

Mathematical modeling of a rotary hearth coke calciner

H. C. MEISINGSET† and J. G. BALCHEN†

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A mathematical model of a rotary hearth coke calciner is developed. The model is based on first principles including the most important dynamic phenomena. The model is a thermodynamic model involving heat and mass transfer and chemical reactions. Fundamental mass and energy balance equations for the coke phase, the gas phase and the lining are formulated. For the gas phase, a stationary model is used. The equations are solved numerically, and simulated temperature profiles are shown in this paper.

1. Introduction

Petroleum coke is a hard and brittle substance, high in fixed carbon and low in ash. It is one of the purest forms of carbon produced in large quantities. Petroleum coke is produced from various petroleum residual fractions. Temperatures of about 500°C convert these resids into green coke within a day (Marsh 1989). A complex series of endothermic pyrolysis reactions produce liquid crystal mesophase which is transformed to a carbon polymer of generally graphitic structure. The result is a coke with a more or less anisotropic structure and related property values.

Most of the petroleum coke produced is used as filler material in the production of anodes for the aluminium industry. Coke for the aluminium industry must be calcined before use to produce quality anode carbon. This calcined coke should be relatively hard, strong, dense, with low electrical resistivity and oxidation sensitivity, high purity and available in aggregate sizing from 26 mm particles to cover standard anode filler sizing requirements (Jones 1986).

Most industrial coke calcination is done using rotary kiln calciners (Perron *et al.* 1988). Some industrial calcination is done in a rotary hearth calciner. Several calciner models have been reported in the literature (Perron *et al.* 1992). However, these models all refer to the rotary kiln calciner and include only steady state models.

In this paper, a dynamic model of a rotary hearth calciner is presented. The final coke quality depends on the thermal treatment of the coke. In order to develop a model based control system, it is therefore important to describe the thermodynamics of the calciner. The model is based on first principles including physical and chemical knowledge.

The paper is organized as follows: In § 2 a short process description is given. In § 3 the chemical reactions are presented. In § 4 heat transfer mechanisms are discussed. In §§ 5 and 6 fundamental mass- and energy balance equations are formulated for the coke

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† The Norwegian Institute of Technology, Department of Engineering Cybernetics, N-7034 Trondheim, Norway. email: hilde@itk.unit.no

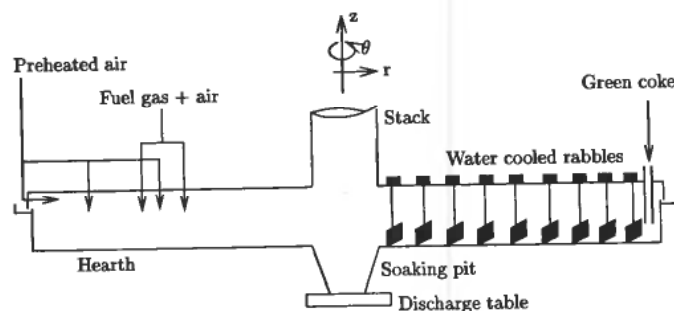


Figure 1. Schematic diagram of a rotary hearth calciner.

bed and the gas phase, respectively. In § 7 the temperature of the lining is modeled. In § 8 simulation results are presented. The conclusions are presented in § 9.

2. Process description

The rotary hearth calciner consists of a horizontal rotating circular table or hearth (Fig. 1). The rotating hearth is inside a furnace chamber. Green coke is fed from a feed bin through a feedshute to the outermost edge of the hearth. On the ceiling a number of rabblers are mounted. The rabblers are guiding the coke in circular paths from the outermost edge to centre of the hearth. The rabblers are water cooled. In the centre of the hearth, the coke falls into a soaking pit before removal from the calciner. Air is supplied through a number of wickets on the ceiling and in the side wall. Several burners are located on the ceiling. During transportation, the coke is heated from the surrounding gas and the lining. Coke moisture is then removed and upon further heating, volatile matter is released and burned in the gas phase. Most of the energy is supplied through volatile combustion. In addition, energy can be supplied by the burners.

The exhaust gas flows through the stack under the influence of a fan controlling the gas pressure. The exhaust gas is further utilized in a steam generator.

During calcination, the overall composition and structural properties of the coke change. The green coke contains typically 8–10% moisture and 8–10% volatile matter. All of the moisture and most of the volatiles are assumed removed during normal operation. Calcined coke is a rather pure carbon except for the sulphur content. Also, metallic impurities of few tenths of one percent are present.

For modeling purposes, the calciner will be divided into three parts

- The coke bed
- The gas phase
- The lining (hearth, roof and walls above the bed)

Mass is exchanged between the coke bed and the gas phase. Heat is exchanged between the coke bed, the gas phase and the lining.

3. Chemical reactions

During calcination several phenomena take place

- Water evaporation from the coke bed
- Release of volatiles from the coke bed
- Combustion of the volatiles and fuel gas in the gas phase

- Combustion of the coke bed
- Dust generation

It is assumed that the hydrocarbons are burned in the gas phase and not in the coke bed. Sulphur release will not be considered. Sulphur release is assumed to occur at higher temperatures than the maximum temperature of the coke during normal calciner operation, (Rhede 1967).

3.1. Evaporation of water

The evaporation of water can be expressed by the reaction



This is an endothermal process. According to Perron *et al.* (1992), the rate of evaporation may be modeled by an Arrhenius rate law. Let g_{H_2O} ($[kg/m^3s]$) denote the rate of evaporation of water written

$$g_{H_2O} = k_{H_2O,0} \cdot e^{-E_{H_2O}/RT_c} \cdot x_{H_2O} \cdot \rho_c \quad (2)$$

where

- x_{H_2O} mass fraction of water in the coke $[kg/kg]$
- $k_{H_2O,0}$ pre-exponential factor $[s^{-1}]$
- E_{H_2O} activation energy $[J/mole\ K]$
- ρ_c coke bed density $[kg/m^3]$
- T_c coke bed temperature $[K]$

The values for k_{H_2O} and E_{H_2O} are taken from Perron *et al.* (1992).

3.2. Release of volatile matter

The devolatilization starts with the release of condensable hydrocarbons. This is followed by the release of noncondensable hydrocarbons, mainly hydrogen and methane (Charette *et al.* 1992). The devolatilization is a complex process. The details will not be considered here. The devolatilization will simply be expressed by a stoichiometric equation of the form



where X represents the green coke, Y the calcined coke and Z the gaseous reaction products. In modeling the release of volatile matter, the following are assumed

- The volatiles are lumped into three components: hydrogen (H_2), methane (CH_4) and tar ($C_{18}H_{12}$)
- The releases are described by independent reactions

According to Dervede *et al.* (1986), the rate of the release of component i may be modeled by an Arrhenius-like rate equation

$$\frac{d\eta_i}{dt} = -k_{0,i} e^{-E_i/RT_c} (\eta_i)^{n_i} \quad (4)$$

where

- $k_{i,0}$ pre-exponential factor $[s^{-1}]$
- E_i activation energy
- i component $i \in [H_2, CH_4, C_{18}H_{12}]$

η_i fraction of component i not converted $\eta_i|_{t=0} = 1$
 n_i reaction order

Let $x_{i,0}$ ([kg/kg]) denote the initial mass fraction of component i in the coke. Let $\rho_{c,0}$ denote the initial coke density. The volatile emission rate, g_i ([kg/m³s]), can then be found

$$g_i = -x_{i,0} \cdot \rho_{c,0} \cdot \frac{d\eta_i}{dt} \quad (5)$$

The parameters used in the rate expressions are taken from Dervede *et al.* (1986).

3.3. Dust generation

Production of carbon dust at the surface of the bed is influenced by several factors. Li and Friday (1974) have developed a rate expression for the generation of dust in a rotary kiln calciner. The variables influencing the dust generation in a rotary kiln are

- (1) kiln rotational speed
- (2) gas density, viscosity and velocity
- (3) coke density
- (4) coke moisture and volatile release

Compared to the dust generation in a rotary kiln calciner, the dust generation in a rotary hearth calciner is much smaller (Brandt 1986). This is mainly due to the reduced mechanical abrasion in the rotary hearth compared to the rotary kiln.

A dust generation rate law will be proposed based on the above discussion. Let g_d ([kg/m³s]) denote the dust generation rate. The generation is written

$$g_d = k_d \cdot \mu_g^{n_1} \cdot v_g^{n_2} \cdot \rho_g^{n_3} \cdot \rho_c^{n_4} \cdot x_{H_2O}^{n_5} \cdot \omega^{n_6} \quad (6)$$

where

μ_g gas viscosity [kg/ms]
 ρ_g gas density [kg/m³]
 ρ_c coke bed density [kg/m³]
 v_g gas velocity [m/s]
 k_d parameter
 ω rotational speed

The gas viscosity is assumed to be proportional to the square root of the gas temperature. Assuming the ideal gas law and approximately constant pressure, the gas density is modeled inversely proportional to the gas temperature

$$g_d = k_d \cdot T_g^{m_1} \cdot v_g^{m_2} \cdot \rho_c^{m_3} \cdot x_{H_2O}^{m_4} \cdot \omega^{m_5} \quad (7)$$

The parameters k_d and m_i should be estimated according to dust generation data.

3.4. Combustion of the coke bed

During normal calciner operation, oxygen excess will be assumed and the temperature regime is below 2000°C. Therefore, only the overall reaction will be considered



It will be assumed that the reaction takes place at the surface of the coke bed and that

the reaction rate is proportional to the diffusion of oxygen from the gas bulk to the coke bed surface (Kanury 1977).

Let y_{O_2} denote the oxygen concentration in the gas phase. The diffusion of oxygen can be written by Fick's first law:

$$J = D_{O_2} \nabla y_{O_2} \quad (9)$$

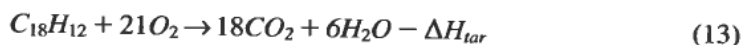
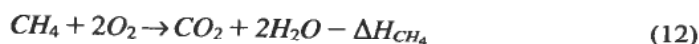
where D_{O_2} is the diffusivity constant. At the coke bed surface, the oxygen concentration will be assumed equal to zero due to the assumed fast reaction kinetics. The burning rate, g_c , will then be assumed proportional to the oxygen concentration in the gas phase:

$$g_c = k_c \cdot y_{O_2} \quad (10)$$

where y_{O_2} is the oxygen concentration in the gas phase and k_c is the proportionality constant. The combustion of dust is assumed to follow the same rate expression.

3.5. Combustion of volatiles

The hydrocarbons are burned in the gas phase. It is assumed that the combustion is complete. The combustion equations can then be written



with $\Delta H_{H_2} = -120000$ kJ/kg, $\Delta H_{CH_4} = -50000$ kJ/kg and $\Delta H_{tar} = -39000$ kJ/kg, (Perron *et al.* 1992).

The following rate expression will be used for the combustion (Perron *et al.* 1988):

$$g_i = k_{0,i} \cdot e^{-E_i/RT} \cdot \rho_g^2 \cdot y_i \cdot y_{O_2} \quad (14)$$

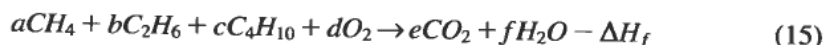
where

- g_i rate of combustion [kg/m³s]
- $k_{0,i}$ pre-exponential factor
- y_i mass fraction of component i in the gas phase
- ρ_g gas density [kg/m³]

The constants used in the rate expressions are taken from Perron *et al.* (1992).

3.6. Combustion of fuel gas

The fuel gas is assumed to be a mixture of methane, ethane, propane and butane. The combustion equation, assuming complete combustion, can be written

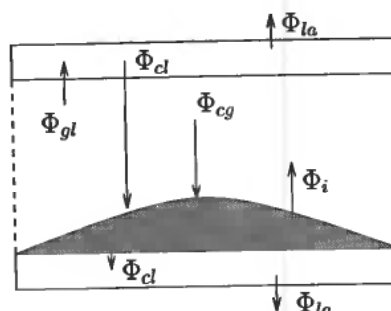


where

$$d = 2 \cdot a + 3.5 \cdot b + 5 \cdot c + 6.5 \cdot d \quad (16)$$

$$e = a + 2 \cdot b + 3 \cdot c + 4 \cdot d \quad (17)$$

$$f = 2 \cdot a + 3 \cdot b + 4 \cdot c + 5 \cdot d \quad (18)$$



- Φ_{cg} radiant and convective heat flux between the gas and the coke bed
 Φ_{gl} radiant and convective heat flux between the gas and the lining
 Φ_{cl} radiant and conductive heat flux between the coke bed and the lining
 Φ_{la} radiant and convective heat flux between the lining and ambient air
 Φ_i heat flux due to evolution of component i from the coke bed to the gas

Figure 2. Heat transfer between the coke bed, the gas phase and the lining.

The following coefficients are chosen: $a = 0.962$, $b = 0.014$, $c = 0$, $d = 0$ (Perron *et al.* 1992).

The fuel gas is supplied together with sufficient air. The reaction rate will be assumed infinitely high due to the assumption of good mixing between the air and fuel gas.

4. Heat transfer in the calciner

There are in general three modes of transfer which can be defined

- (1) Conduction
- (2) Convection
- (3) Radiation

The heat transfer in the calciner is complicated and will involve all three modes of heat transfer. The heat flux pattern between the gas phase, the lining and the coke bed can be described by the following notation (Fig. 2). The figure illustrates a typical cross section of the coke bed in the rotational direction. In addition, heat conduction in the coke bed and in the lining, and heat transfer to the water cooled rabbles are considered. For the soaking pit, a similar illustration can be made.

The relative importance of the modes of heat transfer very much depends on the temperature. In high temperature processes, radiative heat transfer will dominate.

4.1. Radiative heat transfer

For the radiative heat transfer the following assumptions will be made

- Total radiative properties will be considered
- The coke bed and the lining are grey and opaque
 - $\epsilon = \alpha$
 - $\tau = 0 \Rightarrow \rho = 1 - \alpha$
- The gas is grey, transmitting and non-reflecting
 - $\epsilon_g = \alpha_g$

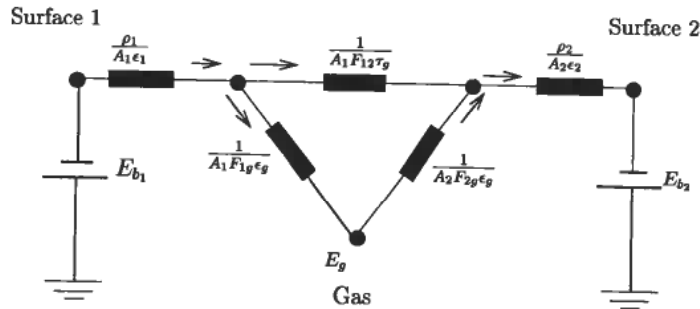


Figure 3. Thermal circuit for two finite plates with intermediate gas. From Kreith and Black (1980).

where ϵ denotes the emissivity, α denotes the absorptivity, ρ denotes the reflectivity and τ denotes the transmissivity. The gas mixture emissivity can be found from emissivity diagrams for H_2O and CO_2 (Hottel and Sarofim 1967). In addition, the soot emissivity must be included. The soot emissivity depends on the soot concentration. The method of Modak (1978) can be used to find the soot radiative properties.

It will be assumed that the furnace length in the direction of gas flow is large compared to its height so that net radiative flux in the gas-flow direction can be ignored. Only flux in the direction normal to the flow will be considered.

Radiation between grey surfaces separated by a grey gas is considered in Kreith and Black (1980). The thermal circuit is shown in Fig. 3.

The radiation will be simplified by assuming that the surfaces are dark grey. The radiative exchange terms can be simplified because the contribution to the radiative exchange by beams that have undergone more than one reflection at the surfaces is small (Hottel and Sarofim 1967).

The radiation between the coke bed and the gas is expressed by

$$\Phi_{r,gc} = F_{gc} \cdot \frac{\epsilon_c + 1}{2} \cdot \sigma \cdot \epsilon_g \cdot (T_g^4 - T_c^4) \quad (19)$$

The radiation between the gas and the lining is expressed by

$$\Phi_{r,gl} = F_{gl} \cdot \frac{\epsilon_l + 1}{2} \cdot \sigma \cdot \epsilon_g \cdot (T_g^4 - T_l^4) \quad (20)$$

The radiation between the coke bed and the lining is expressed by

$$\Phi_{r,cl} = F_{cl} \cdot \epsilon_l \cdot \epsilon_c \cdot (1 - \epsilon_g) \cdot \sigma \cdot (T_c^4 - T_l^4) \quad (21)$$

where

- F_{gc} form factor
- F_{cg} form factor
- F_{cl} form factor
- F_{gc} form factor
- ϵ_c coke bed emissivity
- ϵ_g gas emissivity
- ϵ_l lining emissivity
- T_c coke bed surface temperature [K]
- T_g gas temperature [K]
- T_l lining temperature [K]
- σ Stefan-Boltzmann constant [W/m^2K^4]

4.2. Convective heat transfer

Convective heat transfer between the gas and the lining, $\Phi_{c,gl}$, between the gas and the coke bed surface, $\Phi_{c,gc}$, and between the lining and the ambient, $\Phi_{c,la}$, air are calculated from

$$\Phi_{c,gc} = h_{gc} \cdot (T_g - T_c) \quad (22)$$

$$\Phi_{c,gl} = h_{gl} \cdot (T_g - T_l) \quad (23)$$

$$\Phi_{c,la} = h_{la} \cdot (T_l - T_a) \quad (24)$$

where

- h_{gc} heat transfer coefficient gas to coke [$\text{J/m}^2\text{K}$]
- h_{gl} heat transfer coefficient gas to lining [$\text{J/m}^2\text{K}$]
- T_c coke surface temperature [K]
- T_g gas temperature [K]
- T_l lining temperature [K]
- T_a ambient air temperature [K]

The convective heat transfer coefficients are calculated from correction for the Nusselt number (Nu)

$$\text{Nu} = \frac{hd}{k_g} \quad (25)$$

where h is the heat transfer coefficient, d is the hydraulic diameter, k_g is the gas thermal conductivity. Convective heat transfer between the gas and the lining and between the gas and coke bed are considered as forced convection. The forced convection is assumed to take place in the turbulent regime; $\text{Re} \sim 60000$, (Storaker 1989). For turbulent gas in a circular tube:

$$\text{Nu} = 0.02 \text{Re}^{0.8} \text{Pr}^{0.33} \quad (26)$$

Pr is the Prandtl number. For all diatomic gases and for carbon dioxide, $\text{Pr} = 0.74$. For water vapour it is higher, but for ordinary furnace gases at atmospheric pressure Pr can usually be considered constant at the above figure (Gilchrist 1977).

For other geometries it is possible to use the equation for turbulent flow inside a circular pipe and use some equivalent diameter, d_{eq} , in the place of d (Coulson and Richardson 1988). An equivalent diameter is defined as four times hydraulic radius:

$$d_{eq} = 4 \frac{\text{cross section of channel}}{\text{wetted perimeter}} \quad (27)$$

For the external lining surfaces, a correlation for the Nusselt number for laminar free convection may be used. However, in this work a simplification is introduced by applying constant heat transfer coefficients.

4.3. Conductive heat transfer

Heat flux by conduction is proportional to the temperature gradient (Fourier's law)

$$\Phi_{cond} = -k\nabla T \quad (28)$$

where

- k thermal conductivity [W/mK]
 T temperature [K]

Heat conduction is neglected in the gas phase. For the solid coke bed and the lining, heat conduction is included. The heat conduction is considered to be one dimensional.

The coke bed is considered as a thermally thick medium: This can be expressed by the dimensionless Biot-number (Bi) (Kreith and Black 1980):

$$Bi = \frac{hV}{kA} \quad (29)$$

where

- h heat transfer coefficient from gas/lining to the coke bed [J/m²K]
 V volume [m³]
 k thermal conductivity [W/mK]
 A area [m²]

In the case of $Bi > 1$, the solid is considered as a thermally thick medium.

For the coke bed, the effective heat transfer coefficient is due to both radiation and convection. Consider the case of heat transfer from the gas to the coke bed surface. Due to the high temperatures, the radiative heat transfer will dominate. The heat transfer coefficient can be approximated by

$$h_{eff} \approx \epsilon_g \frac{\epsilon_c + 1}{2} \sigma \frac{T_g^4 - T_c^4}{T_g - T_c} \quad (30)$$

In the case of luminous flames, ϵ_g can be approximated to 1. Consider the case of a gas temperature $T_g = 1000^\circ\text{C}$, let $\epsilon_c = 0.8$ and $k = 1$ and suppose the coke bed height is 0.2 m. h_{eff} and the Bi number for two different coke temperatures are approximately given by

$$T_c = 100^\circ\text{C} \Rightarrow h_{eff} = 73 \Rightarrow Bi = 15 \quad (31)$$

$$T_c = 500^\circ\text{C} \Rightarrow h_{eff} = 115 \Rightarrow Bi = 23 \quad (32)$$

Due to the high Bi numbers computed, the coke bed will be modeled with heat conduction in the axial direction.

The same argument can be used for the lining.

Coke bed effective heat conductivity. The heat transfer in the coke bed is the result of conduction, convection due to volatile release and radiation due to inter particle radiation.

An effective thermal conductivity, k_{eff} , will be used. The effective conductivity accounts for solid conduction and inter particle radiation and neglects the gas conductance (Kolbeinsen 1994).

$$k_{eff} = (1 - \sqrt{1 - \epsilon_b})k_R + \frac{\sqrt{1 - \epsilon_b}}{\frac{1}{k_R} + \frac{1}{k_p}} \quad (33)$$

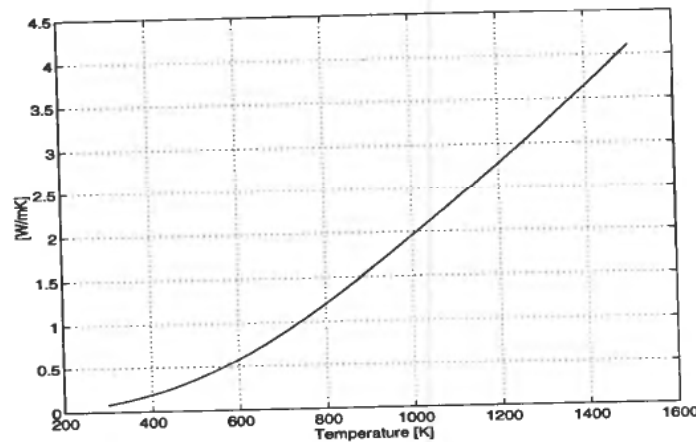


Figure 4. Coke bed effective thermal conductivity.

Where ϵ_b is the bed voidage and k_R is due to radiation given by

$$k_R = \frac{0.04C_R}{\frac{2}{\epsilon} - 1} \cdot \left(\frac{T}{100}\right)^3 \cdot d_p \quad (34)$$

where

- d_p average particle diameter [m]
- ϵ particle emissivity
- T average temperature [K]
- C_R constant

k_p is the thermal conductivity for a particle with porosity

$$k_p = k_s(1 - \epsilon_p) \quad (35)$$

k_s is the thermal conductivity for a coke particle without pores.

The effective thermal conductivity is seen to increase with increasing temperature (Fig. 4).

5. The coke bed

The coke bed can be considered as a packed bed of porous particles of different shapes and sizes. In formulating the coke bed mass- and energy balance equations, only bulk phenomena are considered.

The coke particles are treated as a bulk mass described by a bulk density, ρ_c ([kg/m³]). The green coke enters the outermost periphery of a horizontal rotating hearth. The hearth rotates with rotational speed denoted ω ([rps]). After the completion of one revolution, the coke particles are mechanically moved by the rabbles in the radial direction to the next concentric path (Fig. 5).

It is assumed that the rabbles cause an axial coke bed mixing. The mixing will be described by an operator K . It is assumed that no back-mix flow of the coke bulk exists. After the completion of each concentric path, all the coke mass is transported into the next concentric path. It is assumed that each path has the same area. The paths widen as approaching the centre of the hearth.

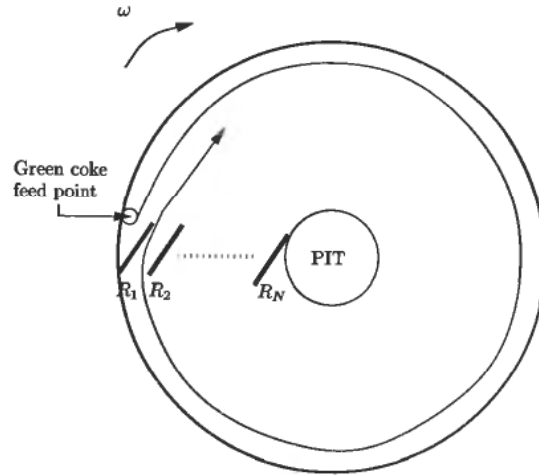


Figure 5. Overview of the rotating coke bed. The coke is transplanted in concentric paths with angular velocity, ω . $R_1, 2, \dots, R_N$ denote the rabbles.

5.1. The mass balance

Let N denote the total number of paths, which equals the number of rabbles. The coke particles are transported from the outer most path denoted $j = 1$ to the innermost path, denoted $j = N$.

Let R_j and R_{j+1} denote the outermost and innermost radii of path j , respectively. The rabbles are assumed located so that each path has the same area

$$\forall i, j: \int_{R_i}^{R_{i+1}} 2\pi r dr = \int_{R_j}^{R_{j+1}} 2\pi r dr \quad (36)$$

Define

$$m_c(\theta, j, z) = \int_{R_j}^{R_{j+1}} \rho_c \cdot r dr \quad (37)$$

$m_c()$ denotes mass of coke per unit radian per unit height. By assuming the density being independent of r , $R_j \leq r \leq R_{j+1}$, m_c can be written

$$m_c(\theta, j, z) = \rho_c \cdot \Delta R_j \cdot (R_j + R_{j+1}) \quad (38)$$

The mass balance can now be written

$$\frac{\partial m_c}{\partial t} + v_\theta \frac{\partial m_c}{\partial \theta} + w_c = 0 \quad (39)$$

with boundary conditions

$$j = 1, \theta = 0 : m_c v_\theta = w_f \quad (40)$$

$$j > 1, \theta = 0 : m_c = \int_0^{Z_c} K(z, \xi) m_c(2\pi, j-1, \xi) d\xi \quad (41)$$

where

- w_c mass loss [kg/m rad s]
- w_f green coke feed rate [kg/s m]
- K mixing operator

Z_c coke bed height
 v_θ coke angular velocity; [rad/s]
 $v_\theta = 2\pi\omega$

w_c is due to water and volatile releases

$$w_c = \sum_i w_{c,i} \quad (42)$$

where

$$\begin{aligned} w_{c,i} &= \int_{R_j}^{R_{j+1}} g_i r dr = -m_{i,0} \cdot \frac{d\eta_i}{dt} \\ &= m_{i,0} \cdot k_{i,0} e^{E_i/RT_c} \cdot (\eta_i)^{n_i} \\ &= m_{i,0} \cdot k_{i,0} e^{E_i/RT_c} \cdot \left(\frac{m_i}{m_{i,0}}\right)^{n_i} \end{aligned} \quad (43)$$

where m_i is the density of component i and $m_{i,0}$ denotes the initial density.

The operator K describes the axial mixing caused by the rabbles. K is determined by the degree of mixing and must fulfill the following condition

$$\int_0^{Z_c} K(\xi, z) d\xi = 1 \quad (44)$$

Coke combustion and dust generation are assumed to occur at the surface of the coke bed. This is modeled as a reduction in the coke bed height

$$m_c(Z_c) \left(\frac{\partial Z_c}{\partial t} + v_\theta \frac{\partial Z_c}{\partial \theta} \right) = w_{c,c} \quad (45)$$

$$w_{c,c} = \int_{R_j}^{R_{j+1}} (g_d + g_c) r dr \quad (46)$$

The coke components mass balances will also be formulated. Let i denote coke component, $i \in [\text{H}_2\text{O}, \text{H}_2, \text{CH}_4, \text{C}_{18}\text{H}_{12}]$. For each of the coke components, the mass balances will be formulated.

$$\frac{\partial m_i}{\partial t} + v_\theta \frac{\partial m_i}{\partial \theta} + w_{c,i} + \frac{m_i}{m_c} \cdot w_{c,c} = 0$$

The boundary conditions are

$$j > 1, \theta = 0 : m_i(\theta, j, z) = \int_0^{Z_c} K(z, \xi) m_i d\xi \quad (47)$$

$$j = 1, \theta = 0 : v_\theta \cdot m_i = w_{f,i} \quad (48)$$

5.2. The energy balance

With the plug-flow assumption the energy balance becomes

$$m_c c_c \frac{\partial T_c}{\partial t} + v_\theta m_c c_c \frac{\partial T_c}{\partial \theta} = \Delta R_j \frac{\partial}{\partial z} \left(k_{eff} \frac{\partial T_c}{\partial z} \right) + \sum_i \Delta H_i w_{c,i} \quad (49)$$

With boundary conditions

$$j = 1, \theta = 0 : T_c = T_{green} \quad (50)$$

$$j \neq 1, \theta = 0 : T_c = \frac{1}{m_c} \int_0^{Z_c} K(z, \xi) T_c(2\pi, j-1, \xi) m_c(2\pi, j-1, \xi) d\xi \quad (51)$$

$$z = 0 : -k_{eff} \frac{\partial T_c}{\partial z} = k_l \frac{\partial T_l}{\partial z} \quad (52)$$

$$z = Z_c : k_{eff} \frac{\partial T_c}{\partial z} = \Phi_{gc} + \Phi_{cl} \quad (53)$$

where

- c_c average coke heat capacity [J/kgK]
- T_c coke temperature [K]
- k_{eff} effective coke bed conductivity [W/mK]
- ΔH_i reaction enthalpy [J/kg]
- T_{green} green coke temperature [K]
- T_l lining temperature [K]
- Φ_{cl} heat flux from the coke bed to the lining [W/m²]
- Φ_{gc} heat flux from the gas to the coke bed [W/m²]
- Φ_{cr} heat flux from the coke bed to the rabbles [W/m²]

The coke heat capacity is dependent on the temperature. The following relationship can be used (Perry and Green 1984)

$$c_c = 2.673 + 0.002617 \cdot T_c - 116900 \cdot T_c^{-2} \quad (54)$$

The heat fluxes can be written

$$\Phi_{gc} = F_{gc} \frac{\epsilon_c + 1}{2} \cdot \sigma \cdot (\epsilon_g T_g^4) + h_{gc} \cdot (T_g - T_c) \quad (55)$$

$$\Phi_{cl} = F_{gl} \epsilon_l \epsilon_c (1 - \epsilon_g) \sigma (T_c^4 - T_l^4) \quad (56)$$

In addition, heat flux between the coke and the rabbles (Φ_{cr}) is considered. Φ_{cr} is expressed as a function of θ in the following way;

$$\Phi_{cr}(j, \theta, z) = \begin{cases} h_{cr} \cdot (T_c - T_r); & \theta = 2\pi \\ 0 & \text{otherwise} \end{cases} \quad (57)$$

where h_{cr} is an effective heat transfer coefficient and T_r is the rabble temperature.

6. The gas phase

The gas phase can be considered as a combustion chamber and serves as a heat exchanger. It is the energy supplied to the coke bed which is of main importance, not the detailed gas flow pattern.

The gas components considered are

- air: O₂, N₂
- volatiles: H₂, CH₄, C₁₈H₁₂
- water from the coke bed
- fuel gas
- combustion products: H₂O and CO₂

A steady state gas model will be used. The dynamics of the gas are much faster than that of the coke bed. The excitations in the gas states are assumed slow compared to the dynamic mode of the gas.

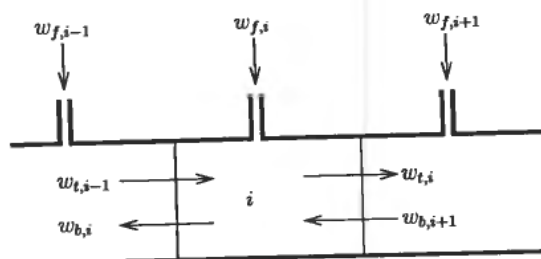


Figure 6. Staged reactor with internal back-mix flow.

6.1. The gas flow model

The gas flow pattern is complicated. The overall bulk gas flow is directed towards the centre of the hearth and further through the stack. Air wickets are distributed on the ceiling and in the side walls. Burners are located on the ceiling. Water vapour and by hydrocarbons enters the gas phase from the coke bed. False air from the outside will also influence the gas phase.

Only gas flow in the radial direction is considered. Mixing in the axial and the angular direction is assumed due to the turbulent character of the gas flow.

Radial flow with radial mixing will be modeled as a series of mixed vessels with an internal back-mix flow (Fig. 6). The vessels have different volumes. Also the vessels have one or several feed streams corresponding to the supply of process air and fuel gas and to the mass transfer from the coke bed. A plug flow model with a dispersion term could alternatively be used. By increasing the number of vessels, the two models can be used to represent the same flow pattern. This is discussed in Froment and Bischoff (1990).

The following notation is used: $w_{f,i}$ denotes the feed stream entering the vessel. For simplicity only a single feed stream is shown. $w_{f,i}$ represents the sum of the process air, fuel gas and mass flow from the coke bed. $w_{t,i}$ denotes the total forward mass flow rate. $w_{b,i}$ denotes the back flow rate. w_i denotes the net mass flow from vessel i to vessel $i + 1$. Then

$$w_{t,i} = w_i + w_{b,i+1} \quad (58)$$

It is assumed that the back-mix flow can be modeled (Singstad 1992)

$$w_{b,i} = b_i \cdot w_i \quad (59)$$

where b_i is the back-mix coefficient for stage i . If N represents the number of stages, the boundary conditions are written

$$w_0 = 0 \quad (60)$$

$$b_I = b_{N+1} = 0 \quad (61)$$

6.2. The mass balances

The total mass balance equation for vessel i can be written

$$\frac{\partial \rho_i}{\partial t} + \frac{1}{V_i} (-w_{i-1} + w_i - w_{f,i}) = 0 \quad (62)$$

where

$$\begin{aligned} \rho_i & \text{ gas density vessel } i \text{ [kg/m}^3\text{]} \\ V_i & \text{ volume of vessel } i \text{ [m}^3\text{]} \\ w & \text{ mass flow [kg/s]} \end{aligned} \quad (63)$$

For each of the gas components j in vessel i the following mass balance can be written

$$\begin{aligned} \frac{\partial(\rho_i y_{j,i})}{\partial t} = & \frac{1}{V_i} (w_{t,i-1} y_{j,i-1} - w_{b,i} y_{j,i} - w_{t,i} y_{j,i} \\ & + w_{b,i+1} y_{j,i+1} + w_{f,i} y_{j,f}) + (S^T \cdot g_i)_j \end{aligned} \quad (64)$$

where

$$\begin{aligned} y_{j,i} & \text{ mass fraction of component } j \text{ in vessel } i \text{ [kg/kg]} \\ y_{j,f} & \text{ mass fraction of component } j \text{ in feed stream [kg/kg]} \\ g_i & \text{ vector of mass rates of combustion [kg/m}^3\text{s]} \\ S & \text{ stoichiometric matrix} \end{aligned}$$

This can be written using vector notation

$$\rho_i V_i \frac{\partial \mathbf{y}_i}{\partial t} = w_{t,i-1}(\mathbf{y}_{i-1} - \mathbf{y}_i) + w_{b,i+1}(\mathbf{y}_{i+1} - \mathbf{y}_i) + w_{f,i}(\mathbf{y}_f - \mathbf{y}_i) + S^T \mathbf{g}_i \cdot V_i \quad (65)$$

The stationary total mass balance can be written

$$\begin{aligned} \frac{\partial \rho_i}{\partial t} = 0 \Rightarrow w_i &= w_{i-1} + w_{f,i} \\ w_i &= \sum_{j=1}^i w_{f,j} \end{aligned} \quad (66)$$

The stationary component mass balance can then be written

$$\frac{\partial \mathbf{y}_i}{\partial t} = 0 \Rightarrow w_{t,i-1}(\mathbf{y}_{i-1} - \mathbf{y}_i) + w_{b,i+1}(\mathbf{y}_{i+1} - \mathbf{y}_i) + w_{f,i}(\mathbf{y}_f - \mathbf{y}_i) + S^T \mathbf{g}_i V_i \quad (67)$$

6.3. The energy balance

The energy balance can be written for each vessel i (Froment and Bischoff 1990).

$$\frac{\partial}{\partial t}(\rho_i u_i) = \sum_j w_{in,j} H_j - \sum_j w_{out,j} H_j + Q_i + W_{s,i} \quad (68)$$

where

$$\begin{aligned} u_i & \text{ specific internal energy [J/kg]} \\ w_{in} & \text{ mass flow rates entering [kg/s]} \\ w_{in} &= W_{t,i-1} + W_{b,i-1} + w_{f,i} \\ w_{out} & \text{ mass flow rates leaving [kg/s]} \\ w_{out} &= W_{t,i} + W_{b,i} \\ H_j & \text{ specific enthalpy [J/kg]} \\ Q_i & \text{ heat transfer to the surroundings [W]} \\ W_{s,i} & \text{ work performed on the surroundings, except for pressure work [W]} \end{aligned}$$

The internal energy can be written

$$u_i = H_i - P_i / \rho_i \quad (69)$$

where P_i denotes total pressure. The enthalpy change in the case of no phase change can be written

$$dH = c_p dT \quad (70)$$

where c_p is the specific heat capacity and T is the temperature.

Neglecting variations in total pressure, considering the case of no phase change and neglecting the work term, the energy balance can be written

$$\begin{aligned} V_i \rho_i \sum_j c_{pj} y_{j,i} \frac{\partial T_i}{\partial t} = & w_{t,i-1}(T_{i-1} - T_i) \sum_j y_{j,i-1} c_{pj} + w_{b,i+1}(T_{i+1} - T_i) \sum_j y_{j,i} c_{pj} \\ & + w_{f,i}(T_f - T_{i-1}) \sum_j y_{j,f} c_{pj} + Q_i + \sum_k \Delta H_k g_{i,k} V_i \end{aligned} \quad (71)$$

where

c_{pj} specific heat capacity of component j [J/kgK]
 ΔH_k reaction enthalpy due to combustion reaction k [J/kg]

The stationary energy balance can be written

$$\begin{aligned} & w_{t,i-1}(T_{i-1} - T_i) \sum_j y_{j,i-1} c_{pj} + w_{b,i+1}(T_{i+1} - T_i) \sum_j y_{j,i} c_{pj} \\ & + w_{f,i}(T_f - T_{i-1}) \sum_j y_{j,f} c_{pj} + Q_i + \sum_k \Delta H_k g_{i,k} V_i = 0 \end{aligned} \quad (72)$$

Suppose that the gas phase can be described by an average heat capacity

$$c_g = \sum_j y_j c_{p,j} \quad (73)$$

The stationary energy balance can then be written

$$\begin{aligned} & \{ w_{t,i-1} c_g (T_i - T_{i-1}) + w_{b,i+1} c_g (T_{i+1} - T_i) + w_{f,i} c_g (T_{f,i} - T_{i-1}) \} \\ & + \sum_k \Delta H_k g_{i,k} V_i + Q_i = 0 \end{aligned} \quad (74)$$

Q_i is the radiative and convective heat transfer between the gas and the surroundings as described in the previous sections

$$Q_i = Q_{i,gc} + Q_{i,gl} + Q_{i,gr} + Q_{i,gs} \quad (75)$$

where

$Q_{i,gc}$ heat transfer gas to coke [W]
 $Q_{i,gl}$ heat transfer gas to lining [W]
 $Q_{i,gr}$ heat transfer gas to rabble [W]
 $Q_{i,gs}$ heat transfer gas to soaking pit [W]

7. The lining

The lining can be considered as two parallel plates. One plate represents the roof and the wall above the coke bed. The other plate represents the floor.

The lining material consists of different brick materials with an outside steel shell. The lining is subject to inside heating and outside cooling. The following approximations are made

- The lining is geometrically approximated by an infinite plate.
This is a good approximation due to the small thickness of the lining.
- The temperature gradient of the steel shell is neglected.
The outside steel shell has large thermal conductivity relative to the brick material. In addition the steel shell is much thinner than the brick and has lower heat capacity. Therefore the steel shell is neglected in the model. It will however determine the radiation to the ambient air.
- The thermal properties of the brick material is constant.
This point means neglecting the temperature dependencies of the heat capacity and the thermal conductivity. Different brick material is used, but not implemented.

Using the given approximations, the lining temperature will be written

$$\frac{\partial T_l}{\partial t} = \alpha_l \frac{\partial^2 T_l}{\partial z^2} \quad (76)$$

The boundary conditions are

$$z = 0 : -k_l \frac{\partial T_l}{\partial z} = \Phi_{in} \quad (77)$$

$$z = D : k_l \frac{\partial T_l}{\partial z} = \Phi_{out} \quad (78)$$

where

- T_l lining temperature [K]
- k_l thermal conductivity of the lining [W/mK]
- ρ_l density of the lining [kg/m³]
- D thickness [m]
- Φ_{in} heat flux at $z = 0$ [W/m²]
- Φ_{out} heat flux at $z = D$ [W/m²]

For the wall and the roof, Φ_{in} is given by the radiative and convective heat transfer between the wall and the gas and between the wall and the coke bed.

For the roof and the walls, Φ_{in} will be written

$$\Phi_{in} = h_{gl} \cdot (T_g - T_l) + \frac{\epsilon_l + 1}{2} \cdot \sigma \cdot \epsilon_g (T_g^4 - T_l^4) \quad (79)$$

For the hearth floor, Φ_{in} is given by the heat transfer between the floor and the coke bed. The floor is in thermal contact with the coke bed. This can be viewed as thermal conduction through composite solid. The total effect is that the coke loses energy to the surroundings and due to the heating of the floor. For the floor, Φ_{in} will be written

$$\Phi_{in} = k_{eff} \frac{\partial T_c}{\partial z} \quad (80)$$

where k_{eff} is the effective coke conductivity. An expression for Φ_{out} is written

$$\Phi_{out} = \sigma \epsilon_o \epsilon_l F_{oa} (T_a^4 - T_{wo}^4) + h_{oa} (T_a - T_{wo}) \quad (81)$$

where

- ϵ_o emissivity of outside shell

- F_{oa} form factor
 T_{wo} outside wall temperature [K]
 T_a ambient air temperature [K]
 h_{oa} convective heat transfer coefficient of outer shell surface [W/m²K]

With $F_{oa} = 1$ the heat flux can be written

$$\Phi_{out} = \sigma \epsilon_o \epsilon_t (T_a^4 - T_{wo}^4) + h_{oa} (T_a - T_{wo}) \quad (82)$$

8. Simulation results

The simulation model is a numerical means of solving the dynamic partially differential equations describing the coke and the lining mass and temperature profiles. Numerical methods for solving partially differential equations are discussed in Patankar (1980). This simulation model uses the finite difference method. Finite difference methods are easy to implement, and they work well under proper conditions (Sælid 1976).

Based on nominal process data, the stationary temperature profile will be presented. Suppose that the hearth is located in the origin of a coordinate system. The stationary temperature profile in the $r-\theta$ plane in the middle of the coke bed is shown in Fig. 7.

Stationary temperature profiles for the coke bed and the gas phase are shown in Fig. 8. The coke bed temperature profiles are shown as a function of coke bed axial coordinate from the outermost path (lowest path number) to the innermost path (highest path number). The coke surface temperature increases very fast and the surface has nearly the same temperature as the gas. This is mainly due to the intense radial heating. The plot also demonstrates the mixing action caused by the rabbles. In this simulation, perfect mixing is assumed.

A step change in the hearth rotational speed is simulated (Fig. 9). The plot shows the temperature response in the middle of the coke bed as a function of time and path number. The step was introduced at time zero. By increasing the rotational speed, the holding time on the hearth is decreased. From the figure it is seen that the coke bed temperature decreases. The reduction in temperature is most significant at the outermost paths (lowest path numbers).

9. Conclusions

A dynamic model of a rotary hearth calciner is proposed.

The model focuses on the thermodynamics of the coke bed including mass and heat transfer between the coke bed and the surroundings. The coke bed is described by a bulk density, mass fractions and temperature. Heat conduction in the coke bed is included. The simulation studies demonstrate that a temperature gradient in the bed is present. However, due to the mixing action caused by the rabbles, the temperature gradients are reduced.

In modeling the gas phase, a stationary model was assumed.

In addition to the thermodynamic model presented in this paper, a more rigorous coke model has been developed describing structural changes in the coke during calcination. The structural changes influence the final coke quality. Coke quality was revealed by properties such as mechanical strength, chemical reactivity and electrical resistivity can be expressed by transformation from the state space. In this framework a model based controller has been developed.

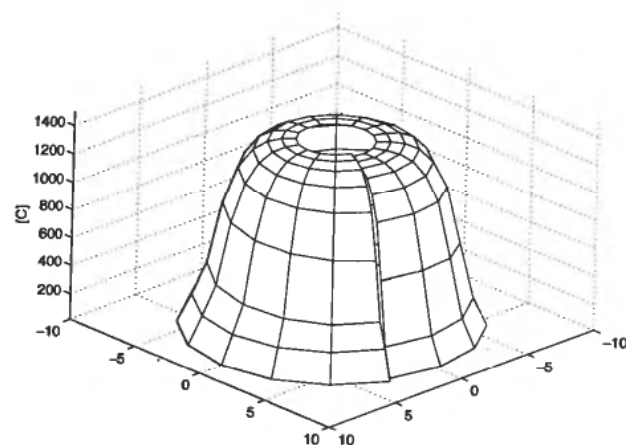


Figure 7. Stationary coke bed temperature profile in the middle $r-\theta$ plane.

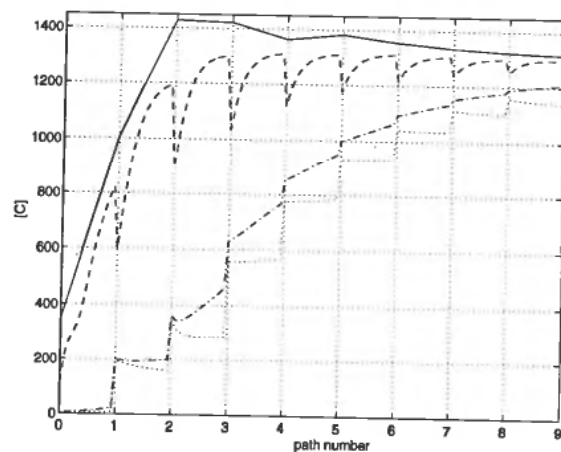


Figure 8. Steady state gas temperature (solid line) and coke bed temperature: Surface temperature (—), middle temperature (---), bottom temperature (-.-.-).

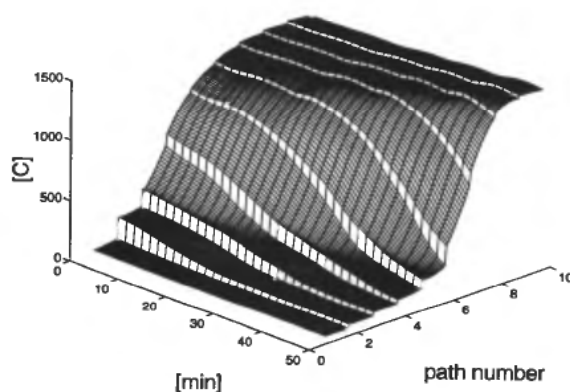


Figure 9. Coke bed temperature response of a step change in the rotational speed.

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