AN ENERGY MODEL OF AN INDUSTRIAL NAPHTHA PYROLYSIS FURNACE

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A model of a pyrolysis furnace is described for calculating the energy consumption of the naphtha pyrolysis in industrial conditions. The values of the overall heat transfer coefficient and products of the overall heat transfer coefficient and heat-transfer area of exchangers were assessed by plant-scale experiments. The radiaton zone of the furnace was identified by a statistical method of the dependence of combustion gases temperature at the radiation zone outlet on the furnace load. The consumption of energy supplied by burning gas within the furnace radiation zone per 1 kilogram of naphtha fed into the furnace decreased with a decrease in both the naphtha flow rate and mass ratio of the diluting process steam to naphtha. When the furnace load dropped to 70% of the design capacity, the specific energy consumption in relation to a weight unit of naphtha decreased by approximately 10%.

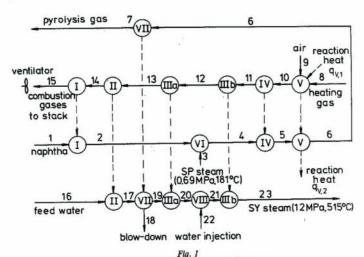
Introduction

A pyrolysis furnace was designed for a certain energy capacity, which could be varied only within certain limits determined by the design parameters of the furnace and by the function of its control elements. An ethylene unit producing ethylene, propylene and other unsaturated hydrocarbons usually comprises several (8–12) pyrolysis furnaces arranged parallelly.

The objective was to asses the energy characteristic of the furnace, i.e. the correlation between the furnace load and consumption of energy, and suggest a model of the pyrolysis furnace that would enable the effect of the furnace load upon energy consumption of the pyrolysis process to be predicted.

The pyrolysis furnace consisted of a system of heat exchangers. One practical solution of the exchangers network arrangement in a pyrolysis furnace is presented in Fig. 1.

Liquid naphtha (stream No. 1) was injected into the pyrolysis furnace, and



Heat exchangers network in pyrolysis furnace

1,2 - naphtha, 3 - SP steam, 4,5 - mixture of naphtha and SP steam, 6,7 - pyrolysis gas,

8 - heating gas, 9 - air, 10, 11, 12, 13, 14, 15 - combustion gases, 16, 17 - feed water, 18

- blow-down, 19, 20, 21, 23 - high-pressure steam, 22 - feed water injection

I, II, IIIa, IIIb, IV - heat exchangers in convection zone of pyrolysis furnace, V - radiation zone of pyrolysis furnace, VI - mixer of naphtha and SP steam, VII - transferline exchanger

after preheating and evaporating, it was mixed with diluting process steam (3). The mixture was heated to the reaction temperature in the radiation zone of the furnace (node V). The product of pyrolysis containing especially ethylene, propylene, and methane in diluting process steam (pyrolysis gas) was cooled in a waste-heat boiler (transferline exchanger, VII), wherein the high-pressure steam (SY) was generated.

Theoretical Section

A general enthalpy balance relationship can be written for each balance node designated by a circle in Fig. 1, i.e.:

$$\left| \sum_{(i)} (mh)_i - \sum_{(i)} (mh)_i \right| = \sum_{(k)} q_{k}, \tag{1}$$

where indices i and j denote the node inflow and outflow resp., k = i + j. Index k refers to heat fluxes incidental to a given node. Heat flow into the surroundings

is neglected in the balances and it is assumed that no changes in the accumulation of mass take place in the individual balance nodes.

For the material balance around each node it holds:

$$\left|\sum_{(i)} m_i - \sum_{(j)} m_j\right| = 0. \tag{2}$$

If no purely thermal flow leads into or out of a node (denoted by a dashed

line in Fig. 1), $\sum_{(k)} q_k = 0$.

Specific enthalpy of liquid streams is calculated with the aid of model mean specific heats c_p of the media and temperature t of the media:

$$h = c_p t. (3)$$

For saturated vapour at the boiling point t, specific enthalpy of the gas phase is given by:

$$h = c_p t + h_{ev} \tag{4}$$

Specific enthalpy of superheated vapour or gas is calculated similarly to the liquid phase according to Equation (3). Specific enthalpies of air and heating gas at the inlet of the node V are considered to be conformable and negligibly small, i.e. $h_8 = h_9 = 0$ (numerical indices of symbols here and henceforth are consistent with those denoting the individual streams in Fig. 1). In addition to the balance relationships (1) and (2) a general equation for heat transfer can be written for each exchanger:

$$\sum_{(k)} q_k = Q = \varepsilon \cdot k \cdot F \Delta t_{1 \cdot m}. \tag{5}$$

$$\Delta t_{1.m.} = (t_a' - t_b' - t_a'' + t_b'')/(\ln(t_a' - t_b') - \ln(t_a'' - t_b''))$$
(6)

On the assumption that the mean specific heats of the media, between which transfer of heat occurs, are roughly constant, the overall heat transfer coefficient can be regarded as a function of the rate of flow w and composition of the medium X:

$$k = k(w, X). (7)$$

The mechanism of heat transfer in the pyrolysis furnace radiation zone V is a very complex one (see e.g. references [5], [6] and [1]). To simplify the procedure, let us confine ourselves to an empirical model of the following type:

$$t_{10} = f(m_1, m_3, c_{02}),$$
 (8)

whose parameters are assessed statistically from data obtained by measurements. Such a simplification, however, is at the cost of restricting the applicability of thus identified model to the conditions under which it was obtained. When the relationship (8) is obtained for constant temperatures t_1 , t_3 , t_{16} and t_{23} , then the application of the pyrolysis furnace model is adequate exclusively for these temperatures. In practical terms, the constancy of these temperatures is the condition that is necessary for a stable regime of the pyrolysis process, which warrants the creation of the model under these marginal conditions.

Let us define the specific energy consumption of the pyrolysis by:

$$A = q_{V,1}/(1000 m_1) \tag{9}$$

i.e. as the ratio of amounts of heat liberated by burning the heating gas $(q_{V,1})$ to the rate of naphtha inlet into the pyrolysis furnace (m_1) .

In a real pyrolysis furnace the heat losses are caused by:

a) combustion gases to stack (flue loss)

b) losses of heat from the furnace surface to the environment

c) inlet of secondary air through leaks in the convection zone of the furnace. Of these three types of heat losses, the flue loss represents a major part (about 70%), those due to heat removal from the furnace surface (caused by nonideal insulation) being roughly 25%. Neglecting the heat losses brought about by the inlet of secondary air through leaks, defining the flue loss as:

$$q_s = m_{15}c_0(t_{15} - t_9) (10)$$

and denoting the flow of heat removed from the furnace surface as q_1 , then the furnace thermal efficiency can be written:

$$\eta = 1 - (q_s + q_1)/q_{V,1} \tag{11}$$

Thus the furnace thermal efficiency is understood to mean the degree of utilization of heat supplied to the furnace by the burning of the heating gas. The heat loss by removal from the furnace surface as given by the project for the design capacity is 2.5% of the heat supplied by burning the heating gas. Hence, the heat flow $(q_{v,1})_{id}$, calculated on the assumption of zero losses to the environment (see Eq. (1)), is corrected by:

$$(q_{V,1})_{real} = (q_{V,1})_{id}/.975$$
 (12)

Practical application of the above relationships is discussed in the following.

Experimental

An important condition for the consistency of data obtained on the pyrolysis furnace at the different furnace loads (varying flow rates of naphtha and SP steam) is to maintain a constant excess of air for burning the heating gas. Therefore, the concentration of oxygen in combustion gases, from which the excess of air can be assessed, must be roughly constant. In the case of a low furnace load – at 60–70% of the design capacity – it was necessary to fully close the openings for air intake to the burners, so that air was sucked in only through leaks and it was no longer possible to control the amount in this way. During the measurements the oxygen concentration in combustion gases mostly fluctuated between 2–3 vol. %.

The experiments were carried out at the constant temperature of pyrolysis gas leaving the radiation zone V, adjusted at $t=829^{\circ}$ C, naphtha feed rate was changed in the range 19,000–26,000 kg per hour, m_3/m_1 ratio was set in the range 0.5–0.8.

The flow rate of combustion gases to the stack was calculated from enthalpy balances of exchangers I, II, IIIa, IIIb, IV and nodes VI and VIII (see Fig. I). The blow-down outlet from the waste-heat boiler was not measured and was regarded as zero in the calculation. Superheated high-pressure steam produced in the pyrolysis furnace was adjusted on p = 12 MPa, $t = 515^{\circ}$ C.

It always took 3-4 hours before a state of dynamic equilibrium of the furnace operation was adjusted, steady conditions were then maintained for roughly

60-90 minutes.

The data for calculating the overall heat transfer coefficient for the waste-heat boiler were measured on a clean and fouled heat-transfer area to assess the

influence of fouling on the overall heat transfer coefficient.

When assessing the overall heat-transfer coefficient for the furnace convection zone it was necessary to consider the real arrangement of the measuring sensors in the convection zone and the fact that the flow rate of the combustion gases passing to the stack was not measured. Some temperatures important for the calculation of Δt_1 . on an exchanger could not be measured directly and had to be calculated from the enthalpy balance of the furnace convection zone. The measured input data balancing the convection zone of the furnace were the values of m_1 , m_3 , m_{22} , m_{23} , t_1 , t_3 , t_{10} , t_{11} , t_{14} , t_{15} , t_{16} , t_{17} , and t_{19} . It was assumed that $m_{18} = 0$ and $t_{20} = 430^{\circ}$ C, i.e. that the thermal capacity of the exchangers IIIa and IIIb was roughly the same. The temperature t_{19} was assessed by measuring the pressure in the waste-heat boiler. The values of temperatures t_2 , t_4 , t_{12} and t_{13} and of the combustion gases flow rate m_{10} were calculated from the balance.

Results and Discussion

A standard programme for the WANG 2200 computer was adopted for the treatment of the measured and calculated data by multiple linear regression [8]. With each relationship obtained by regression, the programme also yielded the value of the correlation coefficient r, which is a measure of accuracy of that relationship. The system of balance equations, including the pyrolysis furnace model, were solved with the aid of the programme KOMAT [2], [3], enabling the statistical adjustment (reconciliation) of redundant measurements and the calculation of unmeasured quantities (i.e. parameters of the mathematical model) to be solved. The calculation was based on the Newton-Rawson method for solving a system of equations. In addition, the propagation of errors was analyzed and the accuracy of the calculated quantities was determined [4]. Using multiple linear regression a correlation was found between the parameter A and naphtha, SP steam feed rates (the rates m_1 and m_3 are uncorrelated with the correlation coefficient r = 0.06) from experimental data:

Let the production of SY steam in the pyrolysis furnace be characterized by the ratio:

$$B = m_{23}/m_8 (14)$$

i.e. by the production of SY steam as related to a weight unit of the heating gas supplied to the furnace for burning. Based on the experimental data the dependence of the parameter B on m_1 , m_3 can be written:

$$B = b_1 - b_2 m_1 + b_3 m_3 / m_1 \tag{15}$$

r = 0.6319.

For modelling the operation of the pyrolysis furnace it was necessary to attempt to find, on the basis of experimental data, relationships for the dependence of the overall heat transfer coefficient of the exchangers on the furnace load.

It was found that the dependence of the overall heat transfer coefficient of the waste-heat boiler is:

1. Clean heat-transfer area

$$k = k_1 + k_2 m_1 + k_3 m_3 / m_1$$

$$r = 0.995$$
(16)

2. Fouled heat-transfer area

$$k = 1.9k_1 + 0.47k_2m_1 + 0.78k_3m_3/m_1$$

 $r = 0.996.$ (17)

In the case of the clean heat-transfer area the effect of the changes in the flow rates of both naphtha and process steam on k was more pronounced.

It was not possible, however, to find such relationships for the product εkF of all exchangers in the pyrolysis furnace convection zone, whose accuracy would be comparable with that of Eq. (16) and (17). Presumably the reason is due to the lower accuracy of calculating the unmeasured temperatures in the furnace convection zone from its thermal balance. When using, in the relationships for heat transfer in the convection zone exchangers, those values of the product εkF correspond to an average furnace load during the measurement, an error is introduced to the calculation of temperatures in the convection zone, particularly in the cases of marginal values of the furnace load (minimum and maximum load). At the minimum load of the pyrolysis furnace an empirical modification of the product εkF depending on the flow rate of combustion gases, applied only to the exchanger I (see Fig.~1), proved correct in the form:

$$\varepsilon kF = (m_{10}/\bar{m}_{10})^{3.4} \, \overline{\varepsilon k}F.$$
 (18)

The symbols marked with bars stand for mean values, while those unmarked correspond to a given flow rate of flue gases m_{10} . In this way the effect of the pyrolysis furnace load on the heat transfer in the convection zone was corrected: the mean values of product εkF were used for exchangers II, IIIa, IIIb, IV in the model. Multiple linear regression was also used to obtain from the experi-

mental data the relationship for the combustion gases temperature at the outlet from the furnace radiaton zone:

$$t_{10} = t_{10}(m_1, m_3/m_1, c_{02})$$

 $r = 0.9883$ (19)

It was found that a considerable deposition of coke in the pyrolysis furnace did not occur during the measurement. Thus all the data necessary for modelling the operation of the pyrolysis furnace were acquired.

Model Input and Output Data

 $Table\ 1$ lists the input quantities and those calculated with the aid of the pyrolysis furnace model. The determination of the oxygen concentration in combustion gases bears the largest relative error.

Table 1

List of input and output variables in the pyrolysis furnace model

Input*	Output*
temperatures t ₁	t ₂
13	t ₄
t ₆	15
to	t ₇
t ₁₆ t ₂₃	110
	. t ₁₁
	t ₁₃
	t14
	t15
	t ₁₇
	t18
	t19
	t ₂₀
mass flows m ₁	m ₈
<i>m</i> ₃	m ₁₀
	m ₁₆
	m ₂₂
pressure p_{19} concentration c_{02}	

^{*)} For indexing see Fig. 1

A conventional process analyzer was used for the measurement of the oxygen concentration in combustion gases. It was also possible to calculate the concentration of oxygen in combustion gases from the known composition of heating gas ($\mathrm{CH_4(97)}$ and $\mathrm{H_2(3)\%}$ by weight) and from the flow rate of the

combustion gases as assessed from the balance of the pyrolysis furnace convection zone. The measured concentrations of oxygen in combustion gases and those calculated from measured flow rates of heating gas and the combustion gases are shown for comparison in *Table 2*. It can be observed, particularly in the concentration range of oxygen in combustion gases at around 2 vol. %, that the value measured by the process analyzer exhibited an error that was as high as 100% relative. However, the mean measured value of oxygen concentration 2.81% vol., differing only by about 5% relative from the average of calculated values (2.97 vol. %), was therefore used in all the examples of model calculations.

The most important parameter for evaluating the energy consumption of the pyrolysis process in a pyrolysis furnace is undoubtedly the consumption of heating gas (m_8) and production of SY steam (m_{23}) . To demonstrate the adequacy of the model relationships, Table III compares the measured flow rates of heating gas and rates of SY steam production with the corresponding values calculated by the model (marked by an asterisk). The relative deviation between the measured and calculated values exceeded 3% relative only in example 1 (feed rate of heating gas m_8) and example 9 (flow rate of SY steam m_{23}).

With the programme KOMAT it was found that the accuracy of determination of the naphtha feed rate m_1 , temperature of pyrolysis t_6 and of the heating gas heat content $q_{V,1}$ are the decisive factors concerning the accuracy of all the calculated quantities of the model. On the assumption that the accuracy of all the input data of the pyrolysis furnace model according to Table 1 is $\pm 2\%$

Table 2

Measured and calculated (')
concentrations of oxygen in combustion
gases

No. 1	°o₂ % vol.	¢′₀₂ % vol.
1	1.15	2.11
`. 2	1.75	2.57
	2.67	3.23
3 4 5	2.84	3.28
5	3.24	3.42
. 6	3.31	2.95
7	3.04	3.03
8	3.28	3.21
9	3.80	3.51
10	1.92	2.74
11	3.17	3.13
12	2.72	2.59
13	3.17	2.85
14	3.24	2.98
Mean concentration	2.81	2.97

Table 3

Consumption of heating gas m₈ and production of SY steam m₂₃ - comparison of measured values and values calculated from the pyrolysis furnace model (*)

No. I	$\frac{m_0^*}{m_0}$	$\frac{m_{23}^*}{m_{23}}$	
1	0.942	0.984	
2	0.988	0.986	
3	1.002	1.009	
4	1.014	0.999	
5	1.008	0.977	
6	0.996	0.997	
7	1.005	0.983	
8	1.011	0.973	
9	1.008	0.962	
10	0.985	0.975	
11	0.995	0.969	
12	0.982	0.978	
13	0.993	0.975	
14	0.996	0.975	

relative, then the accuracy of all the calculated quantities of the model according to $Table\ I$ was better than $\pm 5\%$ relative except for the temperatures t_2 (10%), t_{21} (8%) and feed water injection rate m_{22} (20%).

On the basis of these results, it can be stated that the adopted suppositions are suitable for practical application to the pyrolysis furnaces of an ethylene unit. The model calculations yielded corrected values of consumption of heat per 1 kg of naphtha (A^*) and relative production of SY steam (B^*) , for which the following relationships were obtained by multiple linear regression:

$$A^* = 1.92a_1 + 0.64a_2m_1 + 0.84a_3m_3/m_1$$

 $r = 0.998$ (20)

$$B^* = 0.73b_1 + 0.65b_2m_1 + 9.96b_3m_3/m_1$$

 $r = 0.984$. (21)

A comparison of Eq. (13) and (20) as obtained by the regression of data measured and calculated by the model, resp., shows that the effect of both the naphtha feed rate and the ratio m_3/m_1 on the specific energy consumption as defined by the parameter A is smaller in the case of Eq. (20). Eq. (20) can be considered more reliable since the values calculated by the model are reconciled as well.

If a multiple linear regression is used for the experimental data with the exception of measuring No. 1 in Tab. 3., the dependence of the parameter A on m_1 , m_3 is:

$$A = 1.59a_1 + 0.79a_2m_1 + 0.86a_3m_3/m_1$$
(22)

It can be observed that the parameters in Eqs. (22) and (20) are more similar than the parameters in Eqs. (20) and (13). Hence, this supports the conclusion that the error of measurement can influence the identification of parameters from the experimental data. Eqs. (21) and (15) can be compared in the same way.

Eqs. (20) and (21) were used to calculate the energy consumption for the pyrolysis of naphtha and the relative rate of SY steam production at constant

ratio $m_3/m_1 = 0.7$.

The results of the calculation showing that reducing the feed rate of naphtha from 27,000 to 18,000 kg h⁻¹ brings about a decrease in energy consumption of the pyrolysis by 11.3% are presented in *Table 4*. Viewing the pyrolysis furnace

Table 4

Effect of naphtha feed rate (m_1) on consumption of energy of the pyrolysis process (A^*) and on relative rate of SY steam generation (B^*) at constant ratio $m_1/m_1 = 0.7$

A*/A****	B*/B*
0.887	0.971
0.912	0.977
0.937	0.984
0.962	0.99
1.000	1.000
	0.887 0.912 0.937 0.962

operation purely from the stand-point of energy consumption it can be concluded that it is advantageous to operate it at a lower load compared to the design capacity. A lower furnace load means, however, that the retention time of the reaction mixture in the furnace pyrolysis zone at high temperatures will be longer, which will show itself [7] in the pyrolysis process yield or in the content of the desired pyrolysis products (ethylene, and propylene) in the pyrolysis gas. During the experiments carried out at a roughly constant pyrolysis temperature t_6 , the results of gas chromatography analyzers of pyrolysis gas indicated that the concentrations of both ethylene and propylene varied within 1% relative, which is less than the error of chromatography.

It seems, therefore, that the energy saving advantage in the process of pyrolysis as obtained at lower loads of the pyrolysis furnaces (lower values of the A parameter) are not considerably affected by changes in the pyrolysis products yields. This conclusion can be used especially when the total capacity of the

ethylene unit is not fully utilized.

Conclusion

The creation of a pyrolysis furnace energy model is described, based on measurements carried out under operational conditions. In the model, the calculated heat-transfer coefficients for the individual exchangers (or the product ekF, as the case may be) and their dependence on the furnace load (i.e. on the flow rate and/or composition of the medium flowing through the respective exchanger) are used as the basis. The effect of the other process variables on the temperature of combustion gases leaving the furnace radiation zone was evaluated with the aid of statistical methods. A comparison showed that in most cases the difference between the measured values of the flow rates of the heating gas and produced SY steam and those calculated from the model was less than 3% relative. The model is suitable for assessing the effect of the rate of feeding naphtha and SP steam to the pyrolysis furnace on the consumption of energy for pyrolysis, and to determine the fouling effect of the waste-heat boiler heat-transfer areas on the pyrolysis furnace performance. It can also be used for predicting the heating gas consumption and production of SY steam over a longer period of the furnace operation. It is convenient to determine the model parameters (particularly the products ekF) and the relationship for the temperature of combustion gases at the furnace radiation zone outlet separately for each furnace of the ethylene unit.

SYMBOLS

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A
       energy consumption of the pyrolysis process per unit of naphtha feed, MJ kg-1
a<sub>1,2,3</sub> regression coefficients, 1
       rate of steam production in the pyrolysis furnace per weight unit of heating gas, kg kg-1
b<sub>1,2,3</sub> regression coefficients, 1
C.F
       mean specific heat, kJ kg-1 K-1
       heat-transfer area, m2
       specific enthalpy, kJ kg-1
       specific heat of vaporization, kJ kg-1
       overall heat-transfer coefficient, kJ h-1 m-2 K-1
k<sub>1,2,3</sub> regression coefficient, 1
       mass flow rate, kg h-1
p
       pressure, MPa
9.0
       heat flow rate, kJ h-1
       flue loss, kJ h-1
       fictition heat flow rate as given by burning heating gas, kJ h-1
9v. 1
       fictition heat flow rate as given by the pyrolysis endothermic reaction, kJ h-1
qv 2
       correlation coefficient, 1
SP
       process steam, 0.69 MPa
SY
       12 MPa steam
       temperature, °C
di, logarithmic mean of temperature difference, 1
      symbol of flow rate
W.
X
      medium components vector
      correction factor of At1.m, 1
E
      thermal efficiency of pyrolysis furnace. 1
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Subscripts

a, b denotation of media in heat exchanger

i, j, k denotation of stream in balance diagram

Superscripts

denotation of final temperatures of media at heat exchanger inlet and outlet

* values calculated with the aid of pyrolysis furnace model

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DYNAMIC OPTIMIZATION IN MODEL BASED PREDICTIVE COMPUTER CONTROL: MATHEMATICAL AND CONCEPTUAL BACKGROUND

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Practically all cases of model based optimal predictive control leads one to a constrained optimization of a dynamical system. In continuous systems, the execution of this dynamic optimization requires a two-point boundary value problem to be solved, but it is shown that this problem disappears for discrete recursive difference equation models. The optimization becomes a straight forward constrained optimization from one sampling step to the next, where the soft and hard constraints are encountered now and in the future prediction horizon.

For model based predictive optimal control it is also shown that the recursive difference equation modeling of the process dynamics in discrete time form is the most useful, flexible and direct type of plant modeling. In linear systems, this approach leads to the ARMA model which is the most applicable form of a general empirical process model. The recursive nature of the process model is indeed carried over to the calculation of the sensitivities of the output to the process disturbances and control manipulations.

By way of example, it is shown that optimal predictive control may be applied to the moves of the manipulated variables directly, but also to the parameters of an a priori chosen control algorithm. The model based optimal predictive control becomes cascaded to the original control, just as in traditional cascade control. The PID algorithm was chosen to be the algorithm for the illustration of this particular type of optimal control.

The advantages of models based on recursive nonlinear difference equations are exposed in full when this principle is applied to the optimal setting of the parameters in a PID algorithm from one time step to the next. This illustration uncovers a general concept which may be utilized in the optimization of controller parameters in a wider context.

Keywords: Optimal Control, Model Based Predictive Control, Discrete Time, Modeling, Stability, Constrained Optimization, Parameter Control, PID Control.