

THREE DIMENSIONAL COUPLED SIMULATION OF HEAT TRANSFER WITHIN FURNACES AND REACTOR TUBES FOR THE THERMAL CRACKING OF EDC

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***Abstract.** This work is an application of the numerical code ERHESICS for thermal behavior simulation of a petrochemical furnace based on Vinyl Unit of Braskem S/A. This furnace engenders thermal cracking of EDC (ethylene dichloride) into its monomer VCM (vinyl chlorine monomer). ERHESICS aims to predict the effect of operational parameters of wall burners on load's (tubular reactor skin) overall heat flux. To predict thermal performance of a furnace (where thermal radiation's the more significant way of heat transfer), accurate calculus of radiant transfer between combustion products, furnace enclosure and load must be achieved. For Simulation of Braskem's thermal cracking furnace, thermal radiation was approached using Hottel's integral zone method, assuming participant medium as a weighted sum of gray gases with allowance for isotropic scattering. For a known flue gas flow pattern, a coupled simulation of thermal radiation, convection and conduction was carried out. Basic blocks (direct exchange areas) for formulae of zone method were developed specially for rectangular furnaces, using special transformation of variables to reduce computation effort. Exchange areas were computed using a Monte Carlo-like technique. Simulation results were compared to a real case where experimental data's available to verify model predictions. Good accordance was obtained, with maximum relative deviance of 10% from experimental overall heat transfer to tubular reactors skin.*

***keywords:** heat transfer, cracking furnace, thermal radiation, zone method, erhesics*

1. Introduction

This work (Janny and Sousa, 2005) is a result of the development of a computational code to predict the effect of operational parameters of natural gas-fired wall burners installed in Braskem's cracking unit F-1401-A. Main parameters changed during operation of furnace would be air excess (i.e. air coefficient) and natural gas flowrate on each burner level – see Fig. (1).

Both effects of total power source provided through all burners and distribution of this source over these burners should be simulated: for a given total power source, which distribution of this source over all burner levels would lead to a increase on load's (tubular reactor skin) overall heat flux, hence greater efficiency. Numerical results would be then used as input to a process modeling software like Aspen Plus[®].

The mathematical modeling argued here deals only with furnace region called "radiation chamber" or "radiation section" and, additionally, the following assumptions were made:

- i) Steady state condition;
- ii) Unidirectional flow with allowance for axial mixing, without secondary flow regions (i.e. recirculation);
- iii) Flue gas velocity profile as a sole function of mass flow, temperature and free stream's cross-sectional area;
- iv) Flue gas composition along furnace was calculated from imposed air coefficients (air coefficient $\lambda_{air} = \frac{[\text{effectively used air}]}{[\text{stoichiometry air}]}$);
- v) Sufficient high combustion temperature was admitted, so the only necessary condition to chemical reaction is the mixing of fuel and oxygen;

- vi) Complete fuel conversion (extent of reaction $X = 1$);
- vii) Combustion was admitted as punctual phenomena, as if each burner would be replaced by a punctual source of power related to its "injected" fuel flow rate (power = $\dot{m}_{ng} \cdot SCP_V$, where \dot{m}_{ng} and SCP_V are flow rate and superior calorific power of natural gas, respectively, within control volume V);
- viii) Diffuse reflection over all enclosure or imaginary surfaces;
- ix) There isn't any radiation (in or out) scattering, therefore attenuation of a beam is due only to absorption;
- x) Weak variation of radiosity (emergent radiative flux) along a surface zone.

2. Description of the cracking unit

The radiation section (Fig. (1) for details) has a central plane (symmetry plane) containing 22 reactor tubes on one row, plus 6 reactor tubes on a cross-over plane at section's exiting, before entering convection zone. Furnace can be approximated as a prism with rectangular base, whose dimensions (in meters) are: 6.5 height, 1.6 length and 16.7 width.

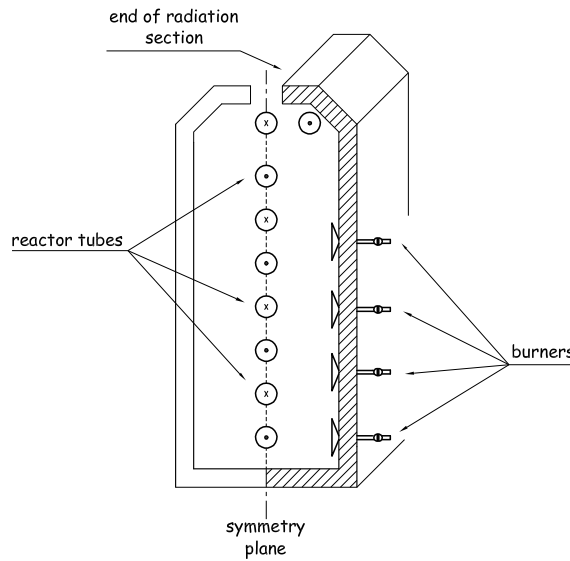


Figure 1: Representation of cracking furnace: load surfaces (reactor tubes) and refractory surfaces (burners)

Heat required for endothermic cracking reaction is provided by means of radiant wall burners located in a parallel plane to reactor tubes. There're 4 rows (levels) of burners on each side of furnace, each row having 10 burners. These burners provide uniform heat distribution through indirect heating of reactor tubes skin: bulk of radiative heat transfer is due to refractory surfaces (these ones first being heated mainly by convective transfer from burner's flame), irradiating to reactor tubes.

3. Zoning and discretization

Usually, zone size is dictated by characteristic length scale of conduction and convection (Hottel and Sarofim, 1967). For this problem, convective and conductive heat transfer answer for less than 15% of the overall heat flux to load, therefore a rough furnace zoning, as detailed on Fig. (2), already gives a good description of the problem, and is coherent with experimental data about reactor tube skin temperatures.

The present zoning scheme is for one half of furnace, as the problem will be admitted plane-symmetric. The zoning is as follows:

- 5 gas volume zones (V_0, V_1, V_2, V_3, V_4): main gas species are O_2 , H_2O , CO_2 and N_2 ; in the first four volumes ($V_0 \dots V_4$) there are heat sources (burners); there aren't burners in fifth volume;
- 6 load surface zones ($S_2, S_6, S_{10}, S_{14}, S_{18}, S_{20}$): discontinued load surfaces composed by spaced tubes and voids; there're strong exchanges by radiation ($S_2, S_6, S_{10}, S_{14}, S_{18}$) and convection (S_{20});
- 16 refractory surface zones (remaining surfaces): made of refractory composites; on some of these surfaces are installed wall burners (S_0, S_4, S_8, S_{12}).

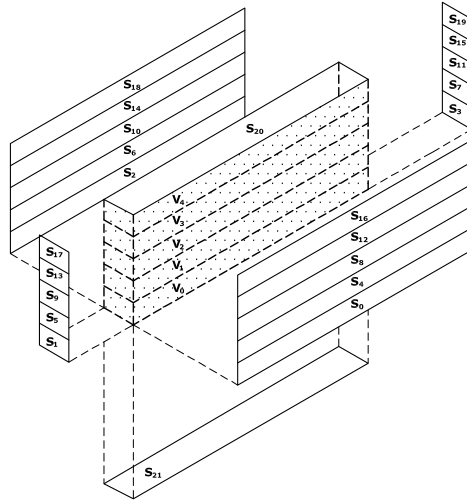


Figure 2: Isometric detail of furnace zoning and identification of all domain zones (surfaces and volumes)

3.1. Mass fluxes in volume zones

Figure 3 gives a detailed view of unidirectional mass fluxes along volume zones.

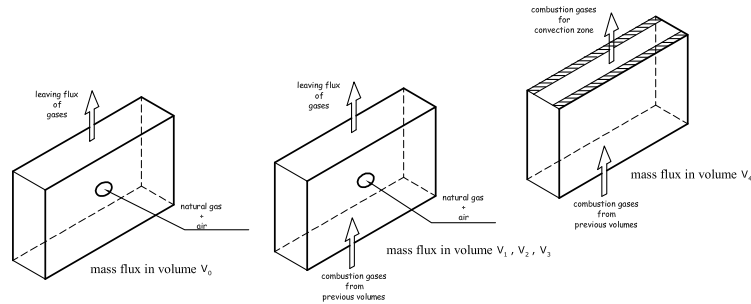


Figure 3: Simplified model for mass flux on each volume zone

4. Zonal analysis

To calculate radiative heat transfer, an integral approach was used employing zonal analysis (Hottel and Sarofim, 1967), a powerful tool to estimate radiative transfer in semitransparent medium. In this method, the domain of interest is divided into a finite number of surface and volume zones – each zone must be small enough so the assumption of uniform and constant properties holds.

Mathematically, the zone method is, perhaps, the simplest numerical quadrature of the differential-integral equation (Radiative Transfer Equation or RTE) which governs radiative transfer. Hottel's method make no approximation or assumption to simplify the RTE. By using the concept of radiosity and the principle of energy conservation, this method transforms RTE into a new set of non-linear algebraic equations.

Together with conventional finite difference techniques to represent convective transports, the zone method provides a way to discretize radiation contribution on a general differential-integral equation.

5. Total balances for zones forming a cavity

Terms related to radiative transport are written as function of exchange factors known as directed flux areas, denoted by \vec{GG} , \vec{GS} , \vec{GS} and \vec{SS} for gas-gas, gas-surface, surface-gas and surface-surface exchanges, respectively.

Using the theory developed by Hottel and Sarofim, directed flux areas can be calculated from more fundamental exchange factors, as shown in Tab. (1):

Table 1: Exchange areas used in zone method for radiation analysis (Rhine and Tucker, 1991)

Exchange Factor	Denomination	Function of
direct exchange area	$\overline{g_i g_j}, \overline{g_i s_j}, \overline{s_i s_j}$	geometry, gray gas, extinction coefficient K .
total exchange area	$\overline{G_i G_j}, \overline{G_i S_j}, \overline{S_i S_j}$	geometry, K , surface emissivity ϵ_i
directed flux area	$\overrightarrow{G_j G_i}, \overleftarrow{G_j G_i}, \overrightarrow{G_j S_i}, \overleftarrow{G_j S_i}, \overrightarrow{S_j S_i}, \overleftarrow{S_j S_i}$	geometry, K , ϵ_i , $T_{s,i}$ and $T_{g,i}$ temperatures.

Directed flux areas are computed from total exchange areas, which in turn are computed from direct exchange areas. Using these exchange factors, the transfer of thermal radiation for a particular zone may be incorporated in a total energy balance. In this balance all others heat transfer modes are accounted.

Equations are written for all gas and surface zones, giving rise to a simultaneous system of non linear equations. This system can be solved to find temperature and overall heat transferred to each zone.

5.1. Total energy balance for a surface S_i with area A_i

$$\underbrace{\sum_j \overrightarrow{S_j S_i} E_{s_j}} + \underbrace{\sum_k \overrightarrow{G_k S_i} E_{g_k}} - \underbrace{A_i \epsilon_i E_{s_i}} + \underbrace{\sum_l h_l A_i (T_{g_l} - T_{s_i})} = \underbrace{\dot{Q}_{all(i)}} \quad (1)$$

Incident power over A_i resulting of the presence of all emitting surfaces.

Incident power over A_i resulting of the presence of all emitting volumes.

Emitted power by A_i .

Incoming power to A_i due to convection.

Overall power transferred to A_i .

where h_l is a bulk convective heat transfer coefficient and E_{z_j} is the blackbody emissive power at zone's (z_j) temperature, and it's given by Stefan-Boltzmann law ($E_{z_j} = \sigma T_{z_j}^4$).

For surfaces S_2, S_6, S_{10}, S_{14} and S_{20} , $\dot{Q}_{all(i)}$ stands for the overall heat transferred to each $i = 2, 6, 10, 12, 14, 20$ load surface (tubular reactor skin). This is the meaningful quantity to evaluate furnace's efficiency. For refractory surfaces, $\dot{Q}_{all(i)}$ stands for losses by conduction through wall.

5.2. Total energy balance for a gas G_i with volume V_i

$$\underbrace{\sum_k \overrightarrow{G_k G_i} E_{g_k}} + \underbrace{\sum_j \overleftarrow{G_i S_j} E_{s_j}} - \underbrace{4 \sum_{\eta} a_{g,\eta} K_{\eta} V_i E_{g_i}} - \underbrace{\sum_l h_l A_l (T_{g_i} - T_{s_l})} - \underbrace{\dot{Q}_{e,i}} + \underbrace{\dot{q}_{v,i}} = 0 \quad (2)$$

Incident power over V_i resulting of the presence of all emitting volumes.

Incident power over V_i resulting of the presence of all emitting surfaces.

Emitted power by V_i .

Leaving power from V_i due to convection.

Enthalpy variation associated with gases flux within V_i .

Power source released from combustion reaction in volume V_i .

Where

$$\dot{Q}_{e,i} = \overrightarrow{\Delta} \mathbf{e} = \sum_{outlet} (\dot{m}_{outlet} \mathbf{e}_{outlet})_i - \sum_{inlet} (\dot{m}_{inlet} \mathbf{e}_{inlet})_i \quad (3)$$

$$\dot{q}_{v,i} = (\dot{m}_{gn})_i PCS_v \quad (4)$$

In volume V_i , outlet and inlet flowrate (kg/s) for O_2 , N_2 , CO_2 , H_2O are expressed by \dot{m}_{outlet} and \dot{m}_{inlet} , respectively. The terms e_{outlet} and e_{inlet} – specific enthalpies (kJ/kg) – are calculated at temperatures of volumes V_i and V_{i-1} , respectively. Combustion air is referenced at temperature $T_{ref} = 298K$. Terms $a_{g,\eta}$ and K_η are weight and absorption coefficients, respectively, of the 1, 2, ..., η gray gas.

5.3. Equations system and convergence loop

Generic form of non linear equations, to be solved for unknown temperature and heat flux, may be written as bellow.

For total energy balance of m surfaces:

$$\begin{pmatrix} \alpha_{s11} & \alpha_{s12} & \cdots & \alpha_{s1m} \\ \alpha_{s21} & \alpha_{s22} & \cdots & \alpha_{s2m} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{sm1} & \alpha_{sm2} & \cdots & \alpha_{smm} \end{pmatrix} \begin{pmatrix} T_{S1}^4 \\ T_{S2}^4 \\ \vdots \\ T_{Sm}^4 \end{pmatrix} + \begin{pmatrix} \beta_{s11} & \beta_{s12} & \cdots & \beta_{s1m} \\ \beta_{s21} & \beta_{s22} & \cdots & \beta_{s2m} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{sm1} & \beta_{sm2} & \cdots & \beta_{smm} \end{pmatrix} \begin{pmatrix} T_{S1} \\ T_{S2} \\ \vdots \\ T_{Sm} \end{pmatrix} - \begin{pmatrix} \dot{Q}_{all(1)} \\ \dot{Q}_{all(2)} \\ \vdots \\ \dot{Q}_{all(m)} \end{pmatrix} + \begin{pmatrix} \gamma_{s1} \\ \gamma_{s2} \\ \vdots \\ \gamma_{sm} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad (5)$$

$$\alpha_{s_{ij}} = \begin{cases} \sigma \left(\overleftarrow{S_i S_i} - A_i \epsilon_i \right), & \text{if } i = j \\ \sigma \overleftarrow{S_i S_j}, & \text{if } i \neq j \end{cases} \quad \beta_{s_{ij}} = \begin{cases} -\sum_k h_k A_i, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases}$$

$$\gamma_{s_i} = \sum_l \overleftarrow{G_l S_i} T_{g,l}^4 + \sum_k A_i T_{g,k} h_k$$

For total energy balance of n volumes

$$\begin{pmatrix} \alpha_{g11} & \alpha_{g12} & \cdots & \alpha_{g1n} \\ \alpha_{g21} & \alpha_{g22} & \cdots & \alpha_{g2n} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{gn1} & \alpha_{gn2} & \cdots & \alpha_{gnn} \end{pmatrix} \begin{pmatrix} T_{g1}^4 \\ T_{g2}^4 \\ \vdots \\ T_{gn}^4 \end{pmatrix} + \begin{pmatrix} \beta_{g11} & \beta_{g12} & \cdots & \beta_{g1n} \\ \beta_{g21} & \beta_{g22} & \cdots & \beta_{g2n} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{gn1} & \beta_{gn2} & \cdots & \beta_{gnn} \end{pmatrix} \begin{pmatrix} T_{g1} \\ T_{g2} \\ \vdots \\ T_{gn} \end{pmatrix} + \begin{pmatrix} \gamma_{g1} \\ \gamma_{g2} \\ \vdots \\ \gamma_{gn} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad (6)$$

$$\alpha_{g_{ij}} = \begin{cases} \sigma \left(\overleftarrow{G_i G_i} - 4 \sum_\eta a_{g,\eta} K_\eta V_i \right), & \text{if } i = j \\ \sigma \overleftarrow{G_i G_j}, & \text{if } i \neq j \end{cases} \quad \beta_{g_{ij}} = \begin{cases} -\sum_k h_k A_k, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases}$$

$$\gamma_{g_i} = \sum_l \overleftarrow{G_i S_l} T_{s,l}^4 + \sum_k A_k T_{s,k} h_k - \dot{Q}_{e,i} + \dot{q}_{v,i}$$

Systems Eq. (5) and Eq. (6), *a priori*, have $2m + n$ unknowns and only $m + n$ equations. Which means ones need to prescribe m boundary conditions to determinate solutions for those systems. About boundary conditions, see **7. Boundary conditions**.

Briefly, Equation (5) and Eq. (6) were solved by means of a modified Newton-Raphson routine with tuned Powell's functions (Powell, 1970), using trust regions and normalized residues within zero curves of possible solutions. This procedure allowed the nonlinear system to be, relatively, "well behaved" for a given arbitrary initial guess for temperature field.

Convergence loop for computing solution of Eq. (5) and Eq. (6) is shown in Fig. (4).

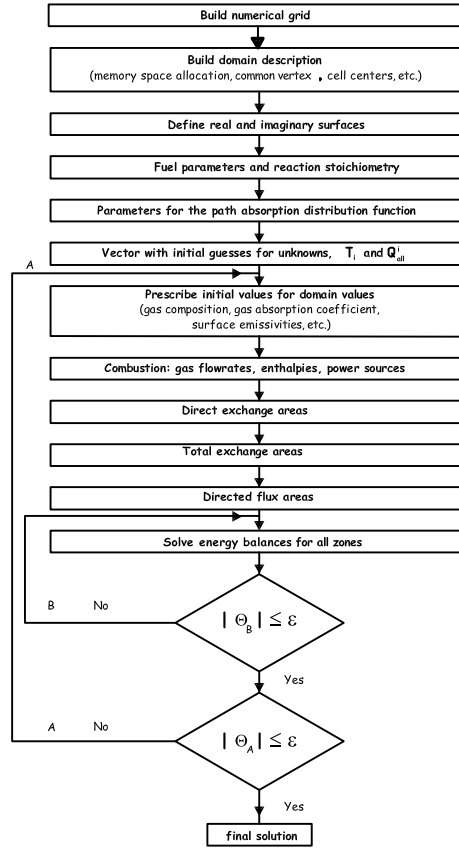


Figure 4: Simplified model for mass flux on each volume zone

Inner loop (B) represents the convergence level of a energy balance equation for each zone (for example, equation Eq. (1) for a zone i). Outer loop (A) involves a global convergence, not just including a particular balance, but energy balances for all zones (surfaces and volumes), effects of participant medium absorptivities, direct exchange areas, total exchange areas and directed flux areas.

In Fig. (4), convergence criteria are expressed by Θ_B and Θ_A (here called convergence error) for inner and outer loops, respectively. Some characteristics of convergence stability cannot be inferred only based on the assumption that both source term and radiative intensity are linear with respect to the blackbody intensity of the medium and walls. When the spectral banded nature of absorption and emission phenomena are taken into account (no grey gas assumption), such linearity is not true because of emissivity's dependence of medium and background temperatures.

In this work we propose a expression to monitor convergence based on eigenvalues stability analysis. For example, to measure convergence advance for gas volumes on an outer loop level at $k + 1$ -th iteration, Equation (7) gives:

$$\Theta_A^{(k+1)} = \chi^{(k+1)} \left(\frac{\chi^{(k+1)}}{\chi^{(k)}} - 1 \right)^{-1} \quad (7)$$

Where $\chi^{(k+1)} = \sqrt{\sum_{i=0}^n (T_{g,i}^{(k+1)} - T_{g,i}^{(k)})^2}$ is a root mean square (RMS) residue. Figure (5) shows a example for convergence-path measured by Θ_A .

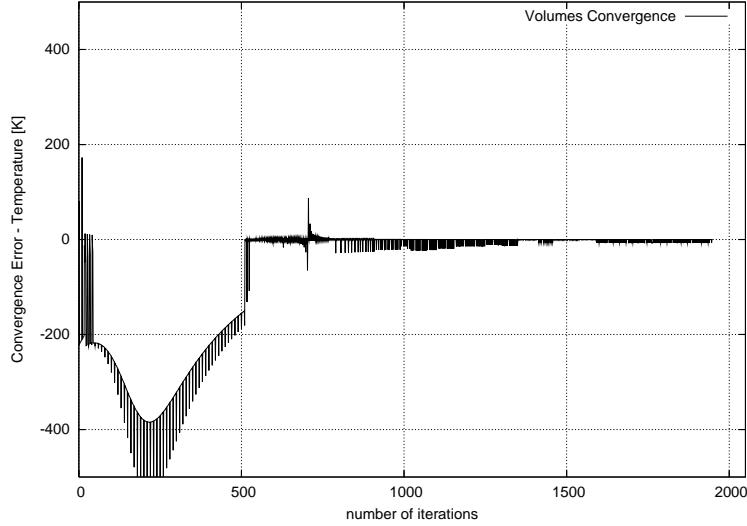


Figure 5: Volume's temperature convergence is measured by Eq. (7)

A more conventional convergence criteria is applied for Θ_B .

$$\Theta_B^{(k+1)} = \sqrt{\delta T_{g,i}^{(k+1)} \delta T_{g,i}^{(k)}} \quad (8)$$

Where $\delta T_{g,i}^{(k+1)} = |T_{g,i}^{(k+1)} - T_{g,i}^{(k)}|$. Total energy imbalance must be also bellow a target criteria, such as a direct residue $\delta = \sum_{i=0}^n \dot{q}_{V,i} - \left(\dot{Q}_{e, \text{exit}} + \sum_{j=\text{loads}} \dot{Q}_{\text{all}(j)} + \text{wall losses} \right)$, where $\dot{Q}_{e, \text{exit}}$ is the enthalpy of fue gases at furnace's exit. This way, one could verify if the problem has, in fact, converged.

5.4. Numerical relaxation

Relaxation factors were used in both outer and inner loops, but outer loop was more affected by stability issues. Figure 5 (outer loop's convergence-path measured in terms of Θ_A) shows a progressive damping of Θ_A amplitude, resulting from an adaptive factor relaxation (AFR). Solver allows software's user to change relaxation factor, if needed, after a certain number of iterations or to let itself apply AFR. With the first choice, user could check, for example, Θ_A and $\delta T_{g,i}$ values and choose suitable relaxation factors to each unknown, dumping iteration instabilities.

One detected source of such instabilities originates from scale differences between terms on equations Eq. (1) and Eq. (2). In other words, there are terms which are small when compared with some other term with higher magnitude order. For a volume zone total energy balance, specifically, when a great air excess ($\lambda_{ar} > 30$) is simulated, the enthalpy term ($\dot{Q}_{e,i}$) becomes, relatively, very big (mainly because of water vapor specific enthalpy). This generates convergence problems in both loops (B and A): for inner loop because of scale differences; and for outer loop because $\dot{Q}_{e,i}$ is an implicit function of temperature.

When ADF is used, different relaxation schemes are applied in loops A and B . For loop B (Newton-Raphson method), solution is iteratively updated accounting to Eq. (9) and Eq. (10). For a zone z_i (either surface or volume)

$$T_{z,i}^{(k+1)} = T_{z,i}^{(k)} + \phi^{(k)} \delta T_{z,i}^{(k)} \quad (9)$$

$$\delta T_{z,i}^{(k)} = - \left(J^{(k)} \right)^{-1} F \left(T_{z,i}^{(k)} \right) \quad (10)$$

where J is the non linear system's Jacobian matrix; ϕ is the relaxation factor; and F is either Eq. (1) or Eq. (2). Factor ϕ is the one (O'Dwyer and O'Donnell, 1995) which minimizes residual L_2 norm in the

direction along the solution update, at each iteration (loop B). That is, $\phi^{(k)}$ is chosen as the value which minimizes $\|F(T_{z,i}^{(k)} + \phi^{(k)} \delta T_{z,i}^{(k)})\|$ or ensures that $\|F(T_{z,i}^{(k)} + \phi^{(k)} \delta T_{z,i}^{(k)})\| < \|F(T_{z,i}^{(k)})\|$. For A loop, Equation (11) was empirically chosen as the relaxation scheme to give best results (great dumping rate and minimum number of iterations needed). Similar method was also proposed by Bastos *et al.*, 1995.

$$T_{z,i}^{(k+1)} = (1 - \phi_1) T_{z,i}^{(k)} + \phi_1 \left(T_{z,i}^{(k+1)} + \phi_2^{(k)} (T_{z,i}^{(k+1)} - T_{z,i}^{(k)}) \sqrt{\frac{T_{z,i}^{(k)}}{T_{z,i}^{(k+1)}}} \right) \quad (11)$$

Equation (11) allows one to choose between two methods: if ϕ_2 (which is an adaptive relaxation factor) is set to 0, this equation simplifies to a traditional under-relaxation method ($0 < \phi_1 \leq 1$); if now $\phi_1 = 1$, only the term under brackets will be evaluated. Of course, if $0 < \phi_1 \leq 1$ and $\phi_2 \neq 0$ a hybrid method will be used (although this case wasn't extensively tested).

The following rules are used to calculate ϕ_2 :

- i) For each unknown, set a initial $\phi_2^{(0)}$ and define an increment $d\phi$;
- ii) For each unknown, calculate $\Delta^{(k-1)} = T_{z,i}^{(k-1)} - T_{z,i}^{(k-2)}$ and $\Delta^{(k)} = T_{z,i}^{(k)} - T_{z,i}^{(k-1)}$;
- iii) Calculate the product $\Delta^{(k)} \cdot \Delta^{(k-1)}$;
- iv) If the product is negative, oscillation in convergence occurred. In this case set $T_{z,i}^{(k)} = T_{z,i}^{(k-1)}$ and $\phi_2 = \phi_{osc}$;
- v) If the product is positive, there wasn't oscillation. In this case set $\phi_2 = \phi_2 + d\phi$.

where ϕ_{osc} is the value affected if the unknown had oscillated, and normally is smaller than $\phi_2^{(0)}$. Unknowns use different relaxation levels determined by their different behavior. Values for $\phi_2^{(0)}$, $d\phi$ and ϕ_{osc} are chosen depending on problem's individuality. Typical values are (Bastos *et al.*, 1995): $\phi_2^{(0)} = -0.6$, $d\phi = 0.05$ and $\phi_{osc} = -0.7$. To solve Eq. (2), an additional under-relaxation scheme (with $\phi_2 = 0$) was utilized to update just the temperature used to calculate $\dot{Q}_{e,i}$, hence minimizing the importance of this term over each iteration.

6. Direct exchange areas for rectangular enclosure

Direct exchange area (DEA) represents the geometric and optic relation between each pair of zones (Hottel and Sarofim, 1967). DEA can also be seen as the energy fraction emitted by a element z_i and absorbed by a element z_j , after a direct transmission – does not include reflection on others surfaces.

Many authors have been applying different methods to calculate DEA for various geometries: Erkkü (Erkkü, 1959) provided solutions to cylinders and slabs; Vercamen (Vercamen and Froment, 1980) obtained DEAs by calculating photon trajectories using Monte Carlo method.

Works by Erkkü (Erkkü, 1959), Tucker (Rhine and Tucker, 1991) and Arima (Arima, 1998) related to formulation and calculus of DEA admitted the simplification of an uniform zoning and a fixed range of optical path lengths (given by $p_g L_m$ product, where p_g is the sum of partial pressures of absorbing/emitting gas species and L_m is the mean beam length). In the works by Tucker and Arima, enclosure was approximated by a collection of cubic gas zones bounded by square zone surfaces.

When emissivity and absorptivity of combustion products are represented through use of multiple gray gases, this uniform zoning limits the usage of DEA tables and zone .description (size) when high extinction coefficients ($K > 10 \text{ m}^{-1}$) are present. In the simulation of cracking furnace F-1401-A, DEAs were formulated for non uniform zones, using special calculus techniques.

Numerical integration of DEA equations were carried out by Monte Carlo statistic method, with an adaptive algorithm (Janny and Sousa, 2005) which evaluates the integrand on a hypercubic region along random directions. The integrand may be seen as radiation beams emitted by a zone which directly arrive on another zone, accounting its interaction with intervenient medium (gases).

6.1. DEA equations

There are tree types of DEA: surface-surface ($s_i s_j$), gas-surface ($g_i s_j$) and gas-gas ($g_i g_j$), which can be expressed by the following equations:

$$\overline{s_i s_j} = \int_{A_i} \int_{A_j} \xi(A_i, \vec{r}_{ij}) \tau(R) \frac{\cos(\theta_i) \cos(\theta_j)}{\pi R^2} dA_j dA_i \quad (12)$$

$$\overline{g_i s_j} = \int_{V_i} \int_{A_j} \xi(V_i, \vec{r}_{ij}) \tau(R) \frac{K_i \cos(\theta_j)}{\pi R^2} dA_j dV_i \quad (13)$$

$$\overline{g_i g_j} = \int_{V_i} \int_{V_j} \xi(V_i, \vec{r}_{ij}) \tau(R) \frac{K_i K_j}{\pi R^2} dV_j dV_i \quad (14)$$

where $\tau(R) = \exp\left(-\int_0^R K(r) dr\right)^1$ is the transmittance; $R = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$ is the absorption path (see Fig. (6)); and $\xi(A_i, r_{ij})$ is the characteristic function which accounts for the presence of shadow zones (Janny and Sousa, 2005). Function $\xi(A_i, r_{ij}) = 1$ when a beam leaving a point (x_i, y_i, z_i) at surface zone A_i (or volume V_i), locally traveling along a per unit solid angle direction \vec{r}_{ij} , is seen when looking from a point (x_j, y_j, z_j) at the other surface zone A_j (or volume V_j). Otherwise (not seen), $\xi(A_i, \vec{r}_{ij}) = 0$.

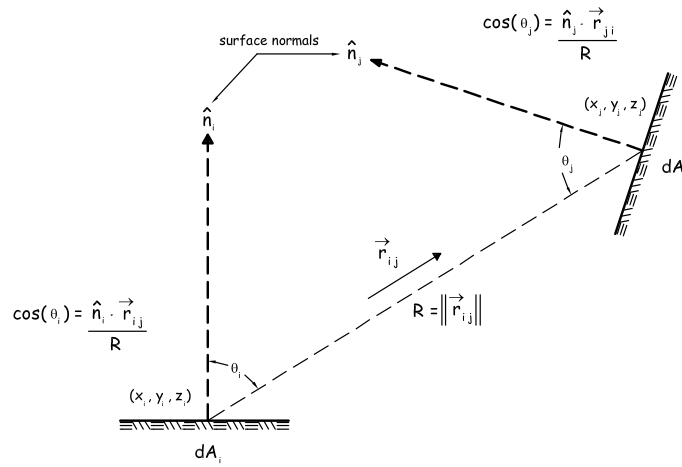


Figure 6: Radiative exchange between two differential surface elements

Transmittance $\tau(R)$ quantifies the energy fraction not transmitted by a radiation beam to the volume zones by which this beam goes through, during a trek from its origin point until its final absorption point. As an approximation, it may be written as

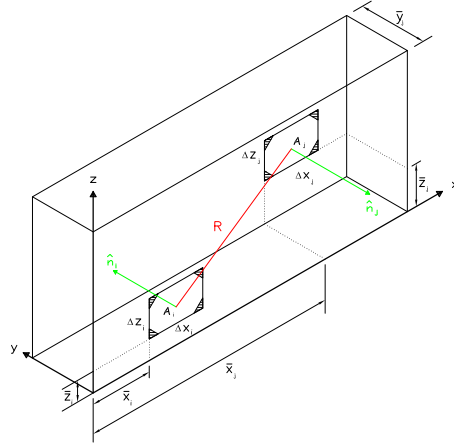
$$\tau(R) \approx \int_{R_{min}}^{R_{max}} \exp\left(-\sum_m K_{r_m} \Delta r_m\right) f(R) dR \quad (15)$$

where Δr_m is the fraction of total beam length (R) which lies inside a given volume zone with absorption coefficient K_{r_m} . It's calculated based on the intersection of the radiation beam with bounding planes of the volume zone. The factor $f(R)$ is a differential distribution of beam lengths, i.e. the probability that an arbitrarily chosen value of beam length lies between R and $R + dR$ (Vercaemen and Froment, 1980). A statistic fit is used because there exist an infinite number of possible absorption paths between a pair of zones.

By example, direct exchange area between a refractory surface and a load surface, without any shadow zones, may be written as (see Fig. (7)):

$$\overline{s_i s_j} = \int_{\bar{x}_i}^{\bar{x}_i + \Delta x_i} \int_{\bar{z}_i}^{\bar{z}_i + \Delta z_i} \int_{\bar{x}_j}^{\bar{x}_j + \Delta x_j} \int_{\bar{z}_j}^{\bar{z}_j + \Delta z_j} \tau(R) \frac{\bar{y}_j^2}{\pi R^4} dz_j dx_j dz_i dx_i \quad (16)$$

¹Instead of fundamental models for transmittance, the exponential law given by Hottel (Hottel and Sarofim, 1967) is used.


 Figure 7: refractory wall zone (A_i) and reactor tube zone (A_j)

6.2. Reduction of the dimension of a multiple integral

A special technique to transform double integral into a sum of simple integrals were developed by Erkkü (Erkkü, 1959). This technique can be extended to non uniform grids using a additional argument, as proposed by Tian (Tian and Chiu, 2003).

This procedure leads, altogether with the reduction of integral dimension, to a minimization of singularities of function $\overline{s_i s_j}$ within its integration domain. This is a result of great importance, since Eq. (13), Eq. (14) and Eq. (15) have integrands with abrupt variation (singularity) within integration domain for some pair of zones (self radiating or adjacent zones).

7. Boundary conditions

As already mentioned, to solve systems Eq. (2) and Eq. (3) it's necessary to specify m boundary conditions. In the case of the actual zoning of furnace F-1401-A, it'll be prescribed 22 conditions. From these, 6 will be Dirichlet boundary conditions – of first kind, which specifies a value $T = b(x, y, z)$ – prescribed to load surfaces ($S_2, S_6, S_{10}, S_{14}, S_{18}, S_{20}$). Experimental data from Braskem's DCS (Distributed Control System) provided information about the temperature of fluid process (inside reactor tube), measured by means of thermocouples allocated immediately upstream (T_{in}) and downstream (T_{out}) from equivalent locations of load surface zones adopted in this work. Starting from arithmetic mean of these values $((T_{in} + T_{out})/2)$, in Tab. (2) tubular reactor skin temperature were calculated accounting for gradients within boundary layer, hence summing a ΔT value to this arithmetic mean.

Table 2: Known (experimental) temperatures of load surfaces

Zone	Temperature [K]	Zone	Temperature [K]
S_2	$T_{S2} = 802$	S_{14}	$T_{S14} = 655$
S_6	$T_{S6} = 767$	S_{18}	$T_{S18} = 579$
S_{10}	$T_{S10} = 732$	S_{20}	$T_{S20} = 542$

The 16 remaining information will be Neumann boundary conditions – of second kind, which specifies a value for $\partial T / \partial \vec{n} = \hat{n} \cdot \nabla T$ – prescribed to refractory surfaces ($S_0, S_1, S_3, S_4, S_5, S_7, S_8, S_9, S_{11}, S_{12}, S_{13}, S_{15}, S_{16}, S_{17}, S_{19}, S_{21}$). In Eq. (2) and Eq. (3), this condition will be associated with term \dot{Q}_{all} .

If furnace walls are not admitted adiabatic ($\dot{Q}_{all} = 0$), there will be losses through these walls and \dot{Q}_{all} wont be null. In this case, \dot{Q}_{all} will be iteratively computed in the following way (Janny and Sousa, 2005):

$$\dot{Q}_{all(i)}^{(k)} = \text{Losses}_i^{(k)} = \dot{Q}_{conduction(i)}^{(k)} = A_i \frac{\kappa_i^{(k)}}{\Delta l_i} \left(T_{si}^{(k)} - T_{i,e}^{(k)} \right) \quad (17)$$

$$\left[T_{i,e}^{(k)} \right]^4 + \left(\frac{\Delta l_i h_{i,e}^{(k-1)} + \kappa_i^{(k-1)}}{\Delta l_i \epsilon_{i,e}^{(k-1)} \sigma} \right) T_{i,e}^{(k)} - \frac{\kappa_i^{(k-1)} T_{s_i}^{(k-1)} + \Delta l_i h_{i,e}^{(k-1)} T_{\infty,e}}{\Delta l_i \epsilon_{i,e}^{(k-1)} \sigma} = 0 \quad (18)$$

were $T_{i,e}$ is furnace external wall's temperature (adjacent to surface S_i); Δl_i is refractor's block thickness (adjacent to surface S_i); κ_i is refractor's thermal conductivity (adjacent to surface S_i); $\epsilon_{i,e}$ is furnace external wall's emissivity (adjacent to surface S_i); $h_{i,e}$ is furnace external wall's convection coefficient (adjacent to surface S_i); and $T_{\infty,e}$ is the environment temperature. The quartic Eq. (20) has a known analytic solution.

7.1. Model to represent an array of tubes

A model was developed (Janny and Sousa, 2005) to replace a set of tubes and voids, by a gray plane (in the same averaged temperature of the array of tubes within the discredited zone), whose emissivity is calculated as follows (see Fig. (8)):

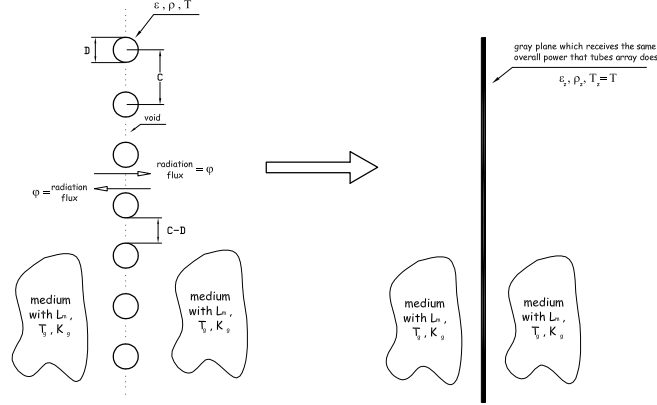


Figure 8: Replacing a set of tubes and voids by a gray plane

$$\epsilon_z = \frac{\epsilon}{\rho} \frac{\pi D}{2C} \left[\frac{D}{2} Y^2 + (C - D)(Y - \pi) \right] \left[\frac{D}{2} Y^2 + (C - D) \left(Y - \frac{\pi}{\rho} \right) \right]^{-1} \quad (19)$$

where $Y = \arcsin\left(\frac{D}{C}\right) + \left[\left(\frac{C}{D}\right)^2 - 1\right]^{1/2} - \frac{C}{D}$. Assuming symmetric conditions on both sides of furnace, equal amount of radiation which comes from the right side and irradiates over a void with $C - D$ width, also leaves the left side towards right side. Therefore, it's like if the void $C - D$ would reflect all incident radiation. In other words, the void $C - D$ behaves like a reflector ($\epsilon = 0$, $\rho = 1$). Similar procedure is detailed by Hottel (Hottel and Sarofim, 1967).

8. Results

Simulation results are compared with measured experimental data presented in Tab. (3). Operating conditions of furnace are given in Tab. (4).

Table 3: Experimental data from furnace F-1401-A operation

Experimental data	Value
Overall heat transferred to reactor tube skin (both sides of furnace)	9206 [kW]
Overall heat transferred to reactor tube skin (one side)	4603 [kW]
Volume V_0 temperature	1144 [K]
Volume V_2 temperature	1184 [K]
Volume V_3 temperature	1189 [K]
Flue gas temperature at radiation section's exit (V_4)	1062 [K]

Table 4: Furnace F-1401-A operating conditions

Condition	Value	Condition	Value
Fuel flowrate in zone S_0	0.0481 [kg/s]	Fuel's carbon content	0.7245
Fuel flowrate in zone S_4	0.0349 [kg/s]	Fuel's hydrogen content	0.2323
Fuel flowrate in zone S_8	0.04134 [kg/s]	Fuel's sulfur content	0.000
Fuel flowrate in zone S_{12}	0.04134 [kg/s]	Fuel's nitrogen content	0.0297
Fuel flowrate in zone S_{16}	0.0 [kg/s]	Fuel's oxygen content	0.0135
Air excess	1.05 [air/stoich air]	Fuel's higher calorific value	49113 [kJ/kg]
Heat input (total)	8137 [kW]	Fuel's density	0.7729 [kg/Nm ³]

Figure (9) gives the simulation results for predicted temperatures and Fig. (10) gives the predicted overall heat transferred to each load (tubular reactor skin) zone, summing a total of 4375 kW. Hence, a deviation of -4.9% from the value in Tab. (3).

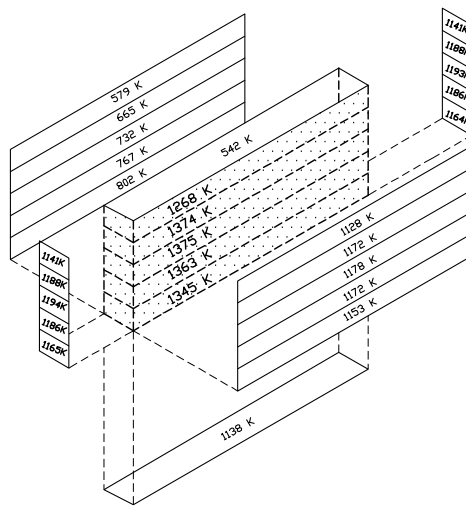


Figure 9: Temperature results from simulation

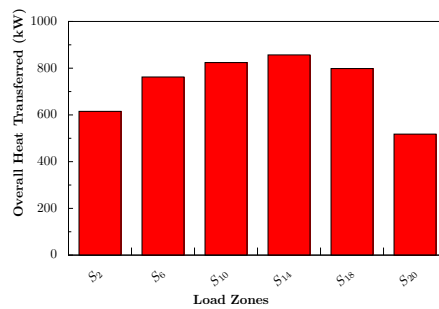


Figure 10: Overall heat transferred to each load surface

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