Dynamic Flowsheet Modeling of MG-Si Production for PV Applications

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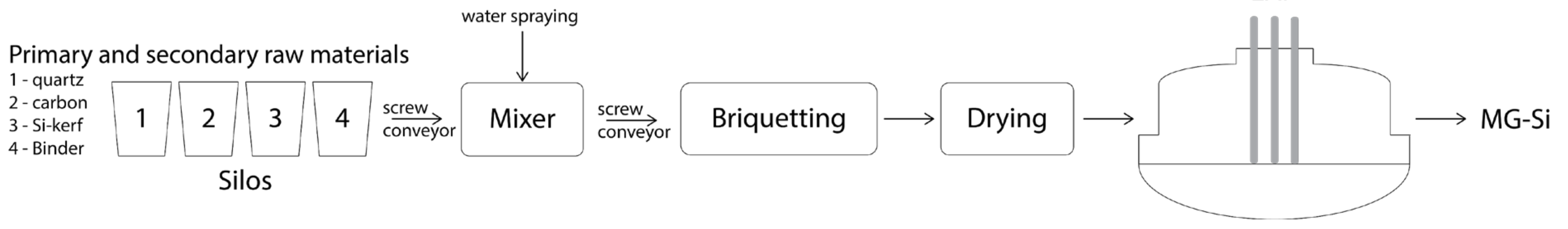
Introduction

The ICARUS project aims to demonstrate modular processing solutions at industrial scale to retrieve 95% of high-value raw materials from silicon ingot and wafer manufacturing, through eco-efficient processing, refining, and transformation of industrial silicon, graphite and silica waste streams.



For this part of the project, the focus is set at silicon production from recycled materials. To optimize the process from the perspective of both Si production and energy consumption, numerical simulations based on flowsheeting will be in use. Flowsheet modeling is a computational modeling technique used to perform steady-state heat and mass balancing, sizing and costing calculations for chemical and industrial processes.

In this work, a dynamic flowsheet model made in HSC Sim is showcased to model the conventional carbothermic reduction of SiO2. A static model is first presented to set reference values for the temperature and the reactivities of the different reactions occurring in the furnace. The model is then run dynamically allowing for, e.g., the varying the input rates over time.

Carbothermic Reduction of Silica

Fig. 1

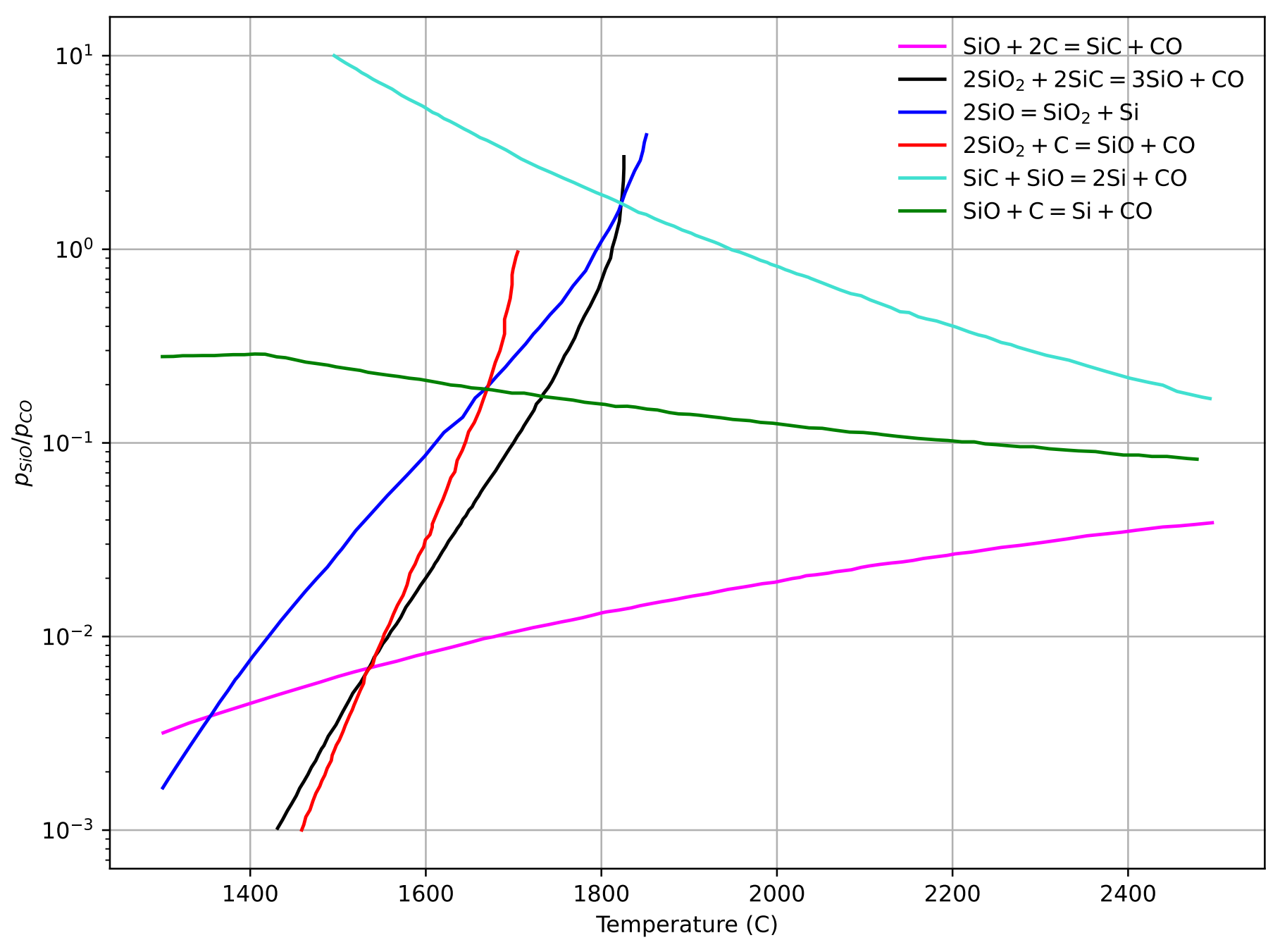
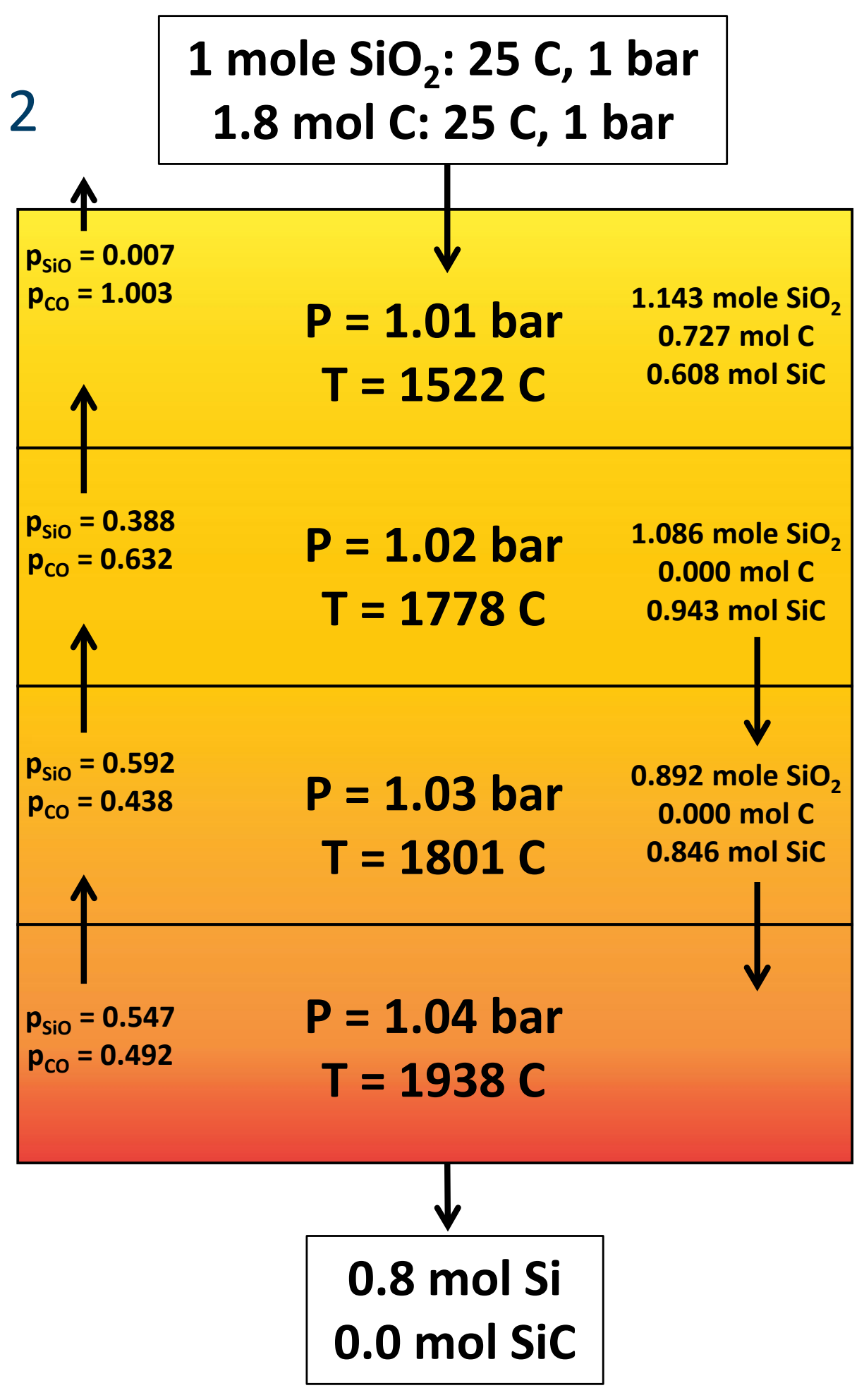


Fig. 2

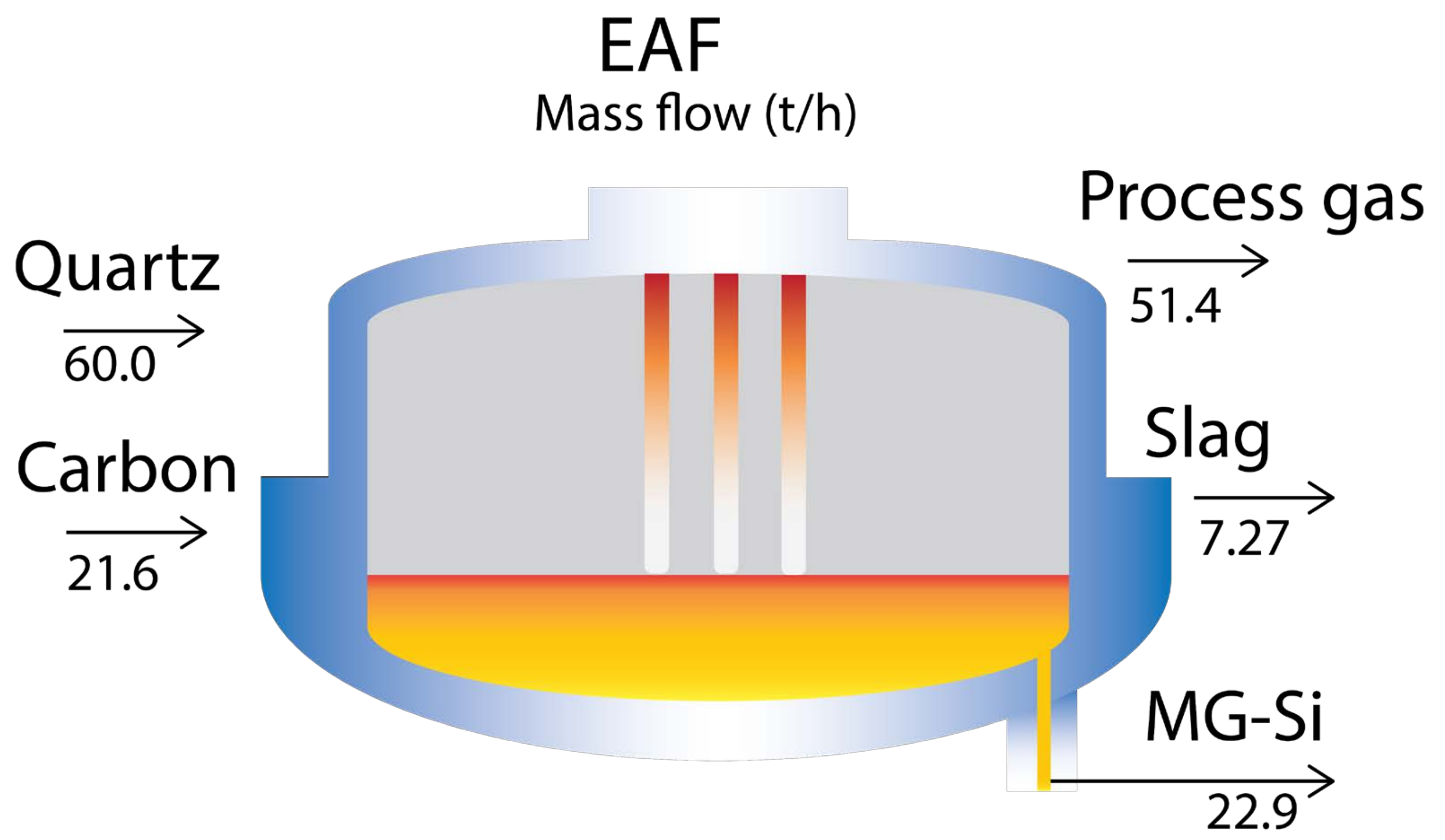


Case of Study

The input streams to the model are labelled “Quartz” and “Carbon”. These consist of 100% pure SiO_2 and C, respectively. In a more realistic application, one could, e.g., set the composition of the “Carbon” stream to be 98% C and 2% SiO_2. Impurities can also be added at this stage. There will be three output streams: “Process gas” containing the CO and SiO produced in the chemical reactions; “Slag” containing the unconsumed SiO_2 and SiC; and “MG-Si” containing the liquid output Si.

The furnace is modeled with four distinct zones, or “tanks”. The temperature and total pressure of each tank is set by the user and the software automatically computes the required energy flow. The chemical reactions presented in Figure 1 are implemented in each of the tanks.

A static simulation is run first to set reference values for the reaction progresses of the chemical reactions occurring within the furnace. For this, an input rate of 60 t/h of SiO_2 and 21.6 t/h of C is used. This gives a ratio of 1 mol of SiO_2 to 1.8 mols of C. The reaction progresses are then estimated according to the partial pressures displayed in Figure 2 and aiming for 80% Si recovery rate. For this static case, an 81 % Si recovery rate is obtained



Results

The model simulated three hours of Si production. The SiO_2 input was linearly increased up to 60 t/h during the first hour while maintaining a constant C input of 21.6 t/h (Figure 3). This is equivalent to reducing the charged C/SiO_2 mol ratio until 1.8/1. This yielded and 82% pure Si recovery rate plus some SiC (Figures 3 and 4). From hours one to two the input C/SiO_2 ratio was further decreased by increasing the SiO_2 input rate up to 80 t/h. This is equivalent to further decreasing the input charged C/SiO_2 ratio (Figure 4). The Si recovery rate achieved a maximum of 83 % when the input SiO_2 rate was 65 t/h (Figure 4). This corresponds to a C/SiO_2 mol ratio of 1.66/1. Further increasing the input SiO2 rate resulted in a decrease in Si recovery rate. From hours two to three, the input SiO_2 rate was linearly decreased to zero. This resulted in a decrease of output Si and an increase in output SiC (Figure 4).

Fig.3

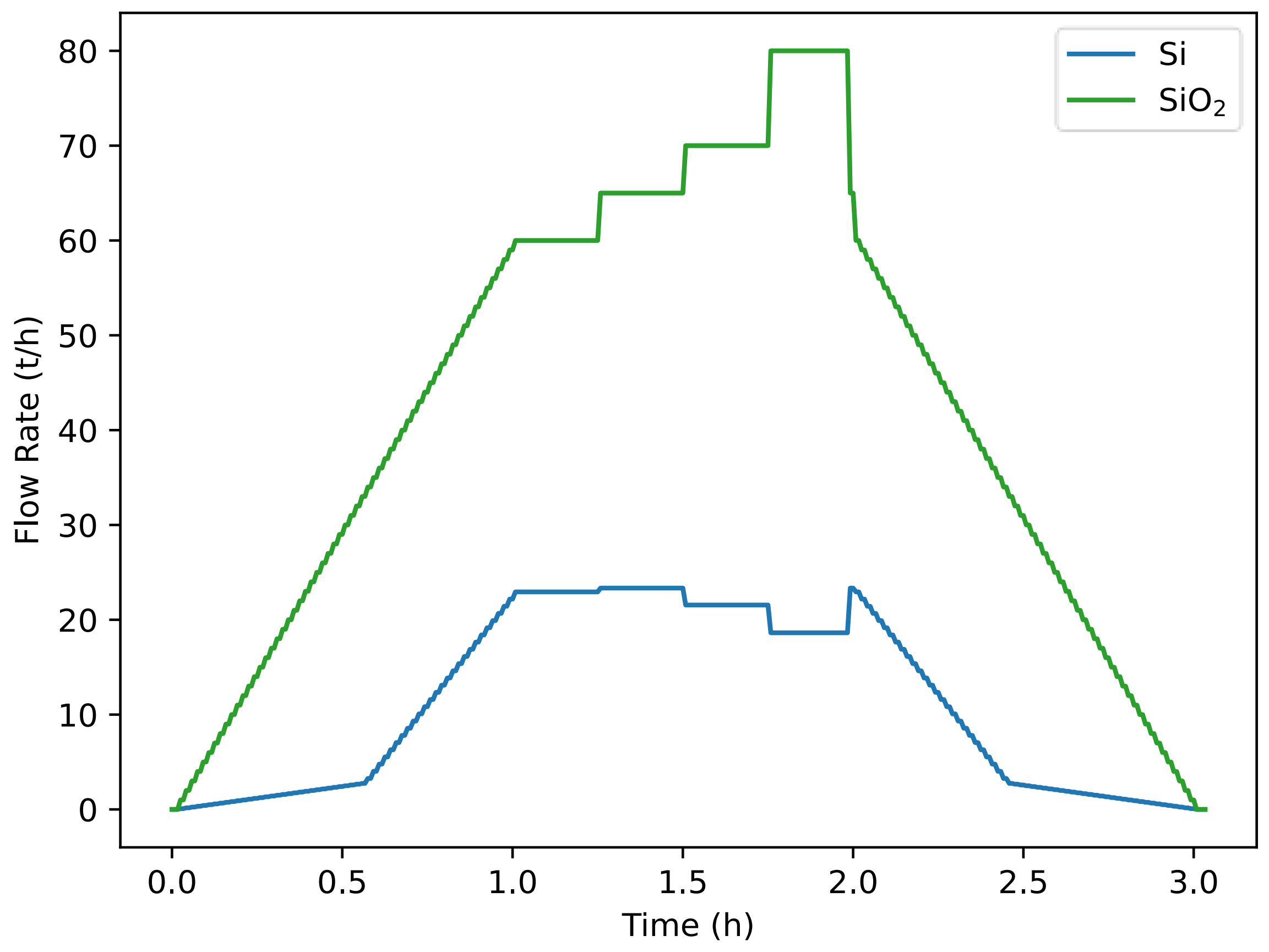
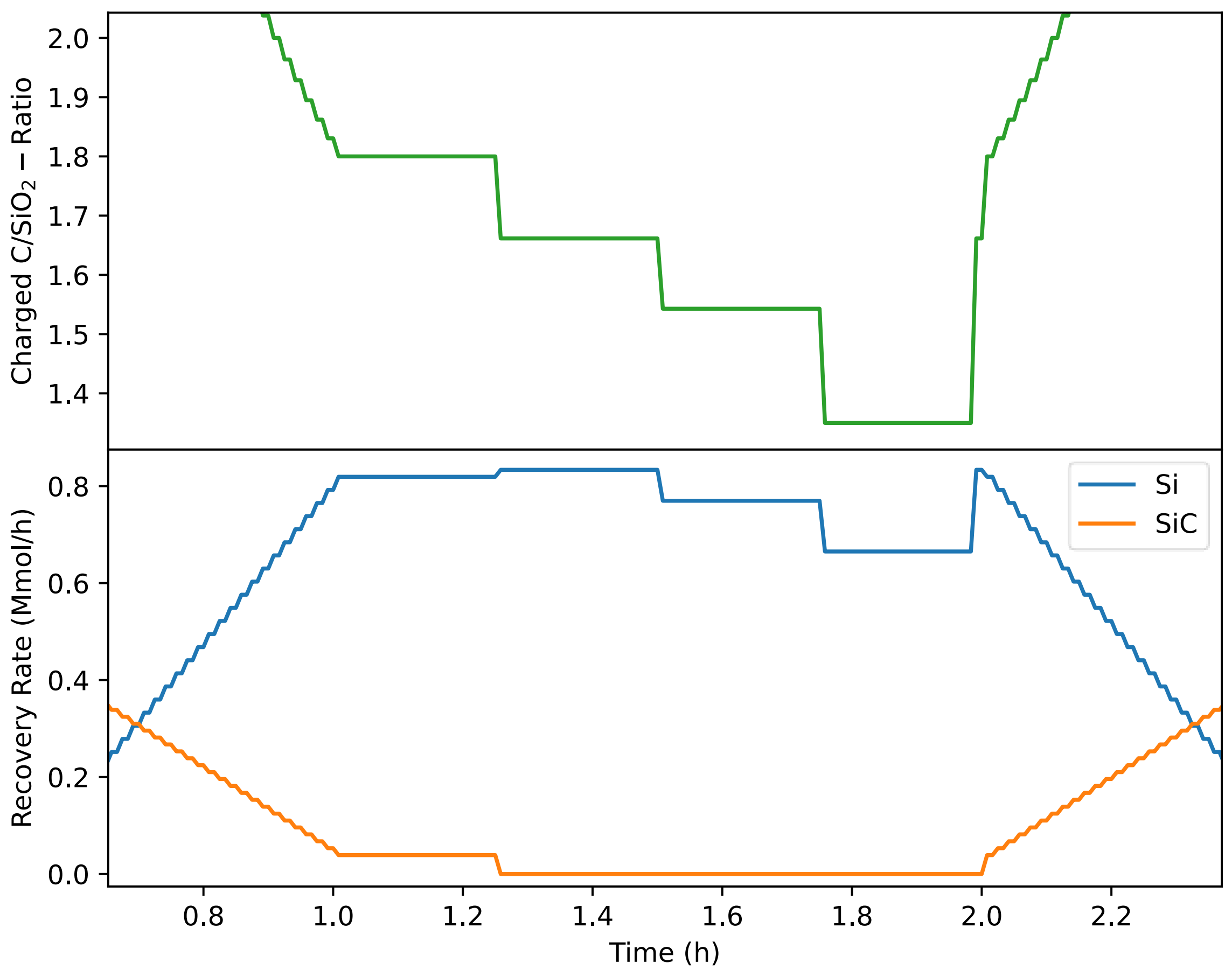
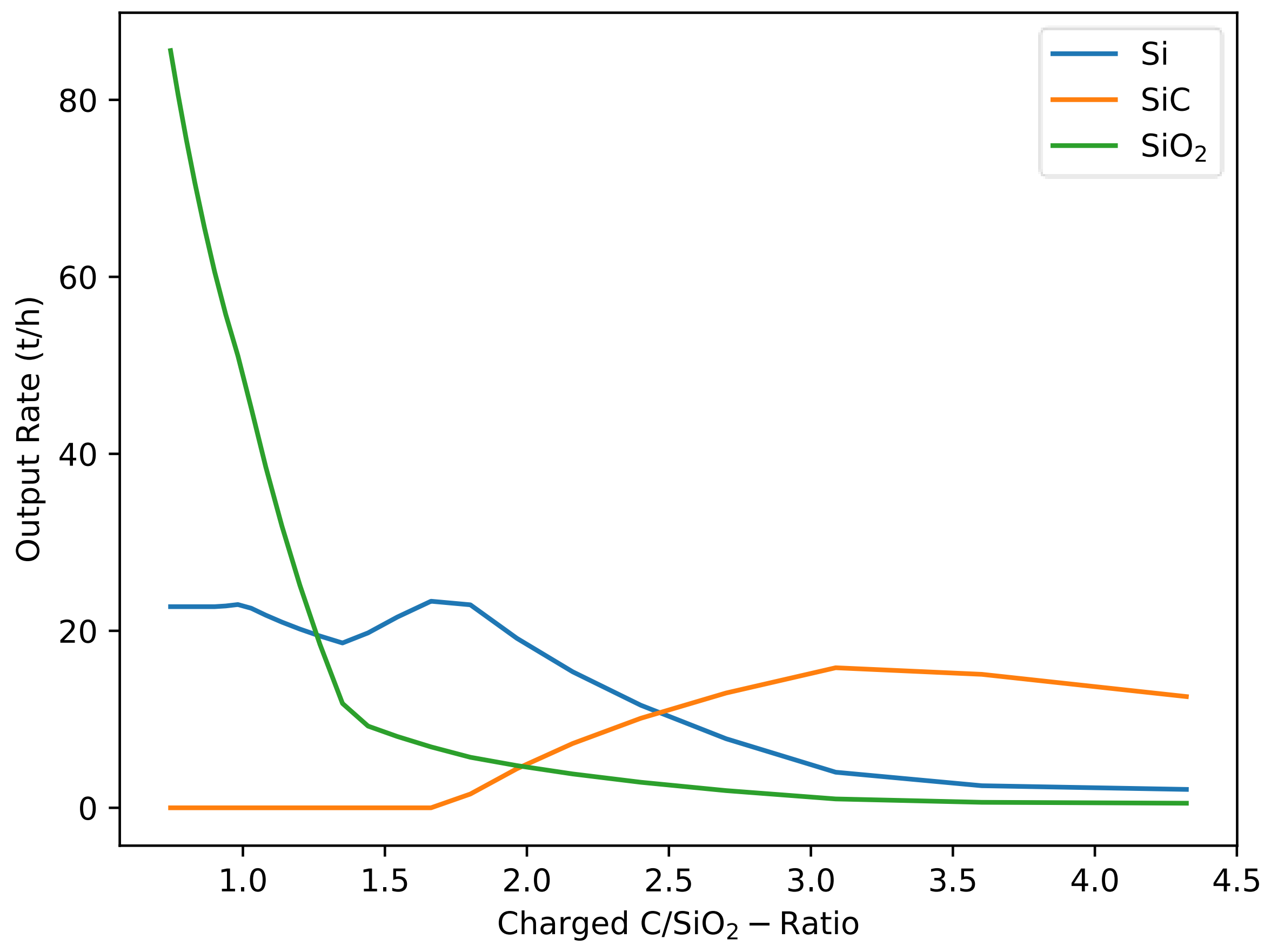


Fig. 4



Finally, in Figure 5, the output rate of SiO_2, SiC and Si displayed as a function of the input C/SiO_2 ratio. Here and as expected from Figures 1 and 2, the Si recovery rate achieves a maximum at a C/SiO_2 mol ratio of 1.66/1. It is also observable that for low C/SiO_2 mol ratios, most of the input SiO2 comes out of the furnace without reacting. SiC is therefore not produced. On the other hand, at higher C/SiO_2 mol ratios, all SiO_2 is rapidly consumed and the production of SiC increases. Because of the low SiO_2 input rate, there is not enough SiO production and therefore the Si recovery rate also decreases.

Fig. 5



Conclusions and Outlook

The presented dynamic model has been proven to be successful in describing the conventional carbothermic reduction of silica. Ideal conditions have been assumed and therefore, modifications need to be implemented if the model is going to be used in industrial applications. For example, in the present model, the temperature of the different zones is set by the user. An external electricity flow should be used for temperature control. The employed reaction progresses, or reactivities of the reactants, are estimated in accordance with mass conservation. Obtaining the real ones will require the implementation of empirical models, or even performing experiments.

Regarding the goals of the ICARUS project, the input flows will be modified to also include recycled secondary raw material. This will allow for obtaining the optimal ratio of secondary to primary materials. Finally, the model will be extended to include remaining mixing, briquetting and drying phases.

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