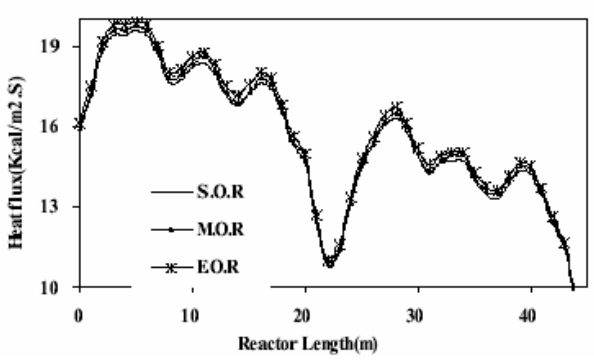

Figure **6**. Profile of Heat Flux in steam cracking of naphtha at Different Run Time.

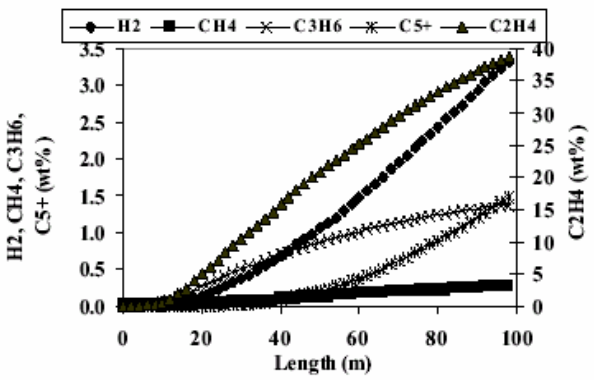

Figure **7**. Profile of productyields in the steam cracking of ethane.

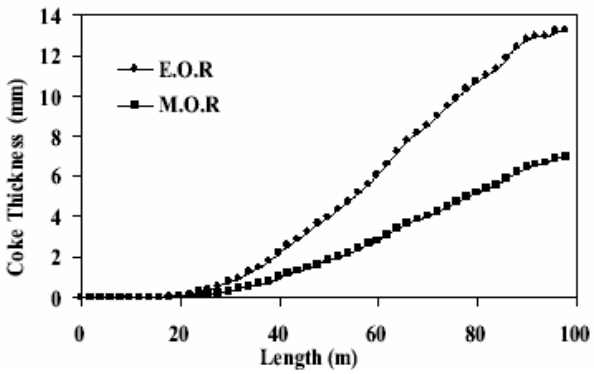

Figure **8**. Coke thickness in steam cracking of ethane.

Nomenclature

A_i Area of a zone (m^2)
C_i Concentration of coke (mole/m^3)
Cp Heat capacity (J/mole K)
d_t Tube diameter (m)
E Black body emissive power (W/m^2)
Eff Fin Efficiency
F Molar flow rate (mole/hr)
Fr Friction factor
G Total mass flux of the process gas (kg/m^2.s)
h_p Process gas convection coefficient (W/m^2oK)
h_o Outside convection heat transfer coefficient (W/m^2 ^oK)
h_i Inside convection heat transfer coefficient (W/m^2 ^oK)
$-\Delta H$ Heat of reaction (J/mole)
k Thermal conductivity of tube (w/m^2 ^ok)
m Mass flow rate (kg/h)
M_m Average molecular weight (kg/mole)
N_f Number of fins per unit length of tube
N_{ij} Stoichiometery factor
Nu Nusselt number
Pr Prandtl number
P_t Total pressure (bar)
Q Heat flux (W / m^2)
r Tube radius (m)
r_e External tube radius (m)
r_i Internal tube radius (m)
r_{ci} Coking reaction rate of precursor i (mole / m^3 .s)
Re Reynolds number
t_c Coke layer thickness (m)
t Time (hr)
T Temperature (K)
T_f Fin thickness
U Overall heat transfer coefficient (kJ/kg. K.m^2)
Z_i Z_j Total exchange area from zone i to j
Z Axial reactor coordinate (m)

Greek Letters

a coking factor
$\mathbf{a}_{abs}$ gas absortivity (w/$m^{2.}$ K^4)
$\in$ Emissivity (w/$m^{2.}$ K^4)
λ Latent heat of vaporization (J/kg)
ζ Parameter of tube bend
ρ_c coke density (kg/m^3)
σ Stefan-Boltzmann constant (w/m^2K^4)
θ Tube perimeter angle

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