6A1. Modeling and Simulation Technologies for Coal Gasification

Research and development: Japan Coal Energy Center
Project type: NEDO-commissioned project

Technology overview

1. Overview of basic technology for advanced coal utilization (BRAIN-C)

The consumption of fossil fuel impacts the environment in a variety of manners. There is also an impact on the environment during the coal production, transportation, and utilization processes. During utilization, in particular, coal dust, ash dust, acid gases (NOx, SOx), and carbon dioxide are discharged, raising concerns of what the unregulated consumption of coal may possibly have on the environment. However, technologies to minimize the harmful impact coal utilization has on the environment, collectively called clean coal technology (CCT), are in widespread use in developed countries, including Japan. Given this, the "Basic Technology Development Program for Advanced Coal Utilization (BRAIN-C)" is focused on coal gasification technology and the rapid commercialization of new high-efficiency and clean coal utilization technologies, such as coal gasification and pressurized fluidized-bed processes. Basic coal data, from a variety of perspectives, has also been collected and compiled. Numerical simulation is a very effective tool to predict the characteristics of a pilot or actual production unit by utilizing the above-mentioned basic data. On the other hand, it can also be used to evaluate and select useful basic data. With this taken into consideration, technology development under BRAIN-C has proceeded from the aspects of both useful basic data retrieval/storage as well as high-precision numerical simulation.

Figure 1 shows the "BRAIN-C technology map." Results from this project are roughly grouped into the following three categories:

(1) An entrained-flow gasification simulator
(2) A predicted model/parameter correlative equation
(3) A coal database

(1) to (3) above are illustrated below and each is as an integral part of the results from this project, indispensable for actual usage in a variety of situations. The appropriate utilization of each in accordance with the application allows for full optimization.

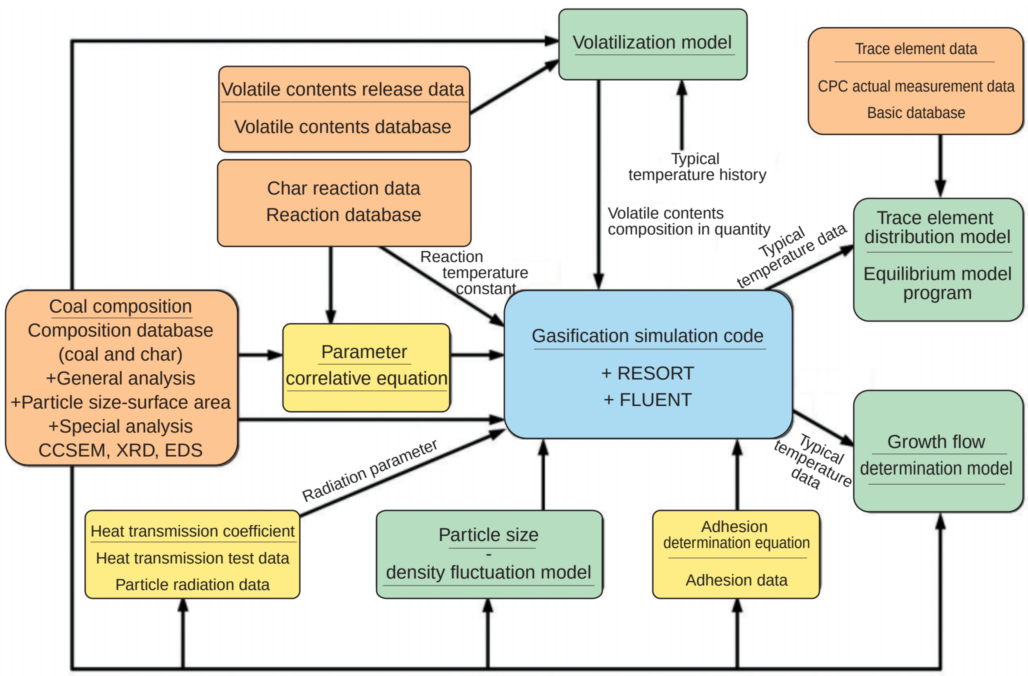


Fig. 1 BRAIN-C technology map

2. Entrained-flow gasification simulator

An entrained-flow gasification simulator, based on thermal fluid analysis software, computational fluid dynamics (CFD), and capable of simultaneously analyzing flow, reaction, and heat transmission, can calculate temperature distribution, ash adhesion locations, gas composition, etc., within a gasifier if given, as input data, such parameters as reactor shapes, operating conditions, coal properties and reaction data (Fig. 2). Highly reliable prediction results can be used for evaluating operating condition validity, reactor design, and other information in advance.

In the BRAIN-C program, the coal gasification reaction model shown in Figure 3 and the particle adhesion model shown in Figure 4 are built within CFD in order to establish technology for an entrained-flow gasification simulator. Simulation results are then compared with gasification furnace operating data in coal-based hydrogen production technology (HYCOL or EAGLE) to examine the validity.

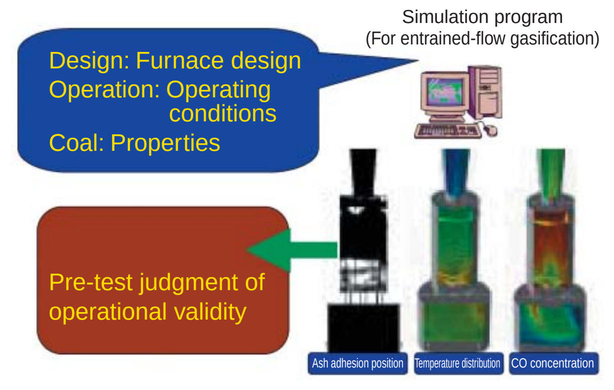


Fig. 2 Functions of entrained-flow gasification simulator

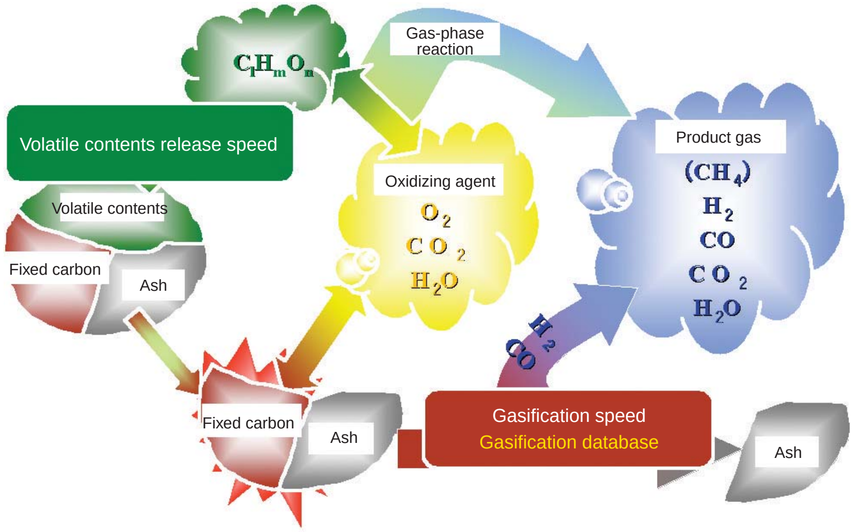


Fig. 3 Coal gasification process modeling

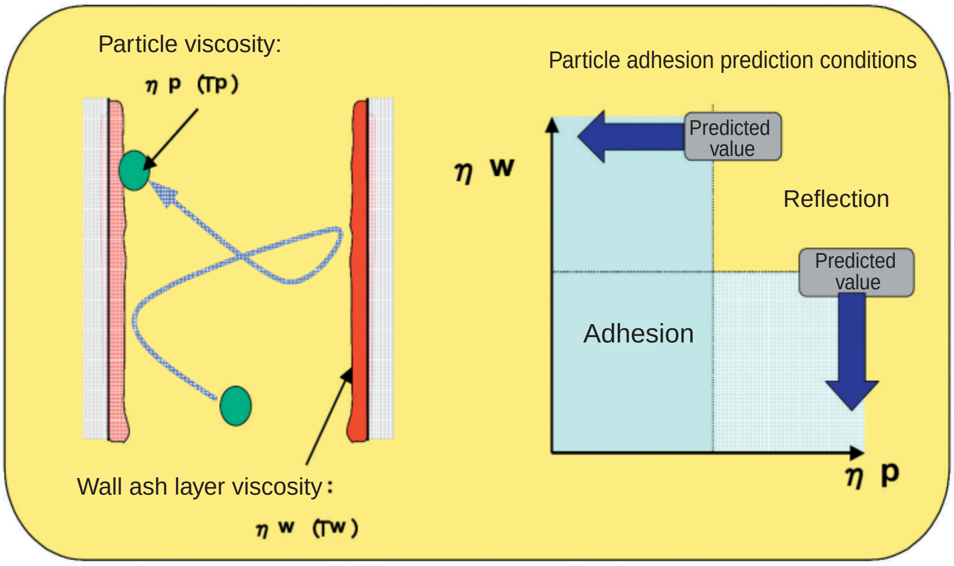


Fig. 4 Ash viscosity-based adhesion prediction model

Figure 5 shows an example of the comparative results between the formation position of a fused ash layer and the internal condition of a gasifier after operations. This showed that the formation position of the fused ash layer as predicted by the simulator corresponded well to the position where the fused ash layer actually existed, confirming the accuracy of the simulation relative to the actual data.

Figure 6 shows the result of case studies on HYCOL using a gasification simulation. The near-wall temperature and ash viscosity on the wall shown on the left side of Figure 6 are those reproduced by simulation after 1,000 hours of operation. The temperature of the bottom area of the furnace (shown in red in upper image) into which slag flows are high versus the low ash viscosity in the bottom area of the furnace (shown in blue in the lower image). The temperature of the upper part of the furnace is low (shown in green in upper image), providing conditions where particles can hardly adhere. On the other hand, the near-wall temperature and ash viscosity on the wall shown on the right side of Figure 6 are the result of simulation under intentionally modified operating conditions. For this case, the oxygen ratio at the top of the chart is higher and that at the bottom is lower than is shown on the right side of the figure. In such cases, it was found that the temperature at the bottom of the furnace decreases (shown in orange) and the low-ash-viscosity region (shown in blue) narrows while the upper part of the furnace becomes hot (the region in red increases) to form a region where it is easier for ash to adhere, categorized as less desirable operating conditions.

By using the gasification simulator in this manner, analysis can be easily made even if gasification conditions are altered. This has resulted in growing expectations for use of the simulator in future gasification projects.

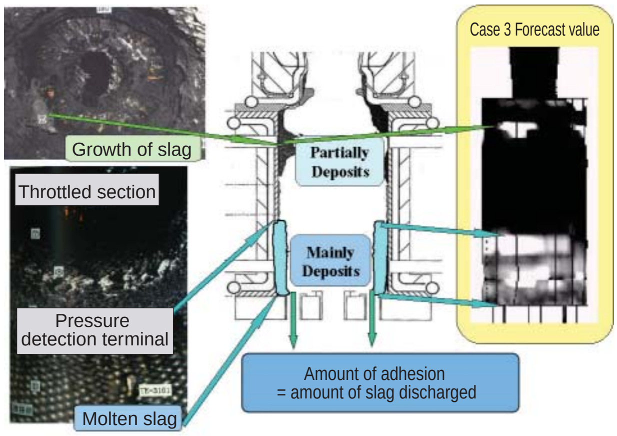


Fig. 5 Ash adhesion position verification results

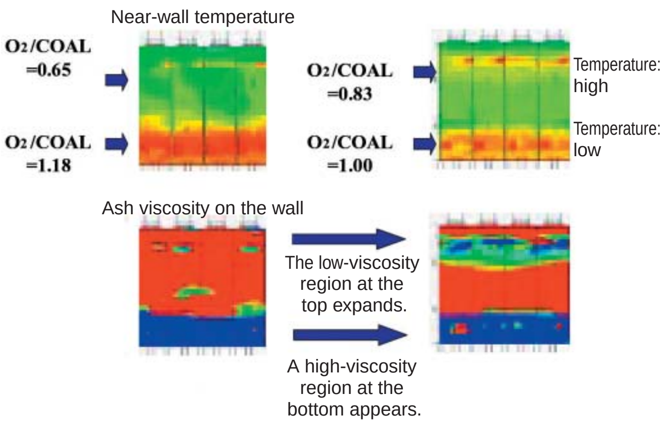


Fig. 6 Simulator-based studies

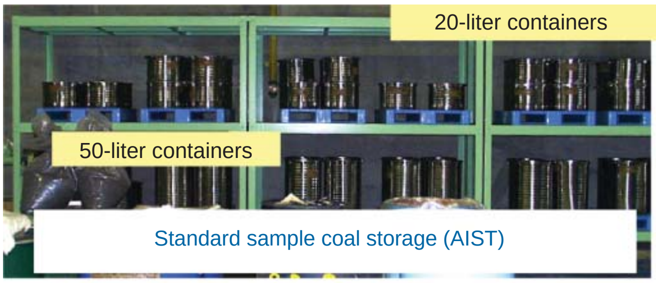
3. Predicted model/parameter correlative equation

The entrained-flow gasification simulator can be applied to various furnace designs and operating conditions, but it is not applicable to all types of coal. It is, therefore, necessary to input coal characteristics into the simulator by coal-type as a parameter. This parameter generally uses the data obtained from basic test equipment but, from the vantage of obtaining a prompt evaluation, it is desirable to establish a means to obtain the parameters from a general analysis of coal or from structural composition data (an advanced model incorporating correlative equations for estimations and experimental conditions). More specifically, a generalized volatilization model and the adhesion determination equation are among the tools to prepare parameters. In the meantime, a trace elements distribution model and an adhesion determination equation model offer determinations from simulation results, playing another important role. Under the BRAIN-C, therefore, prediction equations around a gasification simulator have also been developed so that the simulator can be used effectively and quickly.

4. Coal database

The development of a correlative equation or model indispensably requires physical and basic experiment data, including general analysis data. There is, however, a significant issue in that the characteristics of coal differ by lot, even if the coal has come from the same coal mine. It was, therefore, first necessary for each testing body that obtained physical and basic data to use exactly the same coal samples. Figure 7 shows a coal sample bank built within the National Institute of Advanced Industrial Science and Technology. Such unified management of analytical test samples has enabled the shipment of identical samples to all testing research bodies.

As far as the identical sample-based data is concerned, the measurement of typical data will be completed under this project for 100 types of coal for general/special analysis data, and for at least ten types of coal, depending upon the data criteria, for basic experiment data. Eventually, all of this measurement data will be compiled in an Internet-accessible coal database. Some of the data thus far obtained, as shown in Figure 8, has already been uploaded to JCOAL's server and is accessible or retrievable. Much of this data is stored in an easy-to-calculate/process Excel file (Fig. 9) and can also be downloaded.



Standard sample coal (for delivery)

Fig. 7 Coal sample bank

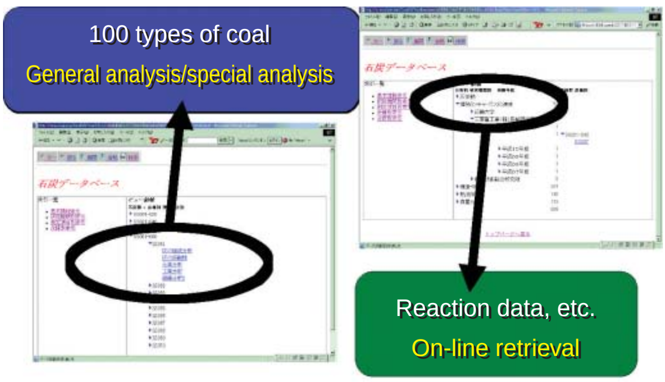


Fig. 8 Coal database

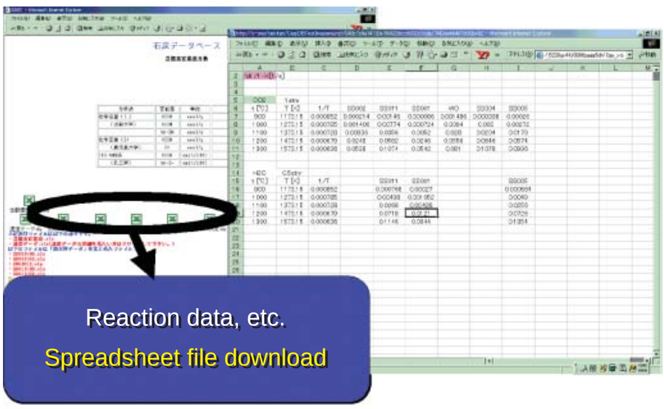


Fig. 9 Basic data acquisition

5. Dissemination of basic coal utilization technology products

An entrained-flow gasification simulator thus far developed under BRAIN-C is capable of making practical predictions through the utilization of various models and basic data. The BRAIN-C Project, finished in 2004, developed a well-equipped system to make a wide selection of programs and basic data available so that the products developed under this project could be used without limitation. Detailed service manuals, as well as workshops for the purpose of encouraging the optimal utilization of these products, were also being prepared.

Despite the predominance of coal gasification technology in this development project, other types of gasification projects are strongly encouraged to use the simulation code, since it can be widely used for combustion simulation as well as in other applications.