Generation of a skeletal mechanism of coal combustion based on the chemical pathway analysis

Seongyool Ahn*†, Hiroaki Watanabe**, Tetsuya Shoji*, Satoshi Umemoto*, Kenji Tnno*

ABSTRACT

A skeletal mechanism of coal combustion was derived from a detailed coal combustion kinetic mechanism through an importance analysis of chemical pathways. The reduction process consists of roughly two parts. The first process is performed based on a connectivity analysis between species. In this process, DRGEPSA is chosen for reduction process. Strongly connected species and related reactions from the important species set as start species by the operator are sorted into the reduced mechanism. About 70% of species and reactions can be removed with a limited accuracy loss. Subsequently the second reduction process, CSP, is performed. This method focuses on an importance of each reaction and can reduce a volume of mechanism appropriately. Through these analyses, a skeletal mechanism is generated that is including 65 species and 150 reactions. The generated skeletal mechanism is verified through a comparison with the detailed mechanism in the homogeneous reactor model of CHEMKIN-PRO under wide range of conditions. The generated mechanism can give an advantage in the analysis of coal combustion characteristics in detail in large scale simulations such as LES and DNS.

Key Words : Coal combustion, Mechanism reduction, Skeletal mechanism, DRGEPSA, CSP

A detailed coal combustion kinetic mechanism which includes high-carbon species such as poly aromatic hydrocarbons (PAH) was presented by Richter in the previous literature[1]. This mechanism is verified by the works predicting coal combustion characteristics and extended to soot formation[2-4]. The combustion kinetic is presented with 257 species 1107 reactions in this mechanism. It is hard to apply this mechanism on large scale simulations such as LES or DNS directly, so it would be reduced through a reasonable process. For this work, we performed two-step reduction process based on a combined process proposed by Ismael et al.[5] as presented in Fig. 1. These combined process can cover drawbacks of single methods and generate a skeletal mechanism more efficiently.

The detailed mechanism is analyzed through a species-based method, directed relation graph with error propagation and sensitivity analysis (DRGEPSA) proposed by Niemeyer et al. first[6]. In this process, ten species such as fuels, oxidant, and interesting species for an analysis of PAH reactive characteristics are determined as important species for reduction operation. Strongly connected species are chosen for a skeletal mechanism based on the reaction rate of each related reaction under wide range of conditions, temperature (1,100~2,000K), equivalence ratio (0.5~1.5), and pressures (1, 2 atm).

Fig. 2 shows the result of the first step, DRGEP[7]. As the threshold increase, the error increase whereas reaction moves opposite tenancy. In this step, the error increase rapidly when the threshold is changed from 8E-4 to 1E-3. So, we set the maximum error to 10%, and determine the optimal condition as 8E-4. From this process, a 118 species is remained.

Subsequently, a sensitivity of each remained species is tested and the result is presented in Fig. 3[6]. As described in the figure, the error touches

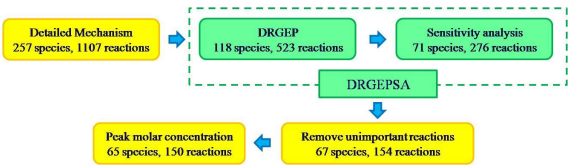

Fig. 1 Flow chart of total process

* CRIEPI in Japan
** Kyushu University
† 연락저자, syahn@criepi.denken.or.jp
TEL : (046)856-2121 FAX : (046)856-3346

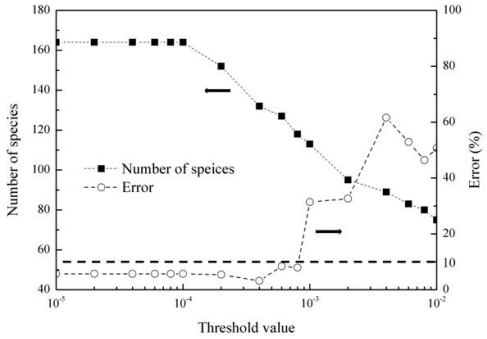

Fig. 2 Number of species and error by threshold values

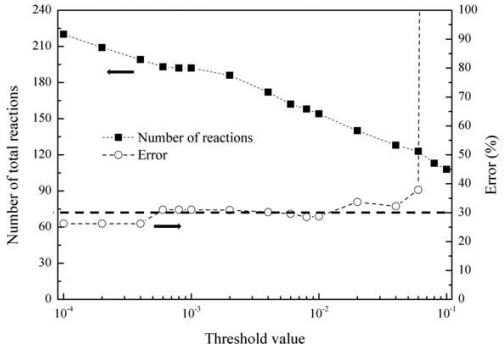

Fig. 4 Number of reactions and error by threshold values

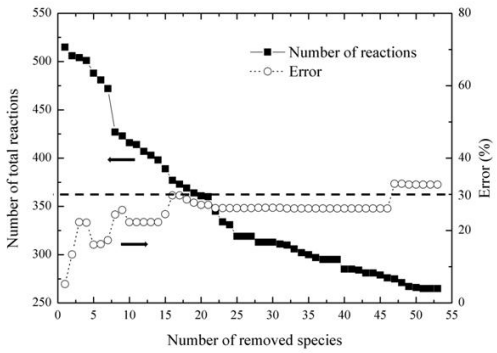

Fig. 3 Number of reactions and error by species removal

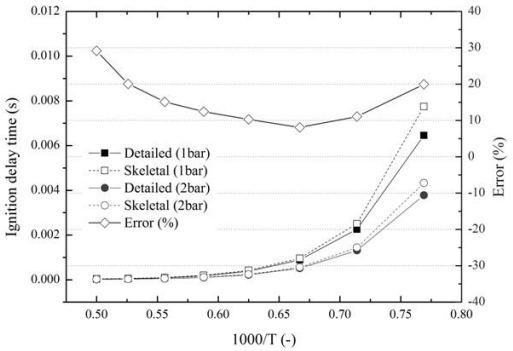

Fig. 5 Ignition delay time of the detailed mechanism and the skeletal mechanism

the 30% line first when the 16 species are removed. Then, the error moves to a lower level and keep the value until the 47 species are removed. Through the comparison of combustion characteristics between two points in the CHEMKIN-PRO, it is confirmed that the second point can be selected as the optimal condition. Through these two species-based analysis, 186 species and 831 reactions are removed well with acceptable accuracy loss, 30% in the ignition delay time and mole fraction of important species.

A reaction-based analysis, computational singular perturbation (CSP) is performed to sort out a redundant part of mechanism[8]. In this process, each reaction is evaluated by importance index presented in the previous literature and the result is presented in Fig. 4[8]. The error increases rapidly at the threshold value 0.08, but we decide to keep the maximum allowed error 30%. The error over the limit slightly at the threshold value 8E-4. However, it does not changed much even the threshold value continuously increase. And then, it over the maximum line at the threshold 0.02 clearly. So, the threshold value 1E-3 is selected as the optimal condition in this analysis.

Two more species which have very low peak mole concentration is eliminated lastly. So, a skeletal mechanism which has 65 species and 150 reactions is generated for a coal combustion, especially PAH reactions. This generated mechanism is verified by a comparison with the detailed mechanism in the homogeneous reactor of CHEMKIN-PRO and the result is presented in Fig. 5. The error is lower than 30% in all test conditions, and it is around 10-15% in the main reaction field, temperature 1200-1500 K. It will give an advantage of calculation in a large scale simulations.

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