GUI program for the calculation of physicochemical properties in VHTR-based SI process

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1. Introduction

The Sulfur-Iodine (SI) process coupled to a Very High Temperature gas-cooled Reactor (VHTR) is well known as a promising technology to produce hydrogen. The SI process consists of a Busen reaction, a sulfuric acid concentration and decomposition, and a hydriodic acid concentration and decomposition [1].

Information on the physicochemical properties of SI process materials is required to design SI process reactors and simulate the performance of the SI process [2][3].

In this study, a Graphic User Interface (GUI) program for the calculation of physicochemical properties in the VHTR-based SI process has been prepared. This program allows a user to easily calculate and evaluate the physicochemical properties of pure or mixture chemical materials in the SI process.

2. Method and Results

2.1 GUI Program description

The GUI program for the calculation of physicochemical properties in the VHTR-based SI process has been developed based on MATLAB (ver. 2010a) and supports a user-friendly graphical user interface. This program consists of four windows for user in/output and can calculate the six physicochemical properties for the chemical material related to the VHTR-based SI process: the solubility, viscosity, thermal conductivity, heat of vaporization, and vapor pressure. Calculation results for each physicochemical property are displayed on the window composed of a chart and spread sheet.

2.2 Design of the User Interface

The functional architecture of the GUI program for calculation of the physicochemical properties is show in Fig. 1. As shown in Fig. 1, this program provides a user with the calculation results for the physicochemical properties through the GUI module using the internal calculation models established by the external reference data such as experimental data.

Fig. 2 shows the navigational user interface (UI) structure of the GUI program. As shown in Fig. 2, the GUI program consists of four windows such as the window for user log-in, the window for selecting physicochemical properties, the window for setting of the calculation conditions, and the window for displaying the calculation results.

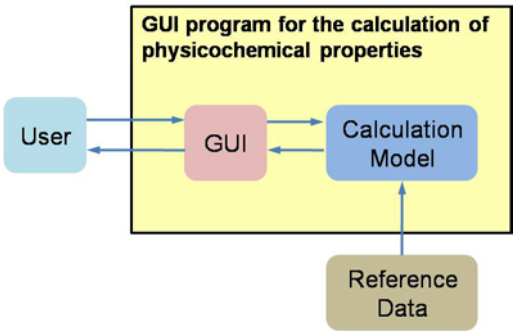

Fig. 1. Functional architecture of the GUI program for analyzing the physicochemical properties.

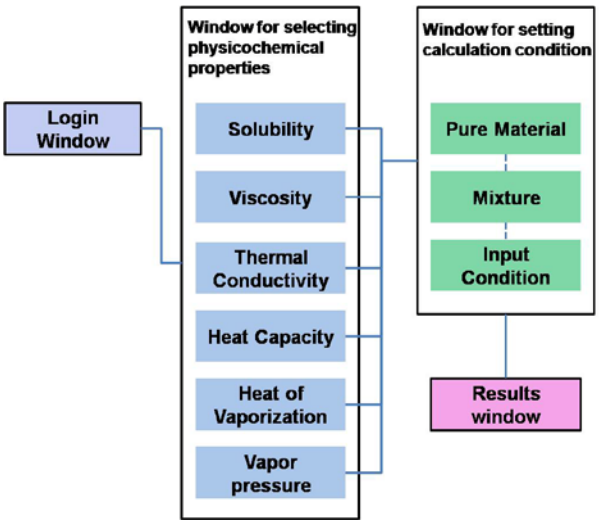

Fig. 2. User interface (UI) structure of the GUI program for analyzing the physicochemical properties.

Based on the UI structure presented in Fig. 2, the windows for user log-in and selecting the physicochemical properties are shown in Fig. 3. In Fig. 3, the window for selecting the physicochemical properties consists of eight buttons. On the other hand, the widow for setting the calculation conditions as shown in Fig. 4, can be executed by clicking the button in the window for selecting the physicochemical properties.

As shown in Fig. 4, the window for setting the calculation conditions can be classified into four menu groups: the selection of the chemical system, the selection of the chemical component, the setting of the temperature, and the setting of the concentration for the selected chemical component.

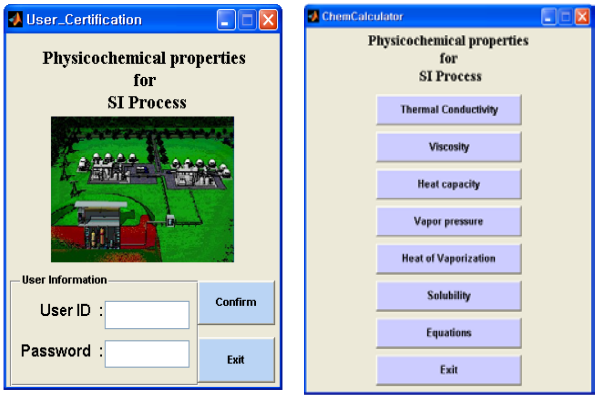

Fig. 3. Window for user log-in and selecting the physicochemical properties.

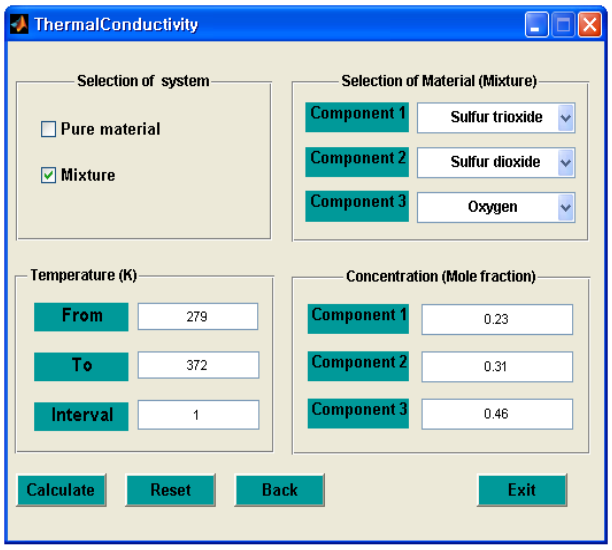

Fig. 4. Window for setting of calculation conditions

2.3 Sample calculation

To identify the performance of the GUI program, a sample calculation for the thermal conductivity of a SO_3-SO_2-O_2 ternary gas mixture at a temperature range of 279 to 372 K has been carried out.

Fig. 5 shows a window displaying the calculation results for the thermal conductivity of sulfur dioxide in the form of a chart and spread sheet.

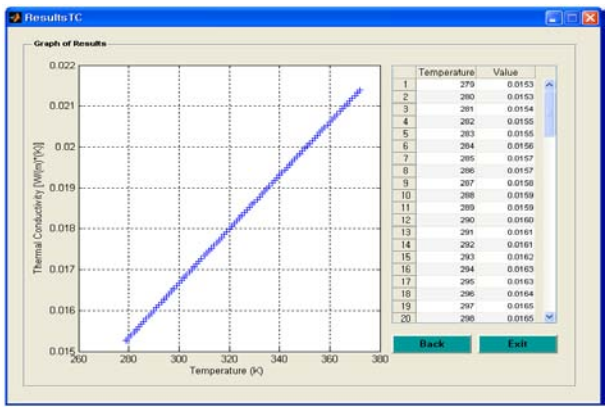

Fig. 5. Window for display of calculation results.

3. Conclusions

A GUI program for the calculation of the physicochemical properties in the VHTR-based SI process has been introduced. This program can be used to calculate and evaluate the physicochemical properties when designing SI process reactors and simulating the performance of the SI process.

Acknowledgments

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