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A PRELIMINARY STUDY OF THE DYNAMIC BEHAVIOUR OF THERMAL CRACKING PROCESSES FOR IMPLEMENTING ADVANCED CONTROL AND OPTIMIZATION

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ABSTRACT. Nowadays industrial chemical processes must operate at maximum efficiency and one of the ways to save energy and still obtain high quality products is by using advanced process control.

The coking furnace is the heart of any thermal cracking installation and the coil outlet temperature influences directly the quality of the end products and the coke deposits on the walls. The major concern is to maintain a constant gas outlet temperature in order to decrease the deposits and implicitly maintain the tube metal temperature and the pressure, constant. Advanced control is a good alternative solution to obtain the desired product yield and still maintain the safety conditions, without changing the system's configuration or replacing the existent components with new ones.

A mathematical model of a thermal cracking coil was developed, based on free radical mechanism and some basic assumptions. In order to predict the coil's behaviour (temperature, product yields and pressure), a simulator for the dynamic process was used.

Keywords: *thermal cracking, coking plant, ethylene furnace, advanced control, optimization, real-time control systems.*

INTRODUCTION

Process models are usually used for the research of an operating strategy of a plant in an optimal mode, advanced process control systems (APC), for the training of operators and for a number of other studies (influences of the operating parameters and processing problems) that can be performed on the model in order to protect the real process from test disturbances. Additionally, a lot of control concepts are based on using a model of the process as part of the controller. This model based controllers' performance depend on the validity of the model. Several thermal cracking

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reactor models can be found in literature ([3], [5], [6], [10], [11] and others) and a full simulation of the reactor and the radiant box is provided by [7]. Some models for a delayed Coker are presented in the chemical engineering thesis of Albers [1].

According to Herink and Belohlav [4], the rigorous models are far more complex than models obtained using artificial neural networks, for example, and could be used for the design of pyrolysis furnaces, fundamental chemical engineering calculations and the prediction of the lighter feedstock cracking yields (ethane or naphtha).

It is not very difficult to implement a dynamic model described by differential equations, using specialized software, but to implement it using a real time control environment, such as Emerson's DeltaV Control Studio, it is a real challenge, because of the need to simplify its conditions and also obtain a valid model.

The purpose of this study is to design an optimal control system for the output variables of the simulated system. The starting point was the development of the dynamic model of an infinitesimal volume of pipe, Fig. 1, using the fundamental equilibrium equations: material balance, thermal balance and momentum balance. The method adopted for solving these equations is the Euler's Method for differential equations, even if efficiency loss may occur in comparison with results obtained applying other, more sophisticated methods, such as Runge-Kutta.

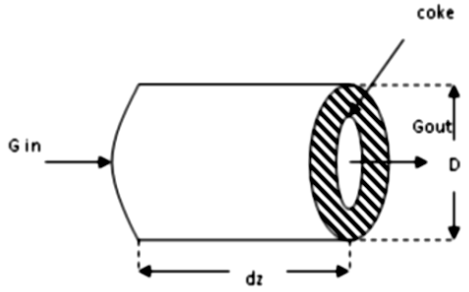

Figure 1. Differential element

The feed-forward control, the state estimators based control and the predictive model control (MPC) are all advanced control techniques that usually need a reliable model of a process. MPC is a method that uses the model of the process to calculate manipulated variable changes from the future predictions of the controlled variables, on the basis of a cost function as an objective which needs to be minimized.

THERMAL CRACKING FURNACES AND PROCESSES

The most frequently used thermal cracking furnaces in today's industry are the cracking furnace from the petrochemical field (cracking of naphtha, ethane, etc.) and the furnace from the coking plant.

The pyrolysis furnaces can be used for any type of raw material; the only implied condition being the boiling point that must be under 600^0 C. The furnace represents the centre of the cracking plant and the consumption of energy is also concentrated in this area. The desired products from this reaction are the light olefins, such as: ethylene, propylene and butadiene.

The furnace, described in this case, is similar to an ordinary fired heater but there are some differences concerning: the added dilution steam, the production of coke layers on the tubes, the testing of the effluent with a GC (gas chromatograph) and the effluent's routing to the TLE's (transfer line exchangers), for generating high pressure steam.

Ethylene is industrially obtained through thermal cracking of hydrocarbons. In order to obtain a larger amount of ethylene and decrease the energy and material loss, the process parameters must be held between certain limits, as follows [10]:

- Residence time inside the coil, between 0.08 and 0.25 [s] – as short as possible. In order to reduce the residence time, tubes' diameters are reduced; the fabrication materials are improved and the burners tend to be much more efficient.
- Dilution steam, measured as the ratio S/Hc (steam/hydrocarbon), between 0.3 and 0.6 – high quantity of steam. The dilution steam is introduced in the process to reduce the coke production and to decrease the gas pressure (minimize the undesired secondary reactions).
- Reaction pressure, between 175 and 240 kPa – as low as possible. Coil output pressure is indirectly controlled by the aspiration pressure of the gas compressor, placed downstream.
- Reaction temperature – at least 900^oC – as high as possible. The pyrolysis is an endothermic reaction and high temperature generates smaller hydrocarbons molecules. Lower temperature favors the production of coke and shortens the tubes' life.

CASE STUDY

The free radicals mechanism represents a universal accepted description of the hydrocarbons pyrolysis. Once the conversion and the olefin concentration increases, the secondary reactions become more frequent. A small segment of pipe, of infinitesimal volume is represented in Fig. 1.

According to the free radicals mechanism [8], the considered reactions are:

Initiation: $C_2H_6 \xrightarrow{k_1} CH_3\cdot + CH_3\cdot$ (1)

Propagation: $CH_3\cdot + C_2H_6 \xrightarrow{k_2} CH_4 + C_2H_5\cdot$ (2)

$C_2H_5\cdot \xrightarrow{k_3} C_2H_4 + H\cdot$ (3)

$C_2H_6 + H\cdot \xrightarrow{k_4} H_2 + C_2H_5\cdot$ (4)

Interruption: $H\cdot + C_2H_5\cdot \xrightarrow{k_5} C_2H_6$ (5)

$C_2H_5\cdot + C_2H_5\cdot \xrightarrow{k_6} C_4H_{10}$ (6)

$C_2H_5\cdot + CH_3\cdot \xrightarrow{k_7} C_3H_8$ (7)

$CH_3\cdot + CH_3\cdot \xrightarrow{k_8} C_2H_6$ (8)

$CH_3\cdot + H\cdot \xrightarrow{k_9} CH_4$ (9)

Dynamic model of the thermal cracking process

The mathematical description of a one-dimensional plug-flow reactor tube is presented, with the following assumptions: laminar flow regime, ideal gas behavior and inert steam used as diluent.

- Mass balance for component *j*:

$$dw_j/dt = -v\cdot(w_j - w_{j_0})/dz\cdot\sum_i r_i \times S(i,j) \quad (10)$$

Where r_i is the i-th reaction rate and it evolves with temperature according to an Arrhenius equation:

$$r_i = A_i\cdot e^{-E_{i_j}/R\cdot T} \quad (11)$$

- Energy balance

$$dT_g/dt = v\cdot(T_g - T_{g\_0})/dz - \frac{[(T_g - T_w)\cdot A\cdot k_{T_g} + \sum_i r_i H_i + \varphi_i(T_0^0 - T_g^0)]}{\rho\cdot C_p} \quad (12)$$

$$dT_w/dt = A\cdot k_t\cdot(T_g - T_w)/(\rho\cdot C_p) \quad (13)$$

- Momentum balance:

$$dP/dt = d\rho/dt\cdot\frac{G_1^2}{(\rho^2\cdot g)}\cdot\left(\frac{2f}{D} - 1\right) \quad (14)$$

For the entire equation system (10), (12), (13) and (14), we have considered as outlet variables:

- w_j (j=1, 9) – components mass fraction for: ethane, methyl radical, methane, ethyl radical, ethylene, hydrogen radical, hydrogen, propane and butane
- Temperatures – T_g, T_W
- Density - ρ
- Pressure – P

The considered inlet variables are:

- Ethane concentration – [C_2H_6];
- Fluid velocity inside the tube- v ($^{dz}/_{dt}$)

Implementation and simulation

The DeltaV system is a part of Plant Web architecture that uses predictive intelligence to improve plant performance. Besides traditional PID control, DeltaV advanced control can be configured to provide model predictive control, neural networks, fuzzy logic and different types of analysis. These digital control technologies can reduce variance in the process, reduce start-up time and improve the performance of processes.

DeltaV Control Studio has an extremely limited ability to solve systems of complex algebraic and differential equations. The idea is to simplify the model to the level it can be represented in Control Studio. Consequently, the simplest way to solve a differential equation is using Euler's integration method.

The differential equations need to be modified in order to be implemented using DeltaV. For a simple equation: $dx/dt = 1 - x$, with the initial conditions $x(0) = 0\ at\ t = 0$ and a sampling time Δt, Euler method can be implemented in Control Studio using the structure presented in Fig. 2 and the equation is modified as: $dx/dt = 1/\tau \cdot (u - x)$.

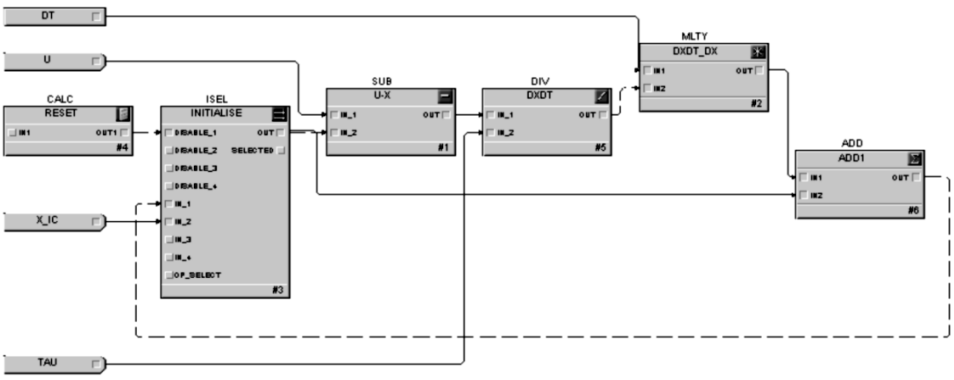

Figure 2. Euler's method DeltaV implementation, for a simple equation

If the equations are more complex, for example:

$$\begin{cases} dx_1/dt = 1/\tau \cdot (u_1 - x_1) - R \\ dx_2/dt = 1/\tau \cdot (u_2 - x_2) + R \end{cases} \quad (15)$$

where:

$$\begin{cases} R = k_f x_1 - k_r x_2 \\ x_3 = x_{3(0)} - x_1 - x_2 \end{cases} \quad (16)$$

and the initial conditions are:

$$\begin{cases} x_{1(0)} = x_1(t=0) = 0 \\ x_{2(0)} = x_2(t=0) = 0 \\ x_{3(0)} = x_3(t=0) = 1 \end{cases} \quad (17)$$

then the implementation has the structure presented in Fig. 3.

The equations are solved using simple arithmetic blocks: multiply, add, divide and subtract. We also needed to use a reset block to restart the integration process. The DT parameter is equal to the scanning rate of the module and has an implicit value of 10.

As a result, the structure used for implementing the *ethylene coil segment* mathematical model is extremely complex and it contains three interconnected derivation blocks. The result is a time and space description of all parameters, depending on the inlet mass flow variation.

In order to be implemented, the balance equations had to be modified as follows:

- Mass balance equation :

$$dw_j = -v \cdot (w_j - w_{j_0})/\mathrm{dz} \cdot \sum_i r_i \times S(i,j) \cdot dt + w_{j\_0} \quad (18)$$

- Energy balance equation:

$$dT_g = \left[v \cdot (T_g - T_{g\_0})/dz - \frac{[(T_g - T_W) \cdot A \cdot k_{tg} + \sum_i r_i H_i + \sigma \cdot (T_W^4 - T_g^4)]}{\rho \cdot C_p} \right] \cdot dt + T_{g\_0} \quad (19)$$

$$dT_W = A \cdot k_t \cdot (T_g - T_W)/(\rho \cdot C_p) \cdot dt + T_{W\_0} \quad (20)$$

- Momentum balance equation:

$$dP_x = G_3^2/(\rho \cdot g) \cdot dt \cdot (2f/D - 1) + dP_0 \quad (21)$$

and $$d\rho_x = \sigma_\rho \cdot dt + \rho_0 \quad (22)$$

where: $\sigma_\rho = \frac{\Delta P \cdot \rho^2 \cdot g \cdot D}{G_3^2 \cdot (2f - D)}$.

For the *entire coil*, the implementation was made using ode15s function from Matlab, solving nine material balance differential equations for: $C_2H_6, \dot{C}H_3, CH_4, \dot{C}_2H_5, C_2H_4, \dot{H}, H_2, C_4H_{10}, C_3H_8$ mass fractions and two energy balance differential equations for gas and wall temperature.

The result is a time and space variation of all parameters, an isobaric process which depends on the inlet mass flow variation and considering the inlet gas temperature as a disturbance.

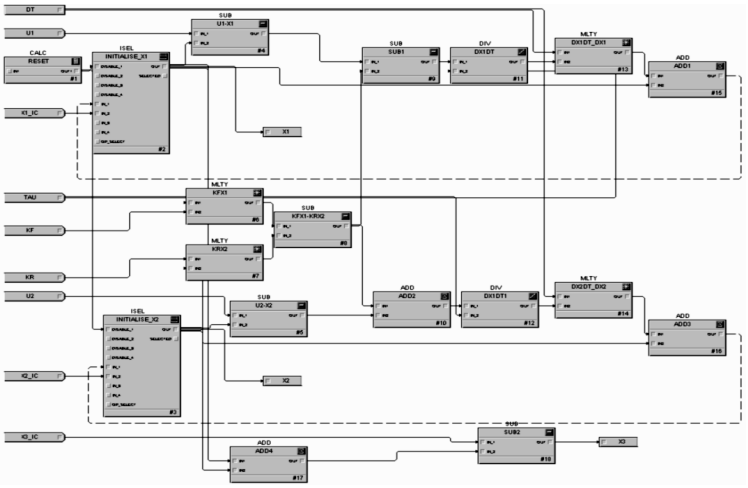

Figure 3. Euler's method DeltaV implementation, for complex equations

The inlet flow represents 97.2% ethane. The ethane concentration decreases in time, along with radicals and final products formation, Fig. 4. The radicals concentrations increase rapidly and afterwards they recombine in final products. In comparison with the other products, the concentration of ethylene is high.

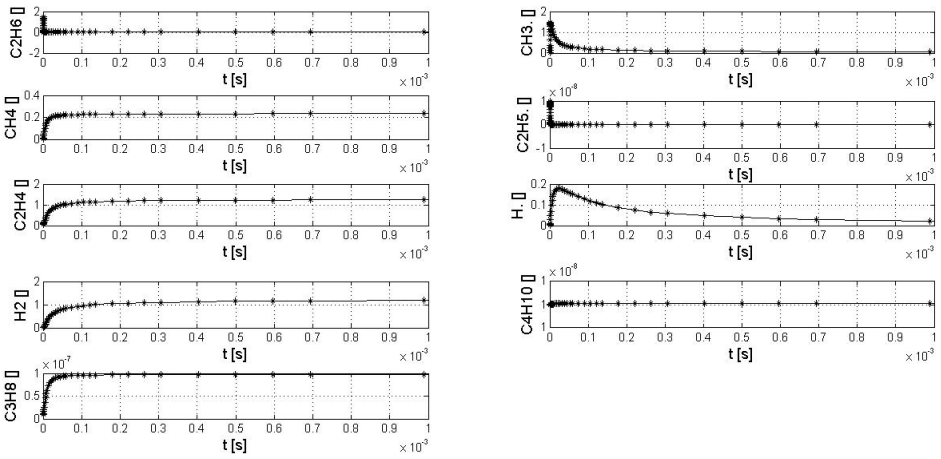

Figure 4. Evolution of products concentration

Due to the fact that the cracking reactions are endothermic, one can observe in Fig. 5, the decrease of the gas temperature. In time, the gas temperature stabilizes. The wall temperature remains constant in time (the change is insignificant).

A reliable dynamic model for this type of coil can be used for a future advanced control project, based on the following techniques: feed-forward control, state estimators based and predictive model controllers.

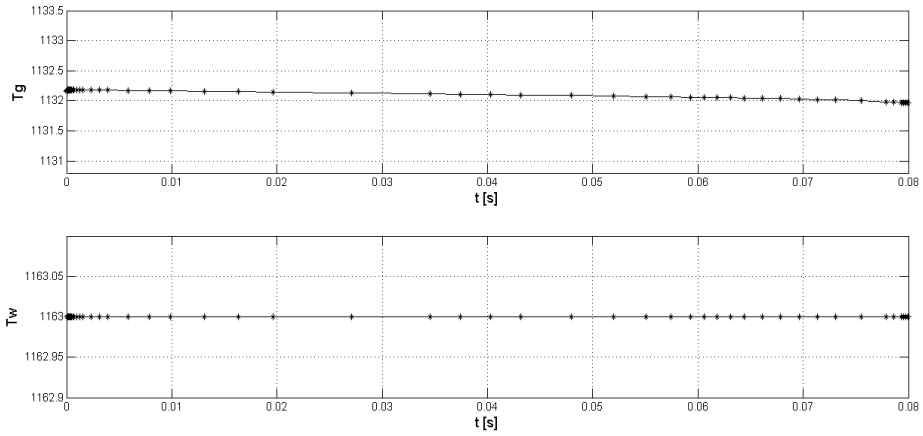

Figure 5. Gas and wall temperatures' evolution

CONTROL SYSTEM ANALYSIS

The operating objectives are to maintain the outlet temperature constant, operate within constraints, while minimizing the excess air and fuel consumption.

The overall control system structure is presented in Fig.6, where one can observe the communication between the optimization and advanced control layers. The MPC receives information from the field and controls the inlet flows and the combustion (air and fuel).

These rules could be applied also in the case of a coking plant when the actual temperature control point is at the heater outlet. The chemical reactions are endothermic and consequently the coke drum temperature (following the heater) will be lower. If the temperature is too low, the coke will be too soft and the other products' specifications will not be met. If the temperature is too high, the coke will be too hard and difficult to remove [1].

The development of a model for this type of furnace is a theme of present interest because of the petrochemical industry evolution and of the increased need of optimization. Studies on the optimization of such a plant were made by Riverol and Pilipovik [9] and Belohlav and Zamostny [2].

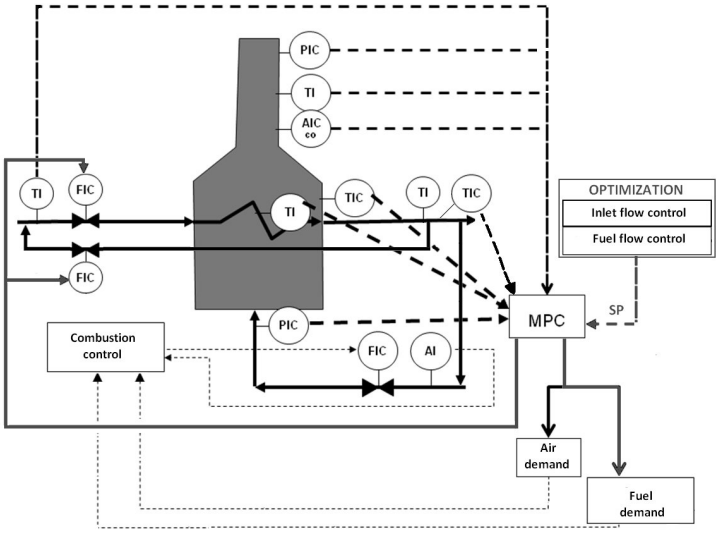

Figure 6. Control system structure

As mentioned earlier, this paper develops a dynamic regime study that can be followed by the implementation of an advanced process control system of the MPC design presented above.

ECONOMIC OPTIMIZATION

The cracking furnace is the heart of the installation and the frequent changes in feed, quality and prices, and the demand for its olefin products are influencing directly the production efficiency. Each reactant in the feed produces a certain distribution of products and, in order to satisfy the demand at the lowest cost, one needs to manipulate the amounts of each reactant, in an optimal way.

The DeltaV Model Predictive Control Professional (MPCPro) function block allows the control of large interactive processes (as large as 40 manipulated variables and 80 controlled variables), within the measurable operating constraints. The optimizer can be used to provide maximum profit or minimum production cost, with respect to the process constraints and the input limits. The MPCPro function block can replace traditional control systems that use feed-forward, decoupling networks and perform multivariable control. Process optimization is implemented using a linear program (LP) optimizer. The predictive control algorithm is based on Dynamic Matrix Control (DMC) technology, but with significant differences. These modifications lead to an improvement in the robustness of the controller, especially those concerning the utilization of the embedded LP optimization, range control and the penalties on manipulated variables moves and errors [12].

PredictPro was used to build an application that has 7 manipulated variables (MV's) and 10 controlled variables or constraints (CV's). The considered MV's are: the inlet feeds (four reactants), the recycle feeds (produced ethane and propane) and the added fuel (including the produced methane and fuel oil). The furnace capacity is limited and the downstream processing limitations have been considered, as well.

The MPCPro works in percentage values, so the ranges associated to each MV and CV need to be carefully chosen when the MPCPro gain matrix is initiated. In operation, in order to simulate nonlinearities the possibility to manipulate the gain matrix at every optimization scan has been considered by using the vectors GAIN_FACT and the module NON_LIN.

The prices for reactants and products are introduced by the operator or from another source and the associated costs and profit are calculated in specific modules (MV_PRC, CV_PRC and COSTS).

With this system the MV's and CV's can be either included or not, in the optimization problem according to different situations, for example: when the MV is no longer under automatic control (operator control) or base-load cases (fixed rates). Their status can be checked in the Optimizer screen, or by using the operator interface.

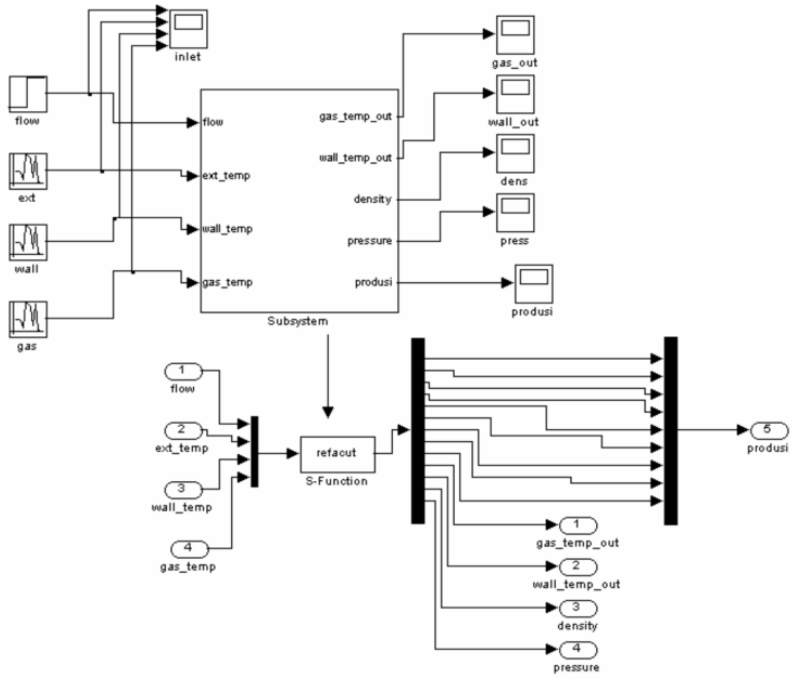

Figure 7. Coking process simulator

The main advantages emerged from the use of DeltaV PredictPro consist in the capability of running its applications on a stand-alone computer interfaced to other automation systems via an OPC communications link and of using up to five different optimization objectives, while increasing the flexibility of the system (different operating modes depending on external conditions).

CONCLUSIONS

This paper stands as the groundwork for the development of a simulator for the entire reactor, with large number of cracking tubes, useful for both monitoring and control of its outlet variables.

By using the simulator, Fig. 7, a steady state optimization built in a real-time control environment was tested, for different configurations, and additionally, a predictive model can be generated in order to build an MPC preliminary structure, for test purposes and operator training. The ethylene coil's developed model can be also the basis for building an equivalent model devoted to the implementation in the real time control environment.

NOMENCLATURE

w_j	[kg/kg]	– Mass fraction of component j
w_{j_0}	[kg/kg]	– Inlet mass fraction of ethane
z	[m]	– Length along coil
t	[s]	– Scanning rate
S (i, j)		– Stoichiometric constant of component j, in reaction i
v	[m/s]	– Fluid velocity
r_i	[kmol/m^3.s]	– Reaction rate
$\overline{C_p}$	[kcal/kg.K]	– Process gas specific heat
H_i	[kcal/kmole]	– Heat of reaction
A	[m^2]	– Transfer tube area
T_w	[K]	– Refractory wall temperature
T_{w_0}	[K]	– Inlet refractory temperature
T_g	[K]	– Flue gas temperature
T_{g_0}	[K]	– Inlet flue gas temperature
k_{tg}	[W/m.K]	– Gas thermal conductivity
k_t	[W/m.K]	– Tube thermal conductivity
σ	[W/m^4 K^4]	– Boltzmann coefficient referring to radiant energy
P	[N / m^2]	– Pressure
P_0	[N / m^2]	– Inlet pressure value
ρ	[kg/ m^3]	– Process gas density
ρ_0	[kg/ m^3]	– Ethane density

G_3 [kg/ s^2.m] – Dimensional constant
f – Friction factor
A_i [s^{-1}] – Frequency factor
E [kcal/mol] – Activation energy
g [m/s^2] – Gravitational acceleration
D [m] – inside tube diameter

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