RESEARCH NOTE

HEAT TRANSFER CALCULATION IN THE FIREBOX OF THE ETHYLENE PLANT FURNACES

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Abstract The thermal cracking of hydrocarbons for olefin production is carried out in long tubular reactors inserted in a furnace. In this process the heat flux along the reactor wall determines the feedstock conversion, the olefin selectivities and rate of coke deposition. A detailed firebox simulation model is therefore a powerful tool in the design and operation of pyrolysis furnaces and reactors to study the effect of process variables. The zone method of analysis is a versatile tool for studying the effects of process variables on furnace operation. A computer program which applies a zoning technique has been written in FORTRAN 77 for analyzing the heat transfer in the radiant chamber of the firebox. The temperature distribution, inside the cracking coils, calculated by the kinetic model [1], has been used for this model. Application of the program to the simulation of the thermal cracking furnace shows that the temperature distributions in such a furnace are highly non-uniform. The results are in agreement with the fundamental results of SPYRO* simulation model [2] for the thermal cracking furnaces.

Key Words Cracking Furnace, Radiation, Simulation, Zone Method

چکیده شکست حرارتی هیدروکربنها برای تولید اتیلن در راکتورهای لوله ای بلند که در داخل کوره های حرارتی قراردارد انجام می شود. دراین فرایند توزیع فلاکس حرارتی در طول راکتور برروی درصد تبدیل، گزینش پذیری محصولات و میزان نشست کک موثر می باشد. لذا یک برنامه شبیه سازی دقیق و با قدرت می تواند ابزاری مفید برای کمک در مسایل طراحی و عملیات کوره های حرارتی و راکتورهای شکست حرارتی باشد تا بوسیله آن بتوان مطالعه اثر پارامترهای فرایند را انجام داد. روش ناحیه بندی که امروزه در شبیه سازی کوره های مورد استفاده قرار می گیرد، دراین مطالعه بکار گرفته شده است. دراین مقاله نتایج یک برنامه کامپیوتری که به زبان فرترن ۷۷ نوشته شده و برای حل معادلات انتقال حرارت در کوره های حرارتی مورد استفاده قرار گرفته است ارائه می گردد. توزیع درجه حرارت در داخل راکتور از مدل سینتیکی [۱] گرفته شده است و دراین برنامه وارد شده است. نتایج برنامه شبیه سازی کوره های حرارتی نشان می دهد که توزیع دما در این کوره ها یکنواخت نمی باشد. نتایج این برنامه ها با داده های نرم افزار استاندارد SPYRO [۲] که برای طراحی کوره های بکار گرفته شده است مقایسه و تطابق نتایج حاکی از دقت محاسبات می باشد.

INTRODUCTION

Direct fired heaters have a vital role in many important petroleum, petrochemical and chemical processes, as demonstrated by their use for heating oils, cracking hydrocarbon feedstocks and for steam reforming processes. The key-factor in large tonnage olefin plant design and operation for optimum flexibility and feedstock utilization is the precise prediction of yields and pyrolysis furnace performance, including on-stream time assessment, for any hydrocarbon feedstock. This can only be satisfactorily achieved

*Simulation of Pyrolysis Reactors for Olefins through rigorous modeling and simulation, using the mathematical representation for the system. By means of simulation, the influences of the firing conditions of the furnace and reactor geometry on the temperature and heat flux distribution in the firebox can be investigated. Usually, the simulation of the thermal cracking coil is uncoupled from the heat transfer phenomena in the firebox by imposing a heat flux profile on the reactor. It is then checked whether or not the firebox allows this heat flux to be attained. In most cases this is done by means of a simplified method like the Lobo and Evants [3] approach, which assumes a uniform temperature throughout the firebox. Vercammen and Froment [4] further developed a zone method initially introduced by Hottel and Sarofim [5] to simulate radiation in industrial heaters.

This paper is concerned with the mathematical representation of an existing box-type furnace which is composed of a preheating convection section and a radiant heated section for the thermal cracking of naphtha. The furnace considered in this work which is designed by KTI (Kinetics Technology International) and is manufactured for the ARAK Petrochemical Complex in IRAN, is fired by 108 radiant burners and mounted in the side walls. A simplified KTI combined coil design is shown in Figure 1. Because of the small diameter tubes at the beginning of the reactor, the surface-to-volume ratio is high in this part of the coil, which permits a fast increase of temperature. After rapid heating, pairs of small tubes are combined to one large tube with a low pressure drop. Cracking coils are usually arranged in the two-row staggered arrangement in which the firebox becomes smaller as this arrangement is very compact. This results in lower investment costs. A disadvantage of this arrangement is the unsymmetric heat flux profile on the tube circumference. This effect is under investigation by using an advanced three dimensional conduction model in the reactor wall of the furnace [6]. The major fraction of the released heat enters the fire box with the combustion gases through radiation and convection. The simulation model is limited to the radiant section while the convection section has been simulated separately [7]. The combined radiation and convection modelling then may be used to obtain the furnace firing performance. The convective heat transfer to the tubes and to the refractory walls in the section was calcualted by

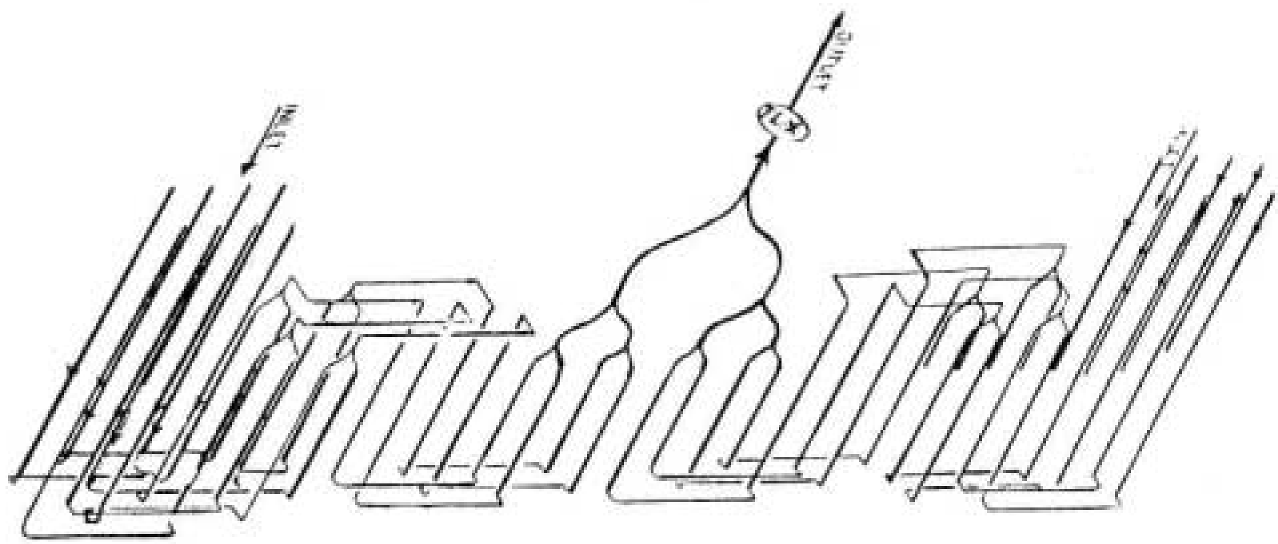

Figure 1. Coils configuration inserted in the furnace.

means of the usual correlations for immersed bodies. A computer program which applies a zoning technique has been written in FORTRAN 77 for analyzing the heat transfer in radiant chambers of the fired heater. In this program the firebox is divided into three main sections; refractory, tubes (sink) and combustion gases. The box also is individed into M volumes for the gas section and N squares for the refractory walls as shown in Figure 2. For each zone the temperature and the physical properties are assumed to be uniform and constant. The program can handle any type of tube lay-out in a rectangular fire box.

FIREBOX HEAT TRANSFER

Convective Heat Transfer- Heat transfer from the flue gas to the surrounding surfaces and to the tubes by convection is only a small contribution to the total heat exchange. The convective heat transfer to the tubes and to the refractory walls in that section was calculated by [6]:

$$h_c = 0.211 \frac{k_g}{D} Re^{0.651} Pr^{0.34} \qquad (1)$$

Heat loss by conduction through the refractory walls and by natural convection at the outside of the furnace walls was neglected.

Radiative Heat Transfer- The furnace considered in this work, schematically shown in Figure 3, is fired by 108 radiant burners, placed in the side walls. The main dimensions and operating conditions of the simulated naphtha cracker are presented in Table 1. Cracking coils are arranged in the radiant section in two rows with variable diameters. The advantage of the two row, staggered arrangement is that the fire box becomes smaller as this arrangement is very compact. This results in lower investment costs. A disadvantage of this arrangement is the unsymmetric heat flux profile on the tube circumferences. The circumferential tube skin temperatures were found to vary over 30°C and more due to "shadow effects" [10].

A small fraction of the heat of combustion is transferred to the radiant burner cup itself. The major fraction of the released heat enters the fire box with the combustion gases through radiation and convection. In the multizone model for the simulation of radiation section, as outlined by Hottel and Sarofim [5], the space in which radiation heat transfer has to be calculated is divided into a number of surface and volume elements which are isothermal and have uniform properties. The model considers individual band absorption and emission of radiation by carbon dioxide and water and accounts explicitly for the position of the burners in the oven walls. The zone approach reduces the set of integro-differential equations describing the energy transfer into a set of non-linear algebraic equations. The set of energy balances for the zones in a closded radiation system in which heat transfer by conduction and convection (partly also with the surroundings) is accounted for, can be written as:

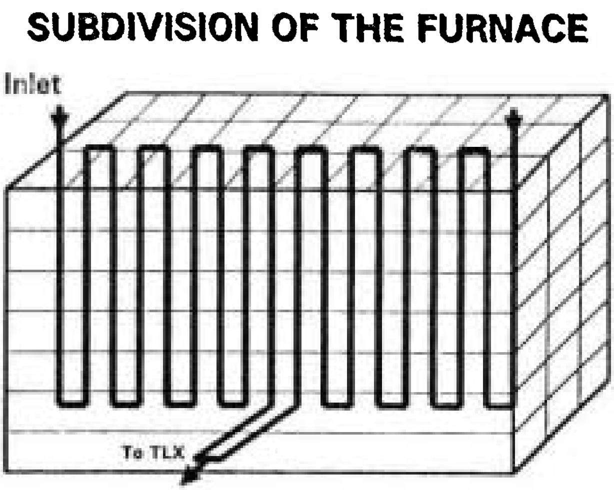

Figure 2. Subdivision of the furnace in isothermal zones.

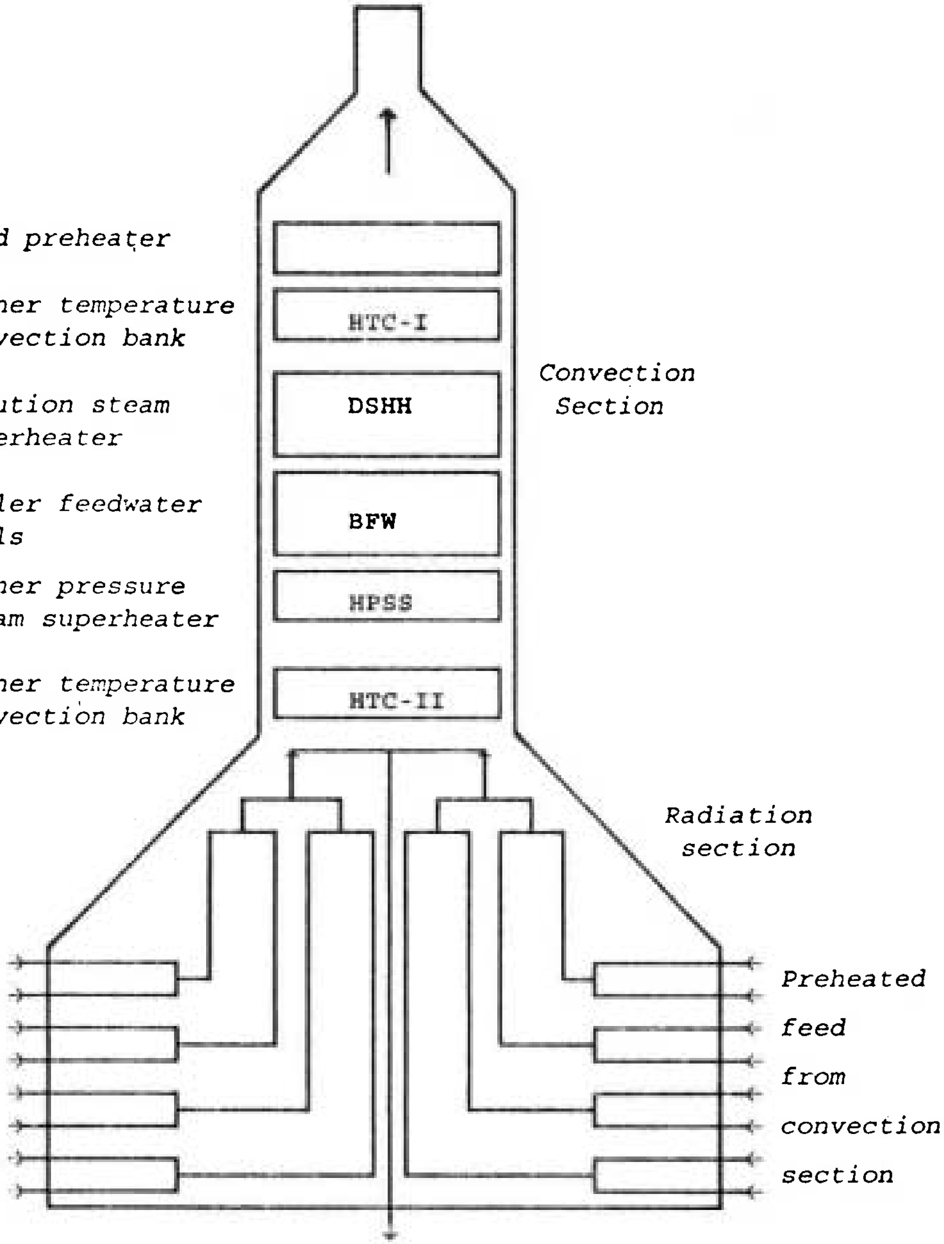

Figure 3. Representation of the thermal cracking furnace.

$$\begin{bmatrix} \overline{Z_1Z_1} - \sigma_j \overline{Z_1Z_j} & \overline{Z_2Z_1} & \cdots & \overline{Z_nZ_1} \\ \overline{Z_1Z_2} & \overline{Z_2Z_2} - \sigma_j \overline{Z_2Z_j} & \cdots & \overline{Z_nZ_2} \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \overline{Z_1Z_n} & \overline{Z_2Z_n} & \cdots & \overline{Z_nZ_n} - \sigma_j \overline{Z_nZ_j} \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \\ \cdot \\ \cdot \\ E_n \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \\ \cdot \\ \cdot \\ Q_n \end{bmatrix} \quad (2)$$

$\overline{Z_iZ_j}$ represents the amount of radiative energy emitted by zone Z_i, both directly and after reflection on other zones, divided by the black-body emissive power E_i of Z_i. $\overline{Z_iZ_j}$ has the dimensions of an area and is defined as the total exchange area between Z_i and Z_j. In Equation 2, $\dot{Q}_i$ is the non-radiative heat flux leaving Z_i. In each zone Z_i (volume or surface) the net radiation captured is equated to the net non-radiative flux leaving the zone Q_i. The radiative flux from zone Z_j to Z_i is given by $Z_iZ_jE_j$, where $E_j = \sigma.T^4$ and $\overline{Z_iZ_j}$ is the total exchanged area between

TABLE 1: Furnace Configurations

Fire box dimensions:
Length: 10.646 m
Width: 2.10 m
Height: 11.5 m
Emissivites of:
Walls: 0.7
Coils: 0.94
Fuel Gas:
Composition: Co: 0.06%, H_2: 14%,
CH_4: 85.36%, C_2H_6: 0.11%
Quantity: 2012.0 kg/hr
Air excess: 15
Number of burners: 108

Zi and $\overline{Z}_j$.

The calculations leading to the total-exchange areas that appear in Equation 2 are performed in three steps. First, the view factors among surfaces in a transparent medium are calculated. In a second step, absorption by the flue gas is accounted for and the direct-exchange areas among surface zones and gas zones are determined. Finally, the total exchange areas are calculated by considering both direct and reflected radiation. The sequence of calculations leading to the total exchange areas appearing in Equation 2 may be summarized as follows. To start with, the view factors between surfaces in a transparent (non absorbing, non scattering) medium are calculated. The second step is the calculation of view factors between surfaces and volumes in a real medium. This requires accounting for the absorption, which depends upon the gas composition and the temperature distribution. The direct exchange areas between surfaces and volumes can be derived from the direct ecxchange areas between surfaces, provided that the imaginary surfaces bounding the volumes are also accound for. Finally the total exchange areas are calculated by accounting for the radiation received by the receptor by both direct and reflected radiation, using the algorithms of Hottel [5].

The numerical solution of this set of non-linear algebraic equations yields the temperatures in the volume and surface zones. since the equations are non-linear, they have to be solved by iteration. A Newton-Raphson [8] procedure was found to be very efficient for the solution.

HEAT BALANCES

Heat balances are formulated on all surface and gas zones of unknown temperautre. A heat balance on refractory surface zone i as illustrated in Figure 4 gives:

$$\sum_{j=1}^{N} \overrightarrow{S_jS_i}E_{w,j} \,.\, \sum_{j=1}^{M} \overrightarrow{G_jS_i}E_{g,j} - \left(\sum_{j=1}^{N} \overrightarrow{S_jS_i} + \sum_{j=1}^{M} \overrightarrow{G_jS_i}\right) E_{r,i}$$

$$+ h_iA_i(T_{g,i} - T_{r,i}) = Q_{sr,i} \qquad 1 \le i \le N \tag{3}$$

where

$$E_{g,j} = \sigma . T^4_{g,j} \tag{4}$$

$$E_{r,j} = \sigma . T^4_{r,j} \tag{5}$$

$$E_{w,j} = \sigma . T^4_{w,j}$$

h_i is the convective heat transfer coefficient at surface zone i and $Q_{sr,i}$ is the net heat flux to the surface. Since the refractory surfaces are adiabatic, therefore $Q_{sr,i} = 0$.

Similarly, a heat balance on gas zone i (Figure 4) gives:

$$\sum_{j=1}^{N} \overrightarrow{S_jG_i}E_{w,j} + \sum_{j=1}^{M} \overrightarrow{G_jG_i}E_{g,j} + \sum_{j=1}^{N} \overrightarrow{S_jG_i}E_{r,j} +$$

$$\left(\sum_{j=1}^{M} \overrightarrow{G_iG_j} + \sum_{j=1}^{M} \overrightarrow{G_iS_j}\right) E_{g,i} - \sum_{j=1}^{M} h_jA_j\,(T_{g,i} - T_{r,j}) + Q_{c,i} = 0$$

$$1 \le i \le M \tag{6}$$

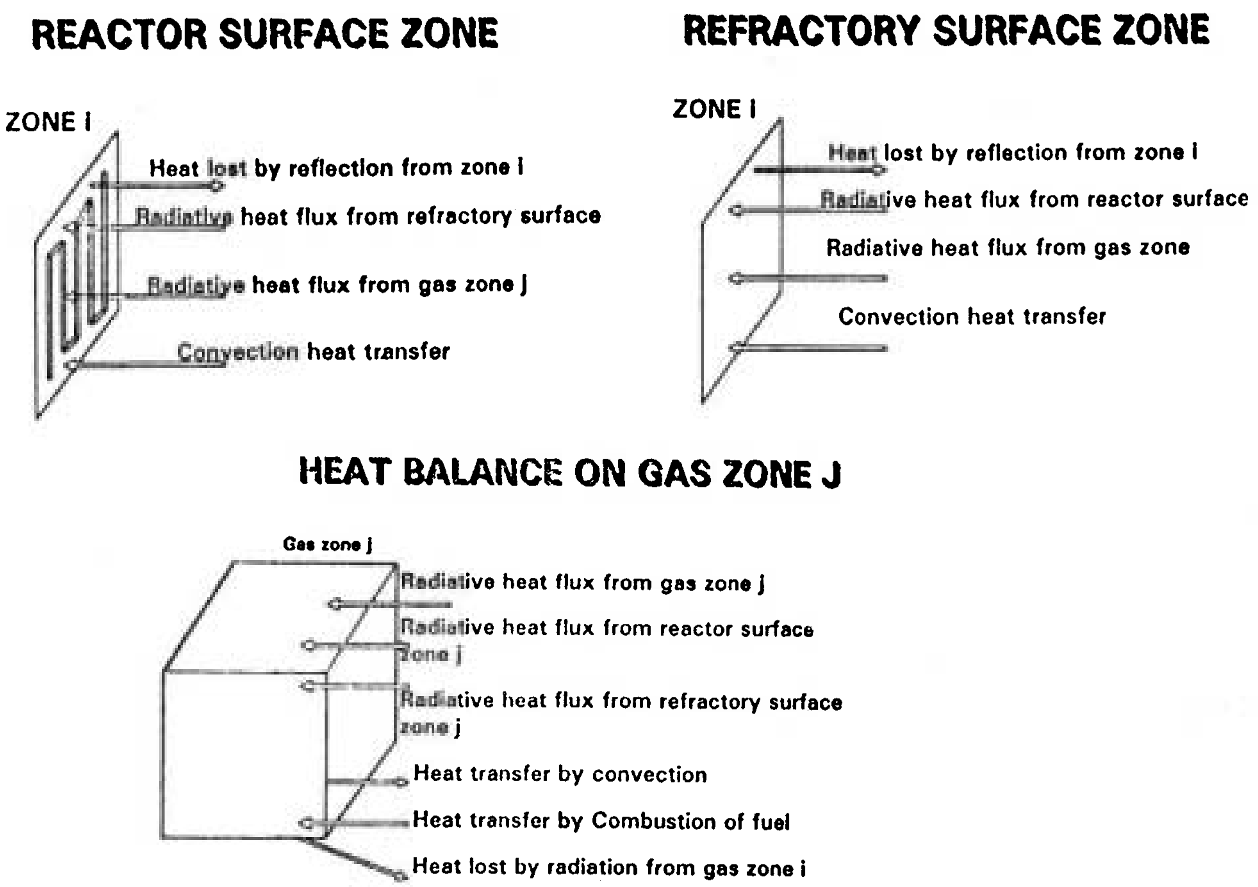

Figure 4. Heat balances on the surface and volume zones.

Where h_j is the convective heat transfer coefficient for convection to an adjacent surface zone at temperature $T_{r,j}$, and $Q_{c,i}$ is the net total heat released due to combustion in the zone.

A heat balance on the surface zone i of the reactor (Figure 4) results:

$$\sum_{j=1}^{N} \overrightarrow{S_jS_iE_{r,j}} + \sum_{j=1}^{M} \overrightarrow{G_jS_iE_{g,j}} - \left(\sum_{j=1}^{N} \overrightarrow{S_jS_i} + \sum_{j=1}^{M} \overrightarrow{G_jS_i}\right) E_{w,i}$$

$$+ h_iA_i(T_{g,i} - T_{w,i}) = Q_{w,i} \qquad 1 \le i \le N \qquad (7)$$

or

$$\sum_{j=1}^{N} \overrightarrow{S_jS_iE_{r,j}} + \sum_{j=1}^{M} \overrightarrow{G_jS_iE_{g,j}} - \varepsilon_iA_iE_{w,i} + h_iA_i(T_{g,i} - T_{w,i})$$

$$= Q_{w,i} \qquad (8)$$

and finally the total heat balance on the reactor gives:

$$U_i \cdot (T_{w,i} - T_{p,i}) = Q_{w,i} \qquad (9)$$

Where U_i is the overall heat transfer coefficient, $T_{w,i}$ is the wall temperature at zone i, and $T_{p,i}$ is the process temperature inside the reactor. By solving these four equations T_g, T_r, T_w and Q_w for zone i can be calculated [9].

RESULTS

By way of example, a simulation of a commercial furnace for the pyrolysis of naphtha is performed.

TABLE 2: Comparison of the Temperature Results and *SPYRO*.

Zone	Gas Temp. Model ∞C	Gas Temp. SPYRO ∞C	Error (%)	Zone	Tube °C Wall Temp. Model	Tube °C Wall Temp. SPYRO	Error (%)
1	1127.62	1097.43	2.77	1	823.23	797.92	3.14
3	1213.08	1181.87	2.69	3	894.46	864.19	3.52
5	1262.21	1230.08	2.66	5	933.90	903.57	2.27
7	1276.57	1243.42	2.68	7	952.03	926.63	2.74
9	1239.40	1206.19	2.77	9	944.62	928.24	1.70
11	1298.16	1264.99	2.67	11	977.04	946.59	2.27
13	1269.09	1238.91	2.45	13	959.95	937.48	2.31
15	1263.14	1232.86	2.52	15	966.14	941.80	2.66
17	1289.52	1257.24	2.52	17	992.90	954.44	2.99
19	1244.73	1212.56	2.61	19	967.95	942.57	2.59
21	1180.18	1148.99	2.73	21	927.09	905.76	2.41

The simulated results are tested against industrial data obtained from the *SPYRO*. The *SPYRO* program is a unique coincidence on many years of fundamental work of a highly qualified scientific team, together with the indispensable practical experience and know-how of a company specializing in the design of steam crackers. KTI (Kinetic Technology International) has designed the furnaces by using the *SPYRO* results. Therefore, these values are used as design data for the comparison of the simulation results.

Forty-four surface and volume zones are considered. For the present simulation the temperatures of the process gas inside the tubes, were obtained from the reactor simulation proposed by Towfighi [1].

The computer results of the present work are given in Table 2 and illustrated in Figures 5 to 7. Table 2 compares the temperature results of the model and *SPYRO* for the flue gas and tube wall of the reactor. The agreement of the calculated results with design values obtained by *SPYRO* simply reflects the reliability of the simulation program. In Figure 5 the temperatures of the flue gas, the furnace refractory, the a xial tube walls and the process gas inside the reactor are given as a function of the reactor length. The process gas temperature is relatively insensitive to the reactor wall temperature variation. This is due to the high mass flow rate in the reactor, which dampens changes in heat input, and to the endothermic nature of the pyrolysis process gas temperature, that has a self-stabilizing effect in the process gas temperature. The comparison between the simulated results and the design data for the flue gas and refractory walls temperatures are demonstrated in Figure 6. A fast increase in the gas temperature is due to the fact that at the beginning of the reactor, the diameter is small which permits a rapid heating for the reaction to be initiated in the reactor. The profile also has the same shape as that of the tube skin temperature profile. The peaks correspond with the bottom of the

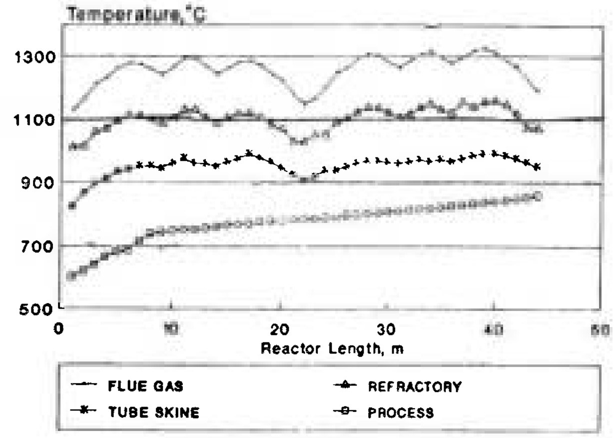

Figure 5. Temperature results of the model for NAPHTHA cracking.

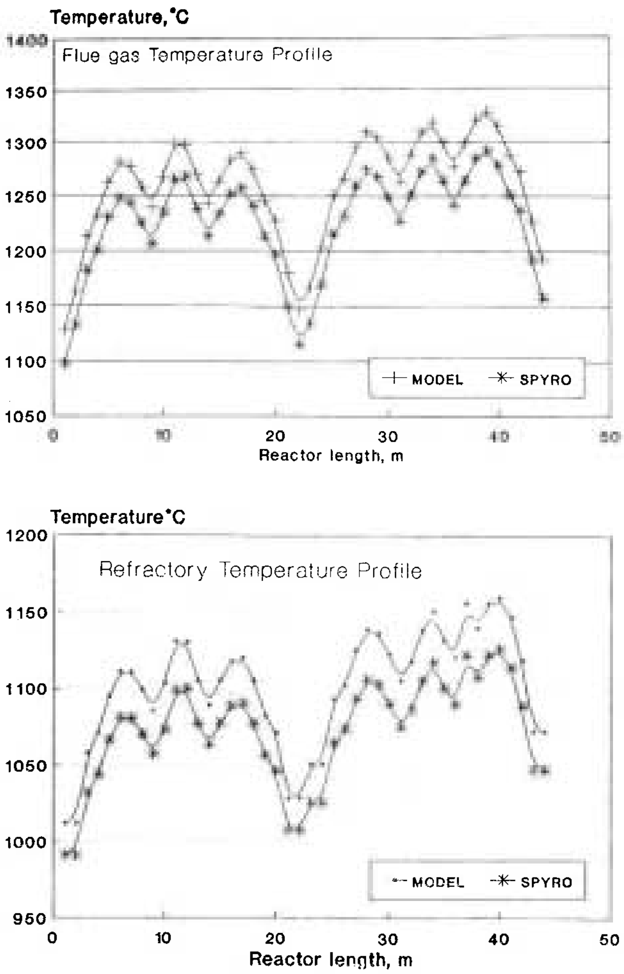

Figure 6. Comparison of simulation results with SPYRO for NAPHTHA.

furnace, where the flue gas temperature reaches its

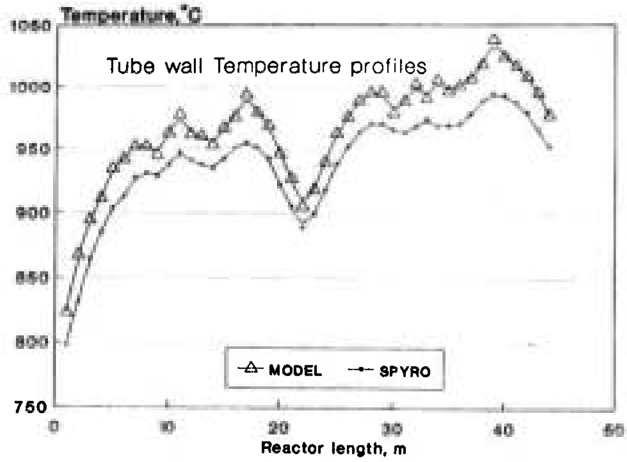

Figure 7. Comparison of the tube wall temperatures with *SPYRO*

highest values. The valleys correspond with the top of the firebox. Figure 7 illustrates the tube skin temperature profile predicted by the model and *SPYRO*. The axial tube wall temperature increases along the tube length of the reactor, but there exists a sharp peak at the middle which corresponds to the increase in the tube diamater. The temperature peaks are very important for the choice of the tube material and are limited by the coil metallurgy. In the present case, the maximum allowable temperature is 1100°C. They also lead to localized coke formation in the lower U-bends, causing a high pressure drop and therefore a loss in the selectivity for the main cracking product, ethylene, and reducing the run length of the furnace between decoking periods.

CONCLUSIONS

In the thermal cracking furnaces, the heat flux along the reactor determines the feedstock conversion, the olefin selectivities and the rate of coke deposition. An average value of the heat flux, obtained via the Lobo and Evants [3] approach, can not be used to predict the furnace performance up to present-day standards. A detailed firebox simulation model is therefore a powerful tool in the design and operation of pyrolysis furnace and reactors. The application of the program to the simulation of the thermal cracking furnace shows that the temperature distributions in such a furnace are highly non-uniform.

ACKNOWLEDGMENT

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NOMENCLATURES

A	Area of a zone, m^2
D	tube diameter, m
E	black body emissive power of zone i, w/m^2
$\overline{GG}$, $\overline{GS}$, $\overline{SS}$	total exchange areas, m^2
h	convective heat transfer coefficient, W/m^2K
M	volume element
N	surface element
Pr	Prandtl number, $Cp\mu/k$
Q_c	non radiative heat flux, W/m^2
Re	Reynolds number
S	surface zone
T	temperature, °C
U	overall heat transfer coefficient, W/m^2K
$\overline{Z_iZ_j}$	total exchange area from zone i to zone j

Greek letters

ε	emissivity
σ	Stephan Boltzman constant, 5.7×10^{-8} W/m^2K^4

Subscripts

c	combustion
g	flue gas
i, j	zone indices
p	process
r	refractory
s	surface
w	wall

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