Modeling and Simulation of Carbonization Chamber Heat Transfer Process in Coke Oven

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Abstract. A novel modeling method based on MATLAB is proposed for heat transfer process of carbonization chamber in coke oven, to achieve time-driving simulation for coke making process. The inter-wall and half of a coal/coke blend are divided into several heat transfer plane units averagely. Based on heat transfer theory of one-dimensional plane, simulation model of heat transfer unit is built by Simulink, and then simulation models of the inter-wall and coal/coke blend are assembled by these unit models. Simulation software used for calculating thermal physical parameters and for analysing carbonization chamber heat transfer process is designed by MATLAB. Temperature curves of plane units in carbonization chamber inter-wall and coal/coke blend are obtained by simulation experiments, which show that the designed modeling method and simulation software are available.

1. Introduction

Recently, coke making enterprises in China are under increasing pressure from falling coke price. Meeting market demand and saving energy are inevitable choices in whole coke making industry. In coke making enterprises, the main product is furnace coke, but now major profits are from coke oven gas and derivative products. Then, some effective measures like delaying carbonization time and optimizing coal blending are applied to reduce coke stock pressure and to increase gas production. But these measures are usually driven from operator’s experiences, and should be tested and corrected by coke making thermal calculation and analysis.

Coke making process is a complex physical-chemistry process with material changing, heat transferring and polymorphic coexistence. In order to study flow-combustion-thermos behavior in coke oven, a three-dimensional transient mathematical model for coupled carbonization chamber and staging combustion chamber in large-capacity coke ovens is developed in [1]. And two types of decoupling numerical methods for coke ovens modeling are proposed in [2]. A two-dimensional transient model of coal carbonization is established in [3]. David Merrick proposes a series of mathematical models for thermal decomposition of coal during coke making process, include the specific heats and heats of reaction[4], the density, porosity and contraction behaviour[5],and the heat transfer and temperature profiles in coke-oven[6]. As an important software tool to study thermal behaviour of fluid-gas-solid coexistence system, CFD is widely used to analyze the thermal behaviours and characteristics in coke oven [7].

The aforementioned heat transfer models of carbonization chamber and combustion chamber are usually used to analyze steady-state characteristics of coke oven and the dynamic performance of coke making process are hard to emulate. In addition, these models are designed for one carbonization chamber or that coupled with combustion chamber, the performances of which cannot represent the whole coke oven, and the whole coke oven model is hard to compose by these models as well. So the
modeling methods of these existing models are inappropriate to build and to analyze continuous production process of coke oven.

In real coke making process, production efficiency are determined both by thermos characteristics of coke oven and performances of heating control system. As a control target, the coke oven model is usually used to test control algorithm in closed-loop [8], but it is obvious that the existing coke oven models are incompetent. So a dynamic simulation model of coke oven with time-driving is required.

2. Principle Analysis

In this paper, the heat transfer process of inter-wall and half of a coal/coke blend in 5.5m stamping-charging coke oven are discussed, and the central plane of coal/coke blend is treated as a heat-insulating layer. Then based on symmetric structure of coke oven, the continuous production process model of whole coke oven will be assembled by these models. Based on assumption that heat transfer process in coal/coke blend is plane heat transfer process, the inter-wall of carbonization chamber and 1/2 coal/coke blend are divided into multi plane units in longitudinal direction, material and temperature in one plane unit are uniform. The structure of carbonization chamber and inter-wall in coke oven is showed in figure 1. The modeling object in this work are inter-wall and carbonization chamber (1/2 coal/coke blend), which are divided into 10 and 50 plane units respectively. Each plane unit is independent and represented by dashed line in figure 1, and they are coded by number 1 to 10 and 1 to 50 in bottom of the figure. The carbonization chamber taper is neglected, and the coal/coke blend is treated as cuboid with width of 500mm, the inter-wall’s width is 90mm.

![Figure 1. Structure of carbonization chamber and wall in coke oven.](image)

2.1. Heat Transfer Process in Carbonization Chamber

The heat transfer process of plane unit in coal/coke blend is heat conduction process of double-layers one-dimensional plane, and heat conduction equation is

$$\rho_c c_c \frac{\partial T_c}{\partial t} = \frac{\partial}{\partial x} (\lambda_c \frac{\partial T_c}{\partial x}) + \sum q$$

(1)

Where $\rho_c$ is density in kg/m$^3$, $c_c$ is specific heat capacity in J/kg$^\circ$C, $\lambda_c$ is thermal conductivity in W/m$^\circ$C, $T_c$ is temperature in $^\circ$C, $\sum q$ is inner heat sources included reaction heat and latent heat of coal/coke blend in W/m$^3$. The subscript $c$ means coal/coke blend.

In coke making process, material in coal/coke blend changes with the increase of temperature, and physical parameters $\rho_c$, $c_c$, and $\lambda_c$, presented in (1), vary as well. Then we suppose that the temperature in one plane unit of coal/coke blend is uniform and parameters of this unit are constant at some instant.

In addition, $\sum q$ in (1) contains thermal energy from water evaporation and coal thermal decomposition reaction. But in this paper, the thermal physical parameters are equivalent parameters obtained by experimental analysis of coal sample. The influence of coal thermal decomposition reaction is included in these parameters. So thermal energy created by coal thermal decomposition reaction will not be included in $\sum q$, but the water evaporation process will be considered.
\[
\sum q = q_{\text{H}_2\text{O}} = \frac{dT}{dt} Q_{\text{H}_2\text{O}} (M_c, T_c)
\]  
(2)

Where \( Q_{\text{H}_2\text{O}} \) is equivalent latent heat of water in unit temperature change, and it is the function of \( M_c \) and \( T_c \). \( M_c \) is moisture percentage of coal blend, \( T_c \) is coal blend temperature.

In coke making process, coal in coal blend is changing from one state to another, after drying, decomposing, becoming metaplast, solidifying and contracting, coal finally turning into coke. The thermal physical parameters change with material changing in coal/coke blend. So thermal physical parameters are functions of temperature and they are usually obtained by experimental analysis [9-12].

2.2. Heat Transfer Process in Inter-Wall
The inter-wall is divided into 10 plane units, and material in wall is stable during coke making process. The heat transfer model of inter-wall is

\[
\rho_w c_w \frac{\partial T_w}{\partial \tau} = \frac{\partial}{\partial x} \left( \lambda_w \frac{\partial T_w}{\partial x} \right)
\]

(3)

Where \( \rho_w \) is density in kg/m\(^3\). \( c_w \) is specific heat in J/kg/°C. \( \lambda_w \) is thermal conductivity in W/m/°C. \( T_w \) is temperature in °C. The subscript \( w \) means inter-wall.

2.3. Heat Transfer Process between Wall and Coal/Coke Blend
In coke making process, before semi-coke is created, there are molten mass with three phases coexisted in coal blend, and gas in this mass will expand coal blend. But after semi-coke is produced, the semi-coke will shrink and crack, the volume of coke blend will be reduced. So there are different thermal boundary conditions between wall and coal/coke blend in low and high temperature stages. At low temperature stage, as coal blend expands, wall and coal blend become very close, heat conduction boundary conditions should be adopted. At high temperature stage, with semi-cokes shrinking, wall and coke blend will separate, and heat transfers from wall to coke blend in radiation form. So heat radiation boundary conditions should be used. The temperature of molten mass turns into semi-coke is 500°C, and heat boundary conditions will be switched when temperature of coal/coke blend central reaches at 500°C.

3. Modeling

3.1. Modeling of Heat Transfer Process in Coal/Coke Blend
As mentioned above, heat transfer process of coal/coke blend plane unit is heat conduction process of double-layers one-dimensional plane, and 1/2 coal/coke blend are divided into 50 plane units. Heat transfer of each plane unit is achieved by (1). Then heat transfer model of one plane unit is built firstly, and by which the whole 1/2 coal/coke blend model will be assembled. The discretization of model (1) should be presented in simulation step \( T_s \). An outside node method is used for this discretization. The expression is

\[
T_{c_p}(k+1) = T_{c_p}(k) + \frac{T_s}{(\Delta x)^2} \lambda_{c_1} \left[ T_{c_{p+1}}(k) - T_{c_p}(k) \right] - \lambda_{c_2} \left[ T_{c_{p-1}}(k) - T_{c_p}(k) \right] + \frac{\rho_c(T_{c_p}(k)) \cdot c_c(T_{c_p}(k)) + Q_{\text{H}_2\text{O}}}{\rho_c(T_{c_p}(k)) \cdot c_c(T_{c_p}(k))}
\]

(4)

Where \( T_{c_p}(k) \) is temperature of the \( p \)th coal/coke blend plane unit at \( k \) instant, \( T_s \) is simulation step. \( \lambda_{c_1}, \lambda_{c_2} \) are average thermal conductivity of plane units. \( \Delta x \) is width of each plane unit. \( \rho_c(T_{c_p}(k)) \), \( c_c(T_{c_p}(k)) \) are density and specific heat at temperature \( T_{c_p}(k) \) respectively, \( Q_{\text{H}_2\text{O}} \) is equivalent latent heat of water.

Heat transfer model of the \( p \)th coal/coke blend plane unit is built by Simulink showed in figure 2. In this model, thermal physical parameters density \( \rho_c \), specific heat capacity \( c_c \) and thermal conductivity \( \lambda_c \) are obtained from lookup-tables by temperature of the \( p \)th plane unit at \( k \) instant \( T_{c_p}(k) \), and following (4), temperature of the \( p \)th plane unit at \( k+1 \) instant \( T_{c_p}(k+1) \) is calculated. This model will be packaged and named ‘C_cell_p’. Then 1/2 coal/coke blend model showed in figure 3 is
assembled by these generic plane unit models. In figure 3, plane unit models (C_cell_p) are connected one by one in chain; each plane unit model provides its temperature at $k$ instant to the last and next plane unit models. The first plane unit model receives temperature of wall surface by signal line ‘T_W2C’, and it provides its temperature by signal line ‘T_C1’. Then temperature curves of plane units in coal/coke blend driven by simulation time are obtained from ‘goto’ tags.

![Figure 2. Model of plane unit in coal/coke blend (C_cell_p).](image)

![Figure 3. 1/2 coal-coke blend model assembled by C_cell_p unit models.](image)

### 3.2. Modeling of Heat Transfer Process in Inter-Wall

The inter-wall is divided into 10 plane units. An outside node method is used for wall plane unit discretization. The expression (3) is turned into

$$
T_{w_p}^{k+1} = T_{w_p}^{k} + \frac{T_{i}}{(\Delta x_u)^2} \cdot \frac{\lambda_{w1} \cdot [T_{w_{p+1}}^{k}(k) - T_{w_p}^{k}(k)] - \lambda_{w2} \cdot [T_{w_p}^{k}(k) - T_{w_{p+1}}^{k}(k)]}{\rho_u \cdot c_u (T_{w_p}^{k}(k))}
$$

(5)
Where $T_{wp}(k)$ is temperature of the $p$th wall plane unit at $k$ instant, $T_s$ is simulation step. $\lambda_{w1}$, $\lambda_{w2}$ are average thermal conductivity of wall plane units. $\Delta x_w$ is width of each wall plane unit. $\rho_w$ is density of wall, $c_w(T_{wp}(k))$ is specific heat of wall at temperature $T_{wp}(k)$.

The same modeling method proposed in part 3.1 is used to construct heat transfer model of wall plane unit following (5). This model will be packaged as a generic heat transfer plane unit model of inter-wall and will be connected one by one in chain for modeling carbonization chamber wall.

3.3. Modeling of Heat Transfer Process between Inter-Wall and Coal/Coke Blend

Based on analysis in part 2.3, as material and shape of coal/coke blend change during carbonization process, the volume of coal/coke blend varies. So heat transfer process between wall and coal/coke blend includes heat conduction in contact state and heat radiation in non-contact state. These two states are switched by coal blend central temperature. The heat conduction model is constructed by 1/2 plane unit of coal blend and 1/2 plane unit of inter-wall, which is built by the mentioned method above.

3.4. Simulation Platform Design

A simulation platform of carbonization chamber heat transfer process in coke oven is designed by MALAB GUI, the software interface is showed in figure 4. Initial parameters of coal blend should be filled in input boxes, and the thermal physical parameters will be created and showed in plots by clicking the ‘Create Parameters’ button. Based on these parameters, combining with given temperature of inter-wall surface close to combustion chamber, the temperature curves of plane units in wall and coal/coke blend will be presented, and the coking time and corresponded temperature of coke blend central are available.

4. Simulation Results

4.1. Temperature Curves of Coal/Coke Blend

The heat transfer process of carbonization chamber is analyzed by designed simulation platform, and initial parameters of model are showed in figure 4. Temperature curves of the 1st, 10th, 20th, 30th, 40th, 50th plane units in coal/coke blend are showed in figure 5 and they are marked as CL1, CL10, CL20, CL30, CL40, CL50, respectively. In figure 5, temperatures in coal/coke blend increase from outside to inside. The surface layer temperature (CL1) increases rapidly after coal blend is pushed into carbonization chamber, but the rate of temperature rise reduces gradually with increasing temperature, and finally it gets close to 1100°C. The coal/coke blend central layer temperature (CL50) starts to increase at about 1/2 coking time and temperature rises slowly. When this temperature reaches coke maturation temperature, the outside layers of coke blend are mature already. At upper right of figure 5, when central layer temperature reaches desired point (500°C), temperature curves of the 1st, 10th and 20th plane units are influenced to different degrees. From results analyzed above, the temperature characteristics of coal/coke blend in coke making process are agreed well with studies in [1, 2, 3 and 7]. And it is clearly indicated that the proposed modeling method is available.
4.2. Temperature Curves of Inter-Wall

In figure 6, temperature curves of the 1st, 3rd, 5th, 7th, 9th, 10th plane units in carbonization chamber wall are presented and they are marked as WL1, WL3, WL5, WL7, WL9, WL10, respectively. The WL1 temperature curve is almost straight in whole coke making process. But WL10 temperature curve which represents temperature of the 10th plane unit in inter-wall is influenced by coke making process clearly. At the beginning of coking, coal blend is pushed into carbonization chamber, and the surface of inter-wall is cooled, whose temperature drops to 900°C rapidly, then coking process start to work, and the temperature rises to 1150°C slowly. As a whole, the changes in temperature of all plane units in inter-wall occur slowly, the closer to combustion charm the slower of change. In addition, the temperature of plane units close to carbonization chamber is impacted by heat transfer mode change. At the bottom right of figure 6, the curves have been greatly influenced around switch point. It is clearly indicated that the temperature curves have the same property with studies in [1, 3 and 7].
4.3. Coking Time
In the designed software, temperature of combustion chamber wall is given by user and it is treated as standard temperature. In coke making enterprise, like Hunan Coal Chemical and New Energy Company Limited in China, the standard temperature of coke side is 1340°C, and theoretical coking time is 26h. Then in figure 4, the filled wall temperature is 1340 °C, and ‘Simulation Results’ column shows that ‘Coking Time (h)’ is 26.1797 and ‘Central Temperature (°C)’ is 1000.01, the simulation result of coking time is almost the same as theoretical value, so the designed modeling method is available. In addition, coking time and temperature will be analyzed roughly in designed software. Maintaining initial parameters filled in figure 4, and providing different standard temperature, simulation results are presented in table 1. Coking time varies 0.68h, when standard temperature changes 10°C, which agrees with theoretical value.

| Temperature(°C) | 1320 | 1330 | 1340 | 1350 | 1360 |
|---------------|------|------|------|------|------|
| Coking Time (h) | 27.55 | 26.89 | 26.18 | 25.5 | 24.85 |

5. Conclusion
This paper proposes a novel modeling method for carbonization chamber heat transfer process in coke oven, the coke making process is driven by simulation time and the dynamic process of temperature in coal/coke blend is showed intuitively. Future work will focus on constructing complete model of coke oven with the designed model of inter-wall and 1/2 coal/coke blend and achieving total process simulation of making coke production.

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7. References
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