Development and Application of Numerical Thermal Model of a Graphitization Furnace

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Green mesophase powder (GP) is heated to above 3000°C in a graphitization furnace to form mesophase graphite powder (MGP), which is subsequently used as negative electrode materials for lithium batteries. The qualified rate of the MGP is low due to insufficient temperature information. In order to improve the qualified rate of the MGP, a numerical thermal model was developed for simulating the temperature distribution of the graphitization furnace. Then, the new power curve from the numerical model was used to produce the GP/MGP with the qualified rate increased to 93.3%.

Keywords: Green mesophase powder, Graphitization furnace, Mesophase graphite powder, Numerical thermal model

1. INTRODUCTION

Green Mesophase Powder (GP) must be heated to 3000°C in a graphitization furnace to complete the Acheson process to form Mesophase Graphite Power (MGP), which can be applied to the negative electrode material of lithium batteries for use in notebooks, cell phones, electric cars, etc.^(1, 2). Formerly, the MGP price was too high because the Acheson process was carried out by overseas foreign factories. In order to decrease the MPG price, the graphitization furnace has been introduced for the Acheson process.

The graphitization furnace is connected to a direct current (DC) source by the copper clad aluminum (CCA) busbars that are located at the ends of the furnace. The heating of electrodes occurs due to joule heat and exothermic chemical reactions. The heat released in the furnace is also consumed for heating the enclosing elements of coke, crucible and GP/MGP⁽³⁾. The graphitization furnace is shown in Figure 1.

Temperature is the main factor affecting the quality of MGP, which is indicated by measurement of electrical

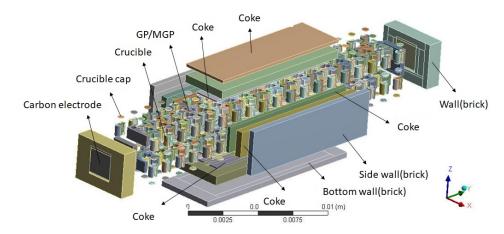


Fig.1. Layout of graphitization furnace

capacity (MEC). Due to the limitation of the field, the graphitization furnace cannot effectively monitor the temperature in real time. Therefore, the GP/MGP was heated according to the experience of the operators. Although the GP can be successfully converted into MPG through the Acheson process, the qualified rate of MEC is low without the information of temperature. To overcome this problem, the numerical thermal model was developed for analyzing the temperature of the graphitization furnace with modification of power curve in this study.

2. NUMERICAL MODEL

2.1 Model Geometry

As shown in Figure 1, a typical graphitization furnace is investigated in this study. The furnace is composed of refractory bricks. The furnace outer dimensions of length, width and height are 14,660mm, 6,100mm and 4,411mm respectively and inner dimensions of length, width and height are 11,860mm, 3,676mm and 1,850 mm, respectively. The CCA busbars are connected to utility power and the dimension of length, width and height are 500mm, 350mm and 350mm, respectively. The coke, which mainly consists of carbon, fills the zone of the furnace core as a heat source with a diameter between 5mm and 25mm. There are 160 crucibles, covered with coke, in the furnace core and the dimensions of height and diameter are 850mm and 500mm, respectively. The GP/MGP are filled in the crucibles and have the diameters between 40µm and 80µm.

2.2 Mathematical Model

All computing zones are solid, and the heat transferred is in the form of conduction. Thus, the partial differential equation of heat conduction is applied as follows:

$$C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) + \frac{(\dot{q} - \dot{q}_s)}{V}$$

where C_p is specific heat (J/(kg · K)); k is heat conductivity coefficient (W/mk); ρ is density (kg/m³); T is temperature (K); x, y, z are the rectangular coordinates (m); V is volume of furnace core (m³); \dot{q}_s is heat power loss by extraction device (W/m³); \dot{q} is thermal power (W/m³) from the power curve.

The thermal properties including brick, coke, crucible, and GP/MGP are shown in References.^(4, 5) The thermal power is specified for the zone of coke and the power loss is estimated by the temperature of exhaust gas. The boundary condition in wall surfaces were assumed to be by natural convection.

2.3 Numerical Method

Gambit is used for generating the mesh of the geometric model. The triangular prism cells were employed in the zones of coke, crucible, and GP/MGP and the structural grids were applied on the brick as shown in Figure 2. The independence of the mesh was tested by developing 320,000, 411,400, 570,000 and 668,000 cells, and the comparative results show that the 570,000 cells produce no noticeable changes in the refined mesh. Therefore 570,000 cells were adopted in the numerical calculation. The power curves represent as a relationship between time and power. Thus, the information of the power curve was established by the User Define Function (UDF). Commercial CFD code Fluent combining with UDF is performed for calculating the partial differential equation in numerical analysis.

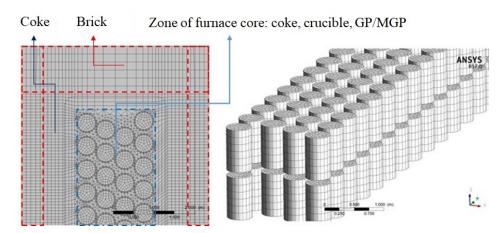


Fig.2. The geometric model of graphitization furnace for mesh

3. EXPERIMENT

Thermal couples are fixed at the center of inner and outer wall surfaces for measuring the temperature. A hollow bar, which is made of carbon, is installed in the center hole of the sidewall. One side of the hollow bar is inside the furnace and the other side is outside the furnace. The inside hollow bar is in contact with the coke and is heated up with the coke through heat conduction. Infrared thermometer (IR) is placed on the opposite side of the hollow bar to measure the temperature of the coke. Figure 3 describes the experiment scheme for temperature measurement. All measurements of temperature information are provided for the numerical thermal model as a basis for verification.

4. RESULTS AND DISCUSSION

The power curve provided for the numerical thermal model test had a heating rate of 290kW/hr to 2900kW. After 2900kW, the heating rate was 410kW/hr until maximum power. Figures 4(a) and 4(b) are the comparison results of temperature progression of the inner and outer wall between simulation and experiment by power curve, and the error is less than 8.2% from 0hr to 38hr. Figure 4(c) shows the comparison results of temperature progression of the coke between simulation and experiment and the error is less than 6% from 0hr to 38hr. After confirming the feasibility of the numerical

thermal model, we simulated the temperature progression by using the historical power curves. Moreover, the relationship of GP/MGP between maximum coke temperature and measurement of electrical capacity (MEC) was established. The temperature of the furnace core was formulated according to the qualified MEC.

A new power curve was formulated and was provided for the numerical thermal model as the input condition to simulate the temperature progression. The heating rate was increased comparing with the previous power curve. Figure 5 shows the simulation results of the coke temperature by the new power curves. The temperature of the furnace coke reached to 745°C at 14.5hr from normal temperature and above 3000°C after 25.7hr. The qualified MEC of MGP was obtained at 28.9hr.

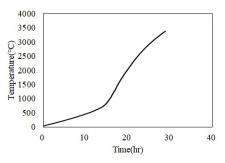
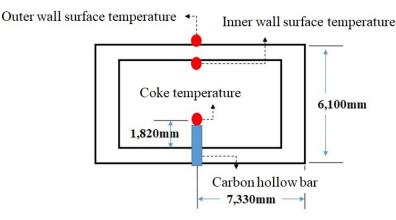
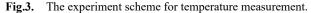


Fig.5. The temperature progression by the new power curves





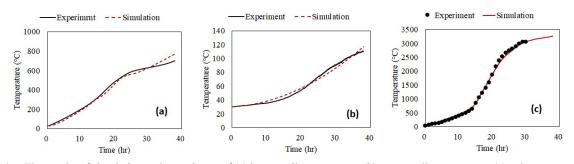


Fig.4. The results of simulation and experiment of (a) inner wall temperature, (b) outer wall temperature, (c) coke temperature

Figure 6 shows the temperature distribution of the furnace core due to the new power curve of HP1.3. It can be seen that the average temperature on both sides of the furnace core does not exceed 2300°C. The temperature in the central area of the furnace core is between 3300°C and 3430°C. The average temperature of the lower furnace core is higher than that of the upper furnace core because there is an extraction device in the upper surface of the furnace to take away excess heat. Regardless of

the upper or lower furnace core, the high temperature is mainly concentrated in the central zone, and the highest temperature is close to 3500°C as shown in Figure 7.

Figure 8 shows that the qualified rate of the MGP was low before PN188 when operators produced the GP/MGP according to their experience. Operators adopted the new power curve to produce GP/MGP after PN188. Obviously, the quality of MGP improved and the qualified rate of MGP increased to 93.3%.

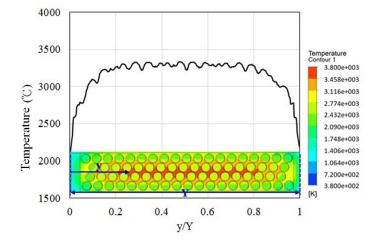


Fig.6. The average temperature of graphitization furnace

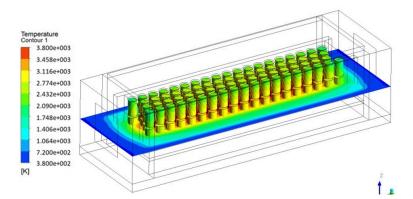


Fig.7. The temperature distribution of graphitization furnace

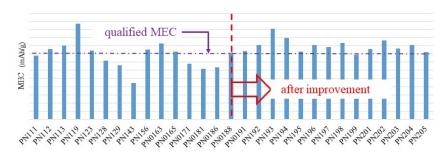


Fig.8. The MEC of MGP after improvement

5. CONCLUSION

The numerical thermal model has been developed for simulating the temperature of the graphitization furnace. The temperature progression of inner wall, outer wall and furnace core can be simulated by numerical thermal model, and the error is less than 6% when comparing with the experiment. Then, the new power curve was formulated and was provided for the numerical thermal model as input condition to simulate the temperature progression. The temperature distribution in the furnace core was observed and the highest temperature was close to 3500°C. Finally, the new power curve was used to produce the GP/MGP and the qualified rate of MGP has been increased to 93.3%.

REFERENCES

- P. Ouzilleau, A. E. Gheribi, and P. Chartrand, Carbon, (2018), 132, pp. 556-564.
- 2. C. Norfolk, A. Kaufmann, A. Mukasyan, and A. Varma, Carbon, (2006), 44, 301-306.
- D. D. Lecce, R. Verrelli, D. Campanella, V. Marangon, and J. Hassoun, ChemSusChem, (2017), 10, pp. 1607-1615.
- 4. B. Zheng, Y. Liu, L. Zou, and R. Li, Mathematical Problems in Engineering, (2016), 2016, pp. 1-9.
- 5. R. E. Taylor and H. Groot, Thermophysical Properties of POCO Graphite, July, 1978.