International Journal of Chemical, Materials and Biomolecular Sciences
ISSN: 2415-6620
Vol:4, No:2, 2010

Feedstock Effects on Selecting the Appropriate Coil Configuration for Cracking Furnaces

Ramin Karimzadeh, Nazi Rahimi, and Mohammad Ghashghaee

Abstract**—**In the present research, steam cracking of two types of feedstocks i.e., naphtha and ethane is simulated for Pyrocrack1-1 and 2/2 coil configurations considering two key parameters of coil outlet temperature (COT) and coil capacity using a radical based kinetic model. The computer model is confirmed using the industrial data obtained from Amirkabir Petrochemical Complex. The results are in good agreement with performance data for naphtha cracking in a wide range of severity (0.4-0.7), and for ethane cracking on various conversions (50-70). It was found that Pyrocrack2-2 coil type is an appropriate choice for steam cracking of ethane at reasonable ethylene yield while resulting in much lower tube wall temperature while Pyrocrack1-1 coil type is a proper selection for liquid feedstocks i.e. naphtha. It can be used for cracking of liquid feedstocks at optimal ethylene yield whereas not exceeding the allowable maximum tube temperature.

Keywords**—**Coil configuration, Ethane, Naphtha, Steam cracking.

I. Introduction

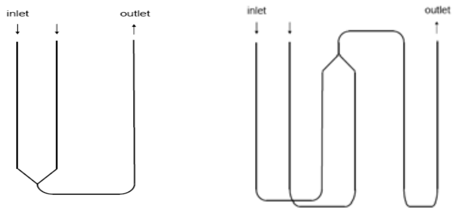
THE technology of olefin production by thermal cracking has been in continuous evolution. Reactor coil and furnace design is subject to constant innovation in search for higher olefin selectivities. The improvement in the pyrolysis reactors has strongly affected the economic benefits of the olefins plants. The coils of pyrolysis furnace in the early stage were horizontally installed with a single-side radiant heating. Later on their installation was changed to a vertical arrangement with a double- side radiant heating. On the sequence of these trends, various new versions of tube–type pyrolysis reactors have come into commercial application and investigated based on parameters and concepts that affect coil design.

In the 70's of 20th century, Kellogg Brown and Root developed the millisecond (short residence time) pyrolysis coils which achieves improvement in yields by incorporating a reaction temperature of 1600-1700 K and contact time of less than 0.1 sec. In 1987, Plehiers and Froment studied reversed split coils geometry in the pilot reactor and proposed the Uno-Quattro coils in 1991 for cracking at high severities to increase ethylene selectivity. The honeycomb high surface to volume ceramic reactor and the shell-and-tube pyrolysis reactor were investigated by Heynericks.and Froment (1991, 1992) in pilot scale for high severity thermal cracking of hydrocarbon to produce olefins [1]-[10].

Some of the mentioned geometries have been compared for a fixed feedstock but the little research work has been done on the evaluation of different configurations utilizing different feedstocks [11]. In the present paper, the steam cracking of both liquid and gaseous feedstocks of naphtha and ethane has been investigated in Pyrocrack1-1 and Pyrocrack2-2 configurations which are the most widely used geometries in industrial olefin plants of Iran. The data obtained by modelling has been validated by Amir-kabir Petrochemical Co. industrial data.

II. Feed Composition and Coil Specification

Naphtha was considered as a typical liquid feedstock and ethane as a gaseous one. Primary naphtha components have been detected by chromatographic analysis. It consists of 42% n-paraffin, 45% i-paraffin, 3.5%aromatic and 9% naphthene. Pyrocrack1-1 (referred to Coil1) and Pyrocrack2-2 (referred to Coil2) coil types are used in Amirkabir Petrochemical plant for liquid and gaseous feedstocks, respectively. Both types are shown in Fig. 1. Each liquid furnace is equipped with 64 ultra short residence time radiant coil type Pyrocrack 1-1 whereas each gaseous furnace is equipped with 16 radiant Pyrocrack 2-2 of longer tube diameter. Coils specifications and feed flow rates are mentioned in Table I.



Pyrocrack1-1 **Pyrocrack2-2**

Fig. 1 Configuration of split1/1and split2/2(right: Split 2/2, left: split1/1)

R. Karimzadeh is with the Department of Chemical Engineering, Tarbiat Modares University (TMU), Jalal Al Ahmad Highway, P.O. Box 14155-4838 Tehran, Iran, corresponding author: phone:0098-21-82883315; fax: 0098-21-88006544; e-mail: ramin@modares.ac.ir).

N. Rahimi is with National Petrochemical Company -Research &Technology (NPC-RT), Iran Polymer and Petrochemical Institute, Pajouhesh Blvd. 17th km of Tehran-Karaj highway , Zip-code: 141851458, Tehran, Iran (e-mail:n.rahimi@npc-rt.ir).

M. Ghashgaee is with the Department of Chemical Engineering, Tarbiat Modares University (TMU), Jalal Al Ahmad Highway, P.O. Box 14155-4838 Tehran, Iran (e-mail: m_ghch@yahoo.com).

Both of the split coils have the varying diameters changed from small to larger diameters and the tube path in each pass is changed from multiple to single along the flow direction of reaction fluid. Based on the coil design, the former part and the inlet of the coil provide both a higher heat transfer surface and heat transfer coefficient. Before reaching the specified pyrolysis severity the feedstock will be heated up so quickly so as to reduce the residence time. The latter part and the outlet of the coil provide low heat, mass and momentum transfer. The lower hydrocarbon partial pressure is obtained, which is favourable to better pyrolysis selectivity.

TABLE I
THE SPECIFICATION OF PYROCRACK 1/1 (COIL1) AND PYROCRACK 2/2 (COIL2)

	Pyrocrack 1/1(Coil1)		Pyrocrack 2/2 (Coil2)	
Number of passes	Pass 1	Pass2	Pass 1 & 2	Pass 3 & 4
Internal Diameter (mm)	43.0	62.0	79.0	106.0
External Diameter (mm)	55.0	76.0	93.0	122.0
Wall thickness (mm)	6.0	7.0	7.0	8.0
Effective tube Length (mm)	10230	11300	12100	12100
Height (mm)	11430		12520	
Naphtha flow rate(kg/h); Steam ratio	29866.9; 0.5			
Ethane flow rate(kg/h); Steam ratio			26017.6; 0.3	

III. MATHEMATICAL MODEL AND SIMULATION

To simulate the cracking coil, models for naphtha and ethane pyrolysis are necessary. Such a model should also account for the coke formation during pyrolysis. For this simulation, an extended version of detailed molecular radical reaction mechanism for ethane and naphtha cracking is used [3], [6], [12], [13]. The model of pyrolysis reaction involves free radical reactions and a set of pure and normal molecular reactions. The conservation of mass, energy and momentum are presented as follows for the system assuming one dimensional plug flow reactor [14]:

$$\frac{dF_j}{dz} = -\left(\sum n_{ij} r_i\right)\frac{\pi d_t^{\,2}}{4} \qquad (1)$$

$$\frac{dT}{dz} = \frac{1}{\sum F_j C_{pj}}\left[Q(z)\pi d_o + \frac{\pi d_t^{\,2}}{4}\sum r_i(-\Delta H)_i\right] \qquad (2)$$

$$\frac{dp_t}{dz} = \frac{\frac{d}{dz}\left(\frac{1}{M_m}\right) + \frac{1}{M_m}\left(\frac{1}{T}\frac{dT}{dz} + F_r\right)}{\frac{1}{M_m Pt} - \frac{Pt}{\alpha G^2 RT}} \qquad (3)$$

Where for tube side :

$$F_r = 0.092\,\mathrm{Re}^{-0.2}/d_t$$

for ellbows :

$$F_r = 0.092\,\mathrm{Re}^{-0.2}/d_t + \mu/(\pi R_b)$$

$$\mu = (0.7 + 0.35\frac{\Lambda}{90})(0.051 + 0.19\frac{d_t}{R_b})$$

The general equation of coke deposition is:

$$\frac{\partial c(coke)}{\partial t} = r_{coke} \qquad (4)$$

The system of non-linear partial differential equation resulted from mass, momentum and heat balances is solved using the method of Steady State Approximation which is based on the assumption that *dF/dz* is zero for all radical components in the integral range. Therefore molar flow of radicals is the same at the beginning and at the end of each individual interval, but the molar flow of the molecules is different. (where *F* is the flow rate and *z* is the reactor length)

Substituting conventional Gear method by Steady State Approximation approach, can substantially improve the capability of simulation programs of olefin furnaces. However, the reliability of this method should be approved first. So the obtained results from this method are compared with industrial information of thermal cracking reactor of Amirkabir Petrochemical complex.

The simulation results have been verified by performance data obtained from Amirkabir Petrochemical plant which are shown in Fig. 2. The results are in good agreement with performance data for naphtha cracking in a wide range of severity (C3H6 wt%/C2H4 wt %), and for ethane cracking on various conversions (50-70) [13]-[15].

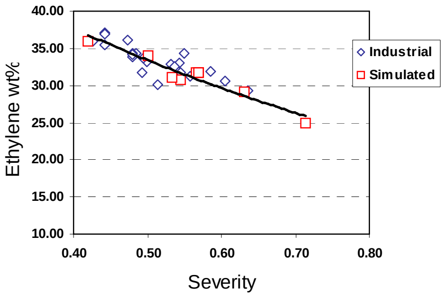


Fig. 2 The comparison between Industrial and Simulated data

IV. RESULT AND DISCUSSION

There are many parameters that affect the coil yield, mostly such as feed composition, radiant coil residence time, severity of cracking, coil outlet pressure, steam to hydrocarbon ratio and etc. Investigating all these parameters together would involve a very complex study. In the present research, steam cracking of two types of feedstocks i.e., naphtha as a liquid type and ethane as a gaseous feed is modelled in the mentioned geometries with regard to the key parameters of coil outlet temperature (COT), residence time (RT) and tube wall temperature using different flow rates.

Both the pyrolysis coils were simulated to satisfy the following operating condition:

- Identical maximum allowable metal temperature
- Identical dilution steam to hydrocarbons for each feedstock

The key operating conditions of both mentioned coil types are presented in Table II.

TABLE II
THE OPERATING CONDITION OF COIL1 AND COIL2 FOR NAPHTHA AND ETHANE

Coil type	Pyrocrack1/1 (Coil1)		Pyrocrack2/2 (Coil2)	
Feed type	Naphtha	Ethane	Naphtha	Ethane
Residence time (s)	0.22-0.7	0.28- 0.5	0.22-0.7	0.23- 0.5
Pressure drop (atm)	0.09-1.23	1.03-1.58	0.08-1.07	1.10-1.94
Coil outlet temperate (^{o}C)	820-880	820-880	820-880	820-880
Max. Tube metal temperature (^{o}C)	1100	1100	1100	1100
Dilution steam/ hydrocarbon	0.5	0.3	0.5	0.3

Cracked gas composition, residence time and tube wall temperature are computed for ethane feedstock at constant coil outlet temperature (COT) of 840 ^{o}C using different flow rates varied from 26017 to 44229 kg/h. The influence of residence time on ethylene yield in both coil types has been drawn in Fig. 3. As shown, the difference between the ethylene yield in coil1 and 2 are almost comparable.

The effect of ethylene yield on tube wall temperature has been investigated in both coil types. As shown in Fig. 4, tube wall temperatures are too much lower in coil1 than in coil2. Furthermore, the enhancement in tube wall temperature with increasing ethylene yield is much faster in coil1 than in coil2.

On the other hand, increasing the ethylene yield over a specific value does not have significant effect on the tube wall temperature therefore the run length of cracking would be higher in coil2 when employing ethane feedstock in spite of the higher ethylene yield is in coil1(Fig. 3). It can be concluded that coil2 is appropriate for steam cracking of gaseous feedstocks such as ethane.

The influence of residence time on steam cracking of naphtha has been also computed in both coil types. As indicated in Fig. 5, the differences between ethylene yields in coil1 and coil2 are considerable. Moreover the enhancements in ethylene yields are best attained by using coil1 because this coil is less sensitive to the variation of residence time.

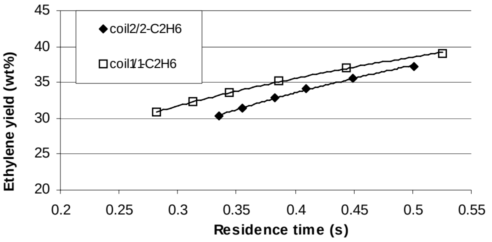


Fig. 3 Effect of residence time on steam cracking of gaseous feedstock in Coil2 and Coil1

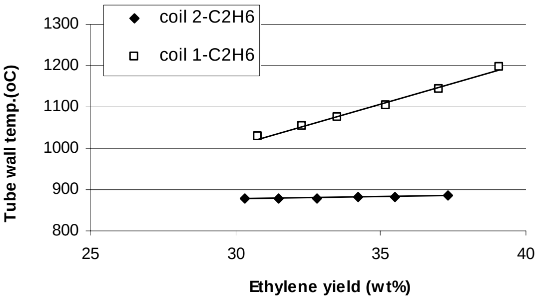


Fig. 4 The variations of ethylene yield vs. tube wall temperature for gaseous feedstock

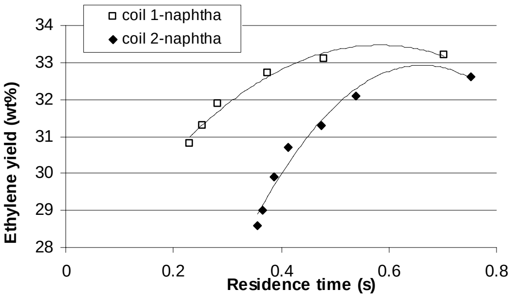


Fig. 5 Effect of residence time on steam cracking of liquid feedstock in Coil2 and Coil1

The variation of tube wall temperature with residence time is illustrated in Fig. 6. The obtained results show that tube metal temperature in coil1 does not exceed the allowable maximum metal temperature. At best condition, the maximum ethylene yield of about 33% corresponds to tube wall temperature of 920^{o}C which is quite acceptable (as indicated by a dashed circle in Fig. 6). It can be concluded that employing coil1 for liquid feedstocks here naphtha, results in higher yields while maintaining the tube wall temperature in the allowable range.

The comparison of the trends observed in Figs. 4 and 6 illustrates that liquid and gaseous feedstocks behave adversely when the ethylene yield increases.

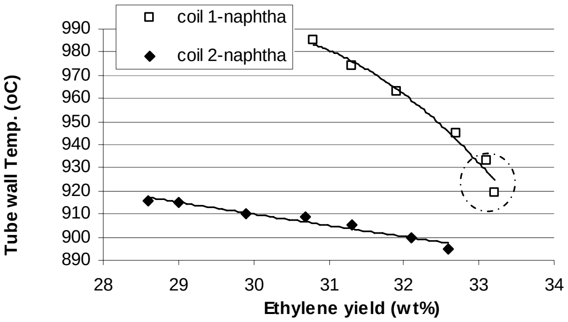


Fig. 6 The variations of ethylene yield vs. tube wall temperature for liquid feedstock

V. CONCLUSION

It was found that Pyrocrack1-1 coil type is not favourable for gaseous feedstocks because the gain in ethylene yield is much less than it is for heavier, liquid feedstocks. Furthermore the sharp increase in the tube wall temperature of coil1 reduces the run length and makes it an inappropriate choice for cracking of gaseous feedstocks. Pyrocrack2-2 coil type is an appropriate alternative for steam cracking of ethane at reasonable ethylene yield while resulting in much lower tube wall temperature.

On the contrary to gaseous feedstocks, Pyrocrack1-1 coil type is a proper selection for liquid feedstocks i.e. naphtha. It can be used for cracking of liquid feedstocks at optimal ethylene yield while not exceeding the allowable maximum tube temperature.

NOMENCLATURE

C_{pj} : Heat capacity of j^{th} component, J/(kmol)(K)
d_t : Inner tube diameter (m)
F_j : Molecular flow rate j^{th} of component (kmol/s)
F_r : Friction factor
G : Total mass flux (kg/(m^2.s))
ΔH_i : Heat of reaction for i^{th} reaction
n_{ij} : Stoichiometric coefficient for j^{th} component in i^{th} reaction
M_m : Mean molecular weight (kg/kmol)
p_t : Total pressure (kPa)
$Q(z)$: Heat flux (W/m^2)
Re : Reynolds number
r_i : Reaction rate for i^{th} reaction
t : Time (h)
T : Temperature (K)
z : Reactor length coordinate (m)

REFERENCES

[1] Z. Renjun, “Fundamentals of Pyrolysis”, Lewis Pub (1993).
[2] B. P. Ennis, H. B. Boyd, R. Orriss, “Olefin manufacture via millisecond pyrolysis” Chemtech, November, 693-703, (1975)
[3] J. L. de. Blieck, A. G. Goossens, "Optimize Olefin Cracking Coils", Hydrocarbon Processing, March, 76-80, (1971)
[4] L. F. Albright, B. L. Crynes, “Industrial and Laboratory Pyrolysis”, ACS Symposium Series, (1976)
[5] P. M. Plehiers, G. F. Froment, “Reversed Split Coil improves ethylene yields”, Oil and Gas Journal-Technology, 41-49, (1987)
[6] A. K. Parameswaran, V. K. Sharma, D. Kunzru, "Modeling of Naphtah pyrolysis in swaged coils" The Canadian Journal of Chemical Engineering, 66, 957-963, (1988)
[7] G. J. Heynderickx, G. F. Froment, P. S. Broutin, C. R. Busson, J. E. Weill, “Modeling and simulation of a honeycomb Reactor for High-Severity Thermal cracking”, AICHE Journal, 37, 1354-1364, (1991)
[8] P. M. Plehiers, G. F. Froment, “The Uno-Quattro Coil: High Severities for Increased Ethylene selectivity”, Ind. Eng. Chem. Res., 30, 1081-1086, (1991)
[9] G. J. Heyderickx, G. F. Froment, G. H. Martin, “A shell and Tube. Pyrolysis Reactor for Olefin Production”, Ind. Eng. Chem. Res., 31, 2080-2087, (1992)
[10] R. Karimzadeh , M. Ghashgaee, "Design of a flexible pilot plant reactor for the steam cracking process" , Chem. Eng. Tech., 31, No.2, 278-286, (2008)
[11] R Karimzadeh, A. Hematian, M. R. Omidkhah, "The Effect Of Coil Configuration On Run Length Of Thermal Cracking Reactors", International Journal Of Chemical Reactor Engineering, Vol. 5, Article A118, (2007)
[12] J. Fernandez, “Factors Affecting Pyrolysis Heater selectivity”, A.I.Ch.E. Journal, Vol. 18, 18-31, (1972)
[13] J. E. Gwyn, “Universal yield models for the steam pyrolysis of hydrocarbons to Olefins”, Fuel Processing Technology, vol 701, 1.7, (2001)
[14] P.M. Plehiers, G. C. Reyniers, G. F. Froment, “Simulation of The Run Length of An Ethane Cracking Furnace”, Ind. Eng. Chem. Res., (Vol.29), 636-644, (1990)