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Validation study of Large-Scale Simulation of CO_2 or H_2O Gasification with Mass Transfer for Metallurgical Coke

Yui Numazawa[1], Yohsuke Matsushita[1], Hideyuki Aoki[1],
Takahiro Shishido[2], Noriyuki Okuyama[2]
[1]Department of Chemical Engineering, Graduate School of Engineering, Tohoku University,
6-6-07 Aoba, Aramaki, Aoba-ku, Sendai, Miyagi 980-8579, Japan
First. yui.numa@dc.tohoku.ac.jp; Second. matsushita@tohoku.ac.jp; Third. aoki@tohoku.ac.jp
[2] Kobe Steel, LTD., 2-3-1, Shinhama, Arima-cho, Takasago, Hyogo, 676-8670 Japan
Forth. shishido.takahiro@kobelco.com; Fifth. okuyama.noriyuki@kobelco.com

Extended Abstract

Gasification reaction of the solid fuel, coke largely affects the operation of iron making process. The metallurgical coke plays a role not only as a reduction agent of iron ore but also as a spacer, which keeps permeability in a blast furnace. In a blast furnace, the coke is degraded by the gasification reaction though the reaction converts the coke to reductants such like H_2 gas and CO gas. Thus, the coke has the possibility to inhibit the permeability. Our research group has made efforts to develop the numerical simulation method for the gasification reaction of metallurgical coke since the reaction field of the coke in a blast furnace is high temperature (> 1000 K). Our analytical object is the coke model developed from the X-ray CT images of coke and has hundreds of millions of voxels. For the object, the gasification reaction with gas diffusion was simulated [1]. In this study, focusing on CO_2 or H_2O gasification reaction individually, the validity was investigated by the comparison with a lab-scale experiment.

Coke sample before reaction was scanned by the X-ray CT (Comscantecno Co, Ltd., ScanXmate-D180RSS270). The screen resolution was 25 μm/pixel. The gasification reaction experiments of CO_2 or H_2O for the sample were individually performed by using the furnace in which the sample was hung from the balance located at the upper part. The reaction temperature and the total gas flowrate were set to the constant value of 1373 K and 10 NL/min, respectively. The volume fraction of gas was also set to CO_2: N_2 = 0.1: 0.9 in CO_2 gasification or H_2O: N_2 = 0.1: 0.9 in H_2O gasification. The sample was reacted until the conversion reached 0.2. The change of the weight of the sample was measured by the balance, and overall gasification reaction rate was obtained from the weight change. In addition, the sample after the reaction was also scanned by the X-ray CT. For numerical simulation, the analytical object was developed from the X-ray CT images of the sample before reaction. The total number of voxels was approx. 700 million. The object was divided into four parts, and gasification reaction with mass transfer by gas diffusion was analyzed in each part assuming that the gasification reaction occurred at the interface between a carbon matrix and gas phase. Also, gasification reactivities of the pulverized coke sample with CO_2 or H_2O were measured by using thermogravimetry individually, and the reactivities were employed as that at the interface in this study. Note that homogenous reaction was not considered in the simulation.

As a result, the overall gasification reaction rate obtained from the numerical simulation almost corresponded that from the experiment in CO_2 gasification reaction. On the other hand, in H_2O gasification reaction, although the gasification reaction rate from the numerical simulation was close to that from the experiment, the calculated value slightly overestimated the experimental value. This is due to homogenous reaction. From the equilibrium calculation, the gas concentration of H_2O was decreased by homogenous reaction between H_2O gas and CO gas generated from H_2O gasification reaction at 1373 K. Therefore, the prediction accuracy of numerical simulation for coke gasification was improved by directly reflecting gas diffusion in a complex structure of coke into the simulation. Regarding H_2O gasification reaction, homogenous reaction also needs to be considered in the simulation.

References

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