

A study on modelling and simulation on reacting flow included in thermochemical conversion process of coal

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論文題名 : **A study on modelling and simulation on reacting flow included in thermochemical conversion process of coal**

(石炭熱化学転換プロセスにおける反応性流体のモデリングと数値解析に関する研究)

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論 文 内 容 の 要 旨

Coal is a major energy resource in the world. Gasification is an old yet still continuously evolving technology, and particularly suitable for the utilization of low-rank coals, such as Victorian brown coal, due to the high gasification reactivity of these coals. Coal thermochemical conversion includes coal pyrolysis, char gasification and volatiles reforming, in which chemical reactions are numerous and complex, including homogeneous and heterogeneous reactions. Kinetic models of reactions are of very significance to understand the chemistry and mechanism of coal thermochemical conversion. CFD approach is a branch of fluid mechanics that using numerical methods and algorithms to solve and analyze problems that involve fluid flows, especially three dimensional (3D) numerical simulation. Therefore, CFD approach coupled with a kinetic model is a powerful tool that enables a better analysis and understanding of both fluid flow and reaction occurring in coal conversion process.

Chapter 1 of this thesis are comprehensively reviewed the existing studies on the importance of low temperature gasification, and the published models of chemical kinetics in coal conversion, especially coupled with CFD simulation. The chapter also includes the main objectives of the doctoral studies.

In **Chapter 2**, Victorian brown coal and char prepared from the same coal were co-fed into an atmospheric DTR. Loy Yang brown coal was converted in a DTR under conditions similar to those typically used in a downer reactor, where coal, char particles, and gas flow co-currently. The effects of reaction temperature (973–1173 K), solid hold-up (8.31×10^{-6} – 2.50×10^{-4}), residence time (0–4.6 s for gas; 0–0.78 s for solid particles), and steam partial pressure (0–0.05 MPa) on the conversion

characteristics were investigated. The temperature showed a significant influence on the rate of every process, and the product yields varied significantly with temperature. The solid hold-up mainly affected the tar-char interaction and tar was decomposed more extensively with increasing solid hold-up. The steam partial pressure only slightly affected the yields of tar, char, and carbon gases, but suppressed soot formation. A 4-lump kinetic model consisting of tar, gases, char, and soot with 6 global reactions was developed based on the experimental results. The lumped kinetic model was integrated with a computational fluid dynamics (CFD) simulation using an Eulerian-Eulerian approach for mixed phase flow to simulate the coal conversion experiments in the DTR. The CFD results for product distribution during coal conversion in the DTR showed reasonable agreement with the experimental results. The CFD approach presented is suitable for use in designing and optimizing a pyrolyzer for a triple-bed combined circulating fluidized-bed coal gasifier, consisting of a downer (pyrolyzer), a bubbling fluidized bed (gasifier), and a riser (combustor).

In **Chapter 3**, a numerical approach is presented for predicting the species concentrations and temperature profiles of chemically reacting flow in the non-catalytic partial oxidation of hot coke oven gas (HCOG) in a pilot-scale reformer installed on an operating coke oven. A detailed chemical kinetic model consisting of 2216 reactions with 257 species ranging in size from the hydrogen radical to coronene was used to predict the chemistries of HCOG reforming. One-dimensional reactor models were developed that considered the heat loss from the reactor wall to the surroundings (plug flow) and axial diffusion, validated with pilot-scale HCOG reforming with partial oxidation measurements. In the plug flow simulations, an ignition temperature option was used initially to calculate the reaction rates, and then the reaction rates were calculated using the gas-phase temperature. The overall heat transfer coefficient for heat losses from the reactor was optimized empirically at $4 \text{ W/m}^2\cdot\text{K}$; with this value, the experimental axial temperature profiles of the HCOG pilot-scale runs were reproduced well. The HCOG was a multi-component gas mixture derived from coal dry distillation, and was approximated with more than 40 compounds: H_2 , CO , CO_2 , CH_4 , C2 hydrocarbons, H_2O , aromatic hydrocarbons such as benzene and toluene, and polycyclic aromatic hydrocarbons up to coronene. The measured gas temperature profiles were reproduced successfully by solving the energy balance equation accounting for the heat change induced by chemical reactions and heat losses to the surroundings. The approach was evaluated critically

by comparing the computed results with experimental data for exit products such as H₂, CO, CO₂, and CH₄, in addition to the total exit gas flow rate. A global sensitivity analysis was used to identify the temperature-sensitive reactions. The axial diffusion model slightly improves the predictions of H₂, CO, and CO₂, but significantly improves those of CH₄ and total exit flow rate. The improvements in the model predictions were due primarily to the improved temperature predictions by accounting for axial diffusion in the flow model.

In **Chapter 4**, a computational fluid dynamics (CFD) approach to simulate reacting flow in a hot coke oven gas (HCOG) reformer is presented. The reforming of HCOG, a multi-component mixture, in a turbulent flow was simulated numerically by considering both chemical reactions and fluid dynamics. A reduced kinetic model developed from a detailed kinetic model, originally consisting of more than 2000 elementary reactions with 257 species, was reduced to 410 reactions with 47 species. Unimportant radical reactions, which did not contribute much in calculating the major product gas phase species concentrations were identified based on a sensitivity analysis, and were excluded with the help of a batch reactor model, because of present software restrictions for handling detailed kinetic models. The reduced kinetic model had a total of 410 reactions with 47 chemical species for realizing a kinetic model of finite rate reactions with a k - ϵ turbulence model. Finally, a greatly reduced model was obtained that showed similar characteristics to the detailed kinetic model. The calculation of a CFD approach was carried out using the eddy dissipation concept (EDC) coupled with the reduced chemical kinetic model, and accelerated using the *in situ* adaptive tabulation (ISAT) algorithm. A thermowell analysis was also considered in the CFD model to incorporate the effect of radiation on thermocouple measurements. Overall, Numerical simulations could reproduce the reformed gas compositions fairly well, such as H₂, CO, CO₂, and CH₄, as well as the temperature profile in a HCOG reformer as measured by thermocouples.

Chapter 5 summarizes the general conclusions of this work and some perspectives are proposed to improve these studies.