CIENCIA, TECNOLOGÍA Y FUTURO

MATHEMATICAL MODEL FOR REFINERY FURNACES SIMULATION

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A mathematical model for simulation of refinery furnaces is proposed. It consists of two different sub-models, one for the process side and another for the flue gas side. The process side is appropriately modeled as a plug flow due to the high velocity of the fluid inside the tubes. The flue gas side is composed by a radiative chamber and a convective section both connected by a shield tube zone. Both models are connected by the tube surface temperature. As the flue gas side model uses this temperature as input data, the process side model recalculates this temperature. The procedure is executed until certain tolerance is achieved. This mathematical model has proved to be a useful tool for furnace analysis and simulation.

Keywords: *furnace, simulation, mathematical models, oil refinery.*

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En este trabajo se presenta el desarrollo de un modelo matemático para simulación de hornos de refinería, el cual consiste en dos sub-modelos diferenciados, uno para simular el lado proceso y otro para simular el gas de combustión. El lado proceso es apropiadamente modelado con un perfil de velocidad plano debido a la alta velocidad del fluido dentro de los tubos. El lado gas de combustión está compuesto por una cámara de radiación y una sección de convección, ambas unidas por una zona de tubos de choque. Los dos sub-modelos interactúan a través de la temperatura de superficie de los tubos, siendo esta un dato de entrada al sub-modelo del lado gas de combustión y es re-calculada por el sub-modelo del lado proceso. Este procedimiento es ejecutado en un ciclo iterativo hasta que cierta tolerancia es alcanzada. Este modelo matemático ha demostrado ser una herramienta muy útil para el análisis y simulación de hornos.

Palabras clave: *hornos, simulación, modelos matemáticos, refinería de petróleo.*

INTRODUCTION

Furnaces for refinery services are considered a key piece of equipment as they provide the necessary heat to carry out distillation processes, cracking reactions and some other processes. They consume considerable amounts of energy and their cost usually ranges between 10% and 30% of the total investment. Given its importance and its cost inside the refination chain it's evidently the significance of a mathematical model for furnaces that can be implemented with the process simulators.

Proper furnace simulation is necessary to analyze variations in regular process conditions such as changes in the feed charge, firing conditions, fuel composition, internal geometry, etc,. A simple mathematical model that takes into account these parameters is, therefore, a very useful simulation tool for refiners. Also considering the increasing necessity of processing heavier oils, this furnace simulator can predict the response of the equipment to changes in the design operating conditions.

Many researchers have modeled furnaces using defined components in the feed especially for thermal cracking processes such as Niaei, Towfighi, Sadrameli & Karimzadeh (2004), Detemmerman & Froment (1998), Joo, Lee, Lee & Park (2000), Heynderickx, Oprins & Marin (2001) but few researchers have used pseudo-components in the feed which is necessary to simulate petroleum crude. Maciel & Sugaya (2001) used 16 pseudo-components to simulate thermal cracking inside refinery furnaces, however, in this work reactions are not considered. Commercial furnace simulators such as FRNC and HTRI Xfh use a separate source to create and calculate properties of pseudo-components; the mathematical model proposed in this work does not need a separate source for that purpose.

DESCRIPTION OF THE MODEL

The process sub-model simulates in detail the behavior of the charge that flows through the furnace tubes. Physical properties, phase equilibrium, pressure drop and flow regimes are calculated for each integration step.

Petroleum feeds are characterized from the True Boiling Point (TBP) curve and the gravity curve. If the gravity curve is not available it can be extrapolated from the total gravity admitting the Watson characterization factor (K_W) constant through the whole curve. The charge is divided into pseudo-components, with the gravity and the normal boiling point known their properties can be calculated using several correlations available in the literature. In this model API TDB (1997) and Aladwani & Riazi (2005) recommendations are used.

The flue gas side sub-model calculates the radiative and convective heat fluxes tube by tube. Tube surface temperatures and fin tip temperatures are calculated using API Standard 530 (2001) and ESCOA (2002) methods respectively. With the flue gas temperatures along the furnace the draft profile can be calculated.

The furnace model proposed manages to calculate the main operational variables for refinery services by combining successfully a process model and a flue gas side model. Data entry for the charge is very simple, only a distillation curve and a gravity curve (or total gravity) are needed. Pure light ends and steam can also be integrated to the charge in order to analyze the process behavior. This capability to analyze different charges that are typical in refinery services makes the model proposed a valuable tool for process engineers who can easily predict operational variables for the daily operation.

The model internally calculates, for every integration step, physical properties and phase equilibrium for petroleum fractions; also calculates heat transfer coefficients, holdup, flow regimes and pressure drop in the case of two phase flow. Pressure drop is an important parameter since it exponentially increases with the vapor fraction in the charge. All this calculations make the performance of the model superior when compared to other commercial software for furnace simulation.

MATHEMATICAL MODEL FOR FURNACE SIMULATION

The mathematical model proposed for furnace simulation consists of two different sub-models connected by the tube surface temperature and a pre-processor for petroleum feed characterization:

- Petroleum feed characterization

- Flue gas side sub-model
- Process sub-model

PETROLEUM FEED CHARACTERIZATION

A TBP curve and a density value must be provided to the simulator. In a first step, the TBP is completed from 0 to 100% of distillated volume using an interpolation polynomial. Then the extrapolated curve is uniformly divided in 30 cuts and the NBP of each cut is calculated using a composite Simpson's rule (See Figure 1). To calculate the density of the 30 pseudo-components, the Watson characterization factor is admitted constant through the whole curve. With the NBP and the SPGR known, molecular weight, critical properties and acentric factor are easily calculated with the correlations recommended by Aladwani & Riazi (2005) and the API TDB (1997), see Table 2.

Flue gas side sub-model

The Hottel one-gas-zone radiation method (Hottel, 1974) has proven to be an appropriate and effective model to simulate radiation chambers when highly detailed radiative conditions are not needed. The flue gas side model uses the mentioned radiation method to calculate the average and maximum heat flux to the tubes and the flue gas temperature. Hottel (1974) proposed that the bridgewall temperature can be considered as the following function:

$$T_{bw} = f(Q_R, Q_F, T_F, d) \quad (1)$$

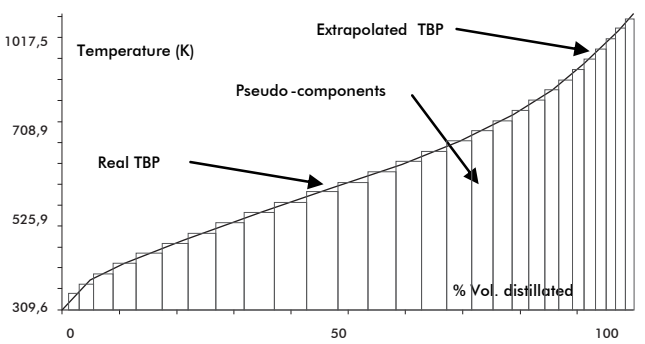

Figure 1. Characterization is pseudo-components for a medium petroleum blend (29.9°API)

Where Q_R is the heat supplied to the sink in the radiation chamber, Q_F is the supplied in fuel, T_F is the so called adiabatic pseudo-flame temperature and d is a dimensionless constant. Based on the analysis of furnace simulation results and industrial data the value of 1,2 is recommended instead of the value of 1,33 suggested by Hottel (1974).

A different model is used in the shield tube zone, a model that includes radiation and forced convection in bare tube bundles. The radiative heat flux to the shield tubes is calculated using the recommendations published by Stehlík, Kohoutek & Jebácek (1996). The tube bundle is replaced by an equivalent plane surface since the first and second row of tubes intercept approximately all the radiation coming from the radiation chamber.

The convective heat fluxes in the bare and extended surface tube zones are calculated with the methods listed in Table 1.

Table 1. Methods available to calculate convective heat fluxes

Bare tube bundles	• Grimson (1938) • Gnielinski, Zukauskas & Skrinska (1983) • Zukauskas (1972) • Khan *et al*. (2006)
Finned tube bundles	• Briggs & Young (1963) • Gnielinski *et al*. (1983) • Weierman (1976) • ESCOA (2002)
Studded tube bundles	• ESCOA (2002)

Pressure drop for the flue gas in convection sections is calculated using the ESCOA (2002) methods. API Standard 560 is used to calculate the draft profile.

Figure 2 illustrates how radiative and convective heat fluxes are calculated from tube surface temperatures, flue gas temperatures and draft profile are also calculated in the flue gas side sub-model. Tube surface temperatures are re-calculated in the process sub-model using API Standard 530 (2001) methods.

Process sub-model

The process side is appropriately modeled as a plug flow due to the high velocity of the fluid inside

the tubes (Maciel & Sugaya, 2001). Liquid or gaseous feeds can be used. Light oils vaporize as walk through the furnace tubes. In this case, two parallel plug flows (vapor and liquid) are modeled and several correlations regarding two-phase flow in tubes are used for a more realistic approach to the industrial process. For a detailed description of the process sub-model procedure see Diaz (2008) and Díaz, Wolf , Sugaya, Maciel & Costa (2008). The equations that describe the process sub-model are as follows:

Energy balance:

$$\left(G_L Cp_L + G_V Cp_V\right)\frac{dT}{dx} = \pi D Flux_{ave} \quad (2)$$

Pressure:

$$P = \left(\frac{\Delta P}{\Delta X}\right)dx + \left(\frac{\Delta P}{\Delta X}\right)_{el} \quad (3)$$

$$\left(\frac{\Delta P}{\Delta x}\right)_{el} = \left(h_L \rho_L + h_v \rho_v\right) X \sin\theta \quad (4)$$

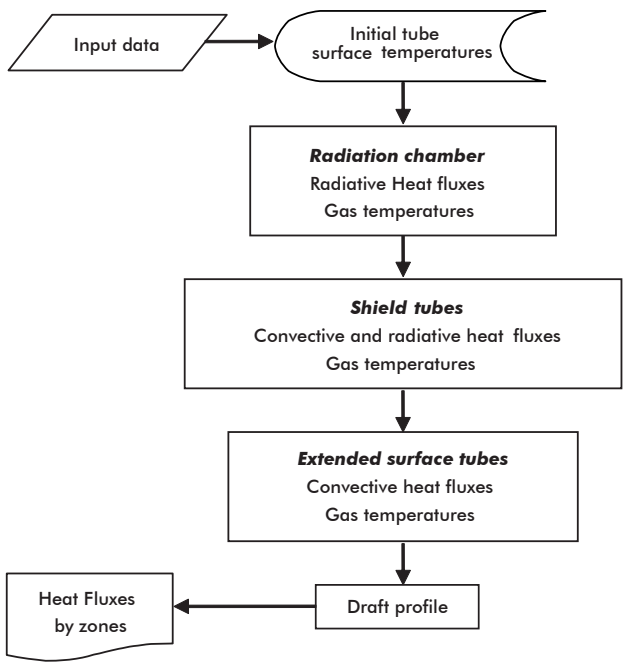

Figure 2. Calculation procedure for the flue gas side sub-model

In the case of vertical flow, the contribution of the static head to the pressure drop is calculated using *Equation 4*; however, this static head is not totally recovered since vaporization takes place as flow proceeds downward through the furnace.

Table 2. Correlations for pseudo-components properties

	Correlations
Molecular weight	Twu (1984) API TDB (1997)
Critical properties	Twu (1984) Riazi-Daubert (1987)
Acentric factor	Lee-Kesler (1975)

Table 3. Methods for physical properties

	Vapor phase	Liquid phase
Density	SRK	Hankinson-Thomson (1979)
Viscosity	TWU (1985) API TDB (1997) Kendall-Monroe (1917)	API TDB (1997) Stiel-Thodos (1961) Dean-Stiel (1965) Bromley-Wilke (1951)
Thermal conductivity	API TDB (1997)	API TDB (1997)
Heat Capacity	API TDB (1997)	API TDB (1997)

Phase equilibrium K-values are estimated using a modified Soave-Redlich-Kwong equation presented in the API TDB (1997); convergence is achieved by using a modified Rachford & Rice (1952) procedure. Since the equations of state are not appropriate to calculate the density of the liquid phase, different methods are used (See Table 3). To calculate the density of the vapor phase the compressibility factor found in the equilibrium calculations is used. Methods for physical properties are listed in Table 3:

If the equilibrium calculations determine the existence of a second phase, alternate procedures are activated to determine parameters for flow in two phases. Two-phase flow parameters are calculated using meth-

ods listed in Table 4. The whole procedure followed by the process sub-model is illustrated in Figure 3.

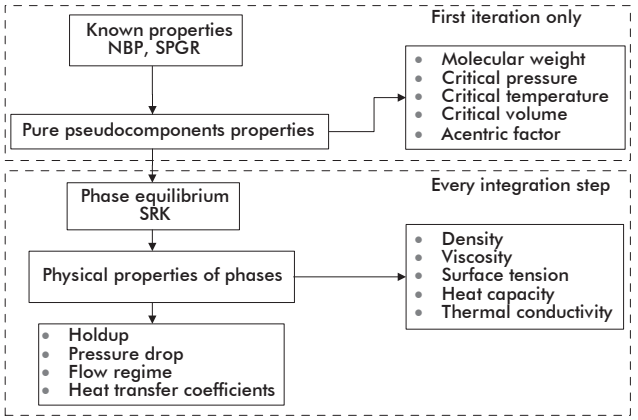

Figure 3. Procedure to calculate properties for the process sub-model

Table 4. Two-phase flow parameters

	Method
Holdup	Hughmark (1962) Chato, Yashar, Wilson, Kopke, Graham & Newell (2001) Rouhani & Axelsson (1970) Dix (Coddington & Macian, 2002) Awad & Muzychka (2005) Woldesemayat & Ghajar (2007)
Pressure drop	Beattie & Whalley (1982) Olujic (1985) García, García, García & Joseph (2007)
Heat transfer coefficient	Kim & Ghajar (2006) API 530 (2001)

CALCULATION PROCEDURE

The flue gas side sub-model uses the tube surface temperature as input data, so the calculations start with an assumed tube surface temperature. Heat fluxes are calculated and then used in the process sub-model to heat up the feed charge. Since tube surface temperatures are highly dependent on bulk process conditions, they are recalculated using the API RP 530 methods. Results are compared and if certain tolerance is not achieved, the procedure starts all over again with the updated temperatures. The whole procedure is illustrated in Figure 4.

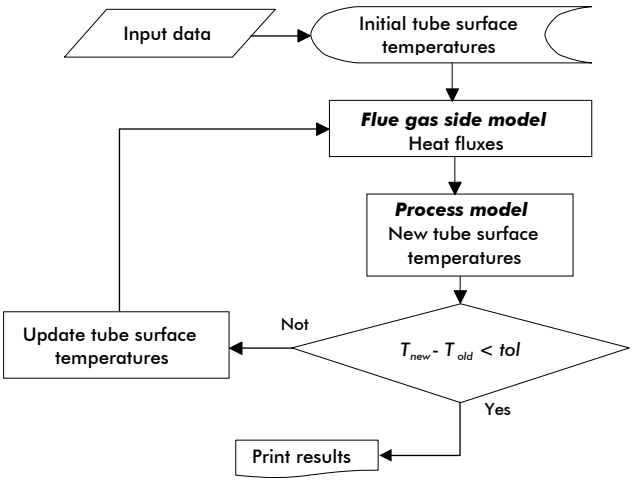

Figure 4. Calculation procedure for the entire model

APPLICATION OF THE MODEL

The mathematical model for furnace simulation proposed has been tested with refinery plant data from the Barrancabermeja Refinery (Barrancabermeja, Colombia). The furnaces are typical box type configuration with burners located in the floor and refractory-backed radiant tubes in a single row (See Figure 5). The feed charges are crude oils in the range of 21,3 to 44,9 API gravity. The results of the simulations are summarized in Table 5. where good agreement between the calculated and the measured data is observed.

CASE STUDY, FURNACE H2001

Results of the simulation of the furnace H2001 are analyzed to evaluate the furnace performance. Three different petroleum feeds are charged to the simulation as seen on Table 6. Tubes are numbered being 1 the entrance and 34 the exit of the feed.

Figures 6 and 7 show how the pressure drop increases exponentially with the vapor fraction. In the last four tubes of the furnace the tendency in the pressure drop changes because the tube diameter changes from 6 to 8 inches. It is also seen a higher pressure drop in the lighter feed since it produces more vapor.

Table 5. Measured vs. calculated data

Furnace		H-201	H-2001	H-253	H-150
API gravity of feed		44,9	41,8	21,3	44,9
T. feed out (K)	Calculated	643,71	652,04	638,71	599,82
	Measured	643,15	649,82	645,37	594,26
	% error	-0,09	-0,34	1,03	-0,93
P. feed out (KPa)	Calculated	668,58	267,86	536,07	509,38
	Measured	620,53	289,58	-	-
	% error	-7,74	7,50	-	-
T. flue gas radiation (K)	Calculated	1099,21	1215,32	938,65	1109,04
	Measured	1109,26	1205,37	922,04	1088,71
	% error	0,91	-0,83	-1,80	-1,87
T. flue gas convection (K)	Calculated	655,59	694,32	543,89	641,48
	Measured	641,48	655,37	551,48	612,59
	% error	-2,20	-5,94	1,38	-4,72

Shield tubes (Tubes 13-16) receive an important heat flux load and consequently show high tube surface temperature (See Figure 8). However the maximum surface temperature appears in the last tubes where the feed is warmer and closer to the peak heat flux in the flame. The change in diameter from 6 to 8 inches decreases the heat transfer coefficient from

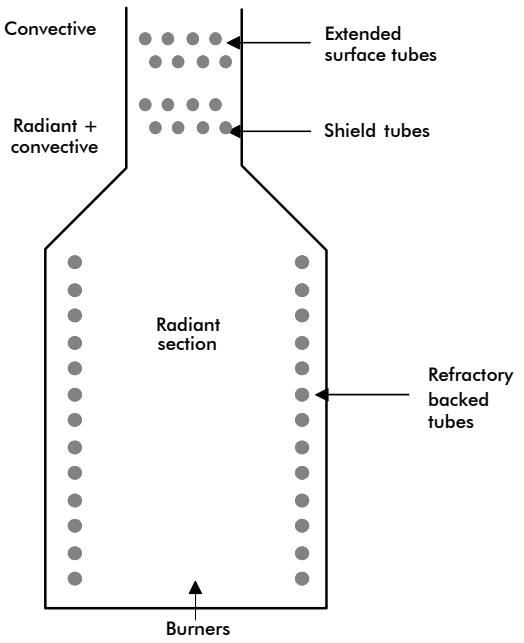

Figure 5. Typical box-type furnace configuration

Table 6. API gravity of feeds to furnace H2001

Feed	API Gravity
F1, medium petroleum blend	26,69
F2, light petroleum blend	36,91
F3, Cusiana crude	41,8

Table 7. Feed and flue gas temperatures

Temperature (K)	F1	F2	F3
T. feed out	653,11	659,58	661,44
T. flue gas out convection	705,99	705,28	704,59

1700 to 1000 W/m²K (See Figure 10.) and the peak heat flux (See Figure 9.) make the tube 31 indicate the higher tube surface temperature. The heavier feed (F1) has the lower heat capacity and removes less heat from the flue gases. It is seen on Table 7, that F1 leaves the furnace 8K cooler than F3.

The higher tube surface temperatures observed in the simulations with the heavier feeds are caused mainly by

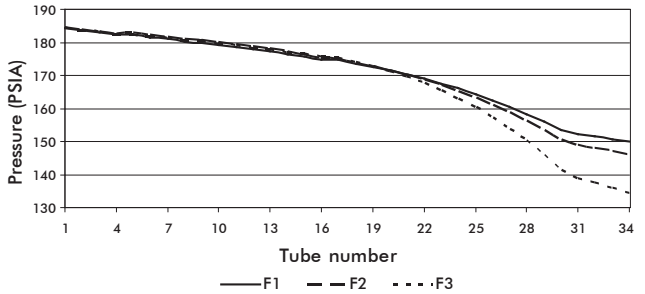

Figure 6. Pressure of feeds through the furnace H2001.

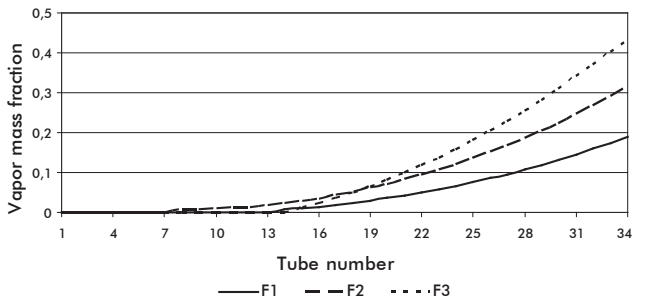

Figure 7. Vaporization of feeds through the furnace H2001

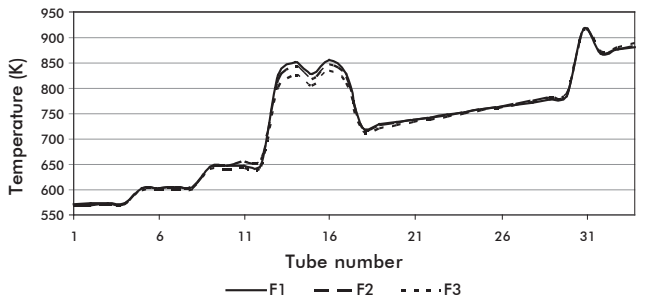

Figure 8. Maximum tube surface temperature, furnace H2001

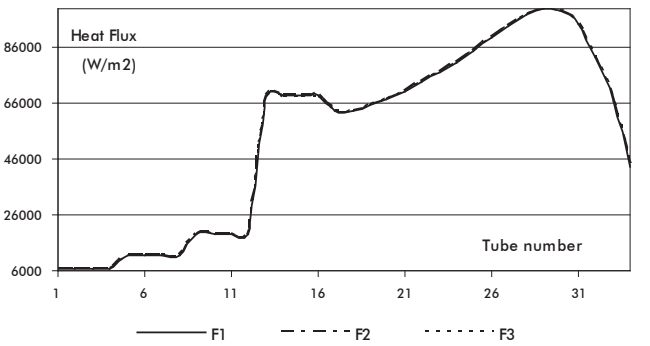

Figure 9. Maximum heat fluxes, furnace H2001

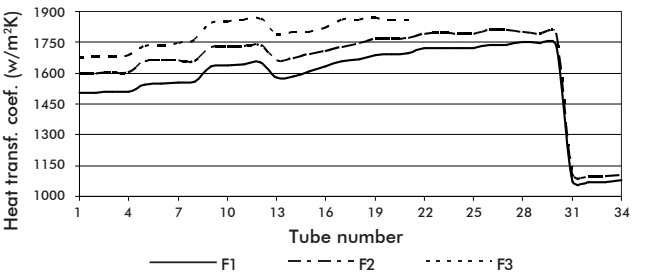

Figure 10. Heat transfer coefficients, furnace H2001

the lower heat transfer coefficient (HTC) (Figure 10) since the heat fluxes remain practically unchanged for the three feeds (Figure 9). The difference among the HTC's in the feeds tends to decrease at the last tubes of the furnace because of two opposite effects: Higher temperature increases the HTC while higher vaporization decreases the HTC. Therefore, the heavier feed is cooler, less vaporized and the HTC tends to increase. HTC's were calculated with the API Standard 530 (2001) methods.

CONCLUSIONS

- Results of the furnace simulations show a higher pressure drop when processing lighter petroleum feeds due to a higher vaporization and higher exit temperature caused by a higher heat capacity.

- Higher tube surface temperature is observed in the simulations with heavier feeds caused mainly by the lower heat transfer coefficient. Heavier feeds also remove less heat from the flue gases and, consequently, higher flue gas temperatures are observed in convection sections.

- The mathematical model for furnace simulation proposed in this work has proved to be a useful tool for analysis of process response to changes in the design operating conditions. Results clearly show how the furnace model appropriately fits the furnace refinery data. Different feeds, fuel gases and operating conditions can be studied providing a fast sight of the furnace performance.

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NOMENCLATURE

Cp	Heat capacity, KJ/Kg K
D	Diameter of the tube, m
G	Mass flow, Kg/s
h	Holdup
Flux	Heat flux, W/m^2
T	Temperature, K
X	Distance, m
ρ	Density, Kg/m^3
P	Pressure, KPa
NBP	Normal boiling point
SPGR	Specific gravity

SUBSCRIPTS

el	Elevation
L	Liquid phase
TP	Two phase
V	Vapor phase
Ave	Average
T	Total
BW	Bridge wall