Simulations of a Fluidized Bed Reactor for Trichlorosilane Production using Barracuda Software

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The production of trichlorosilane (TCS) in a fluidized bed reactor is a widely used process in the polysilicon industry. In many industrial plants, the production of TCS is the first step in producing high-purity polysilicon from metallurgical grade silicon (MGS). In this reactor, solid MGS particles are fluidized by hydrogen chloride gas which reacts to form primarily TCS and hydrogen gas. Silicon tetrachloride, dichlorosilane, and some longer-chain chlorosilanes are produced as byproducts in side reactions.

$$\mathrm{Si} + 3\mathrm{HCl} \rightarrow \mathrm{SiHCl_3} + \mathrm{H_2} \tag{1}$$

Experimental Data

The public availability of thorough experimental data for TCS production is extremely limited. Recently, however, some results have been published. In experiments run by Jain et al (2009), TCS was produced from metallurgical grade silicon in a reactor (2.66 cm ID X 47 cm tall) at 321°C. In these experiments, the reactor was operated under both fixed bed and a fluidized bed conditions. From the fixed bed experiments, Jain et al report a first-order kinetic constant of 0.767 s^{-1} at the operating temperature. The experimental results of the fluidized bed tests are shown in Table 1.

Table 1 - Experimental results from Jain et al. (2009)

Test #	Particle Size (µm)	HCl Gas Flow (L/min)	Temperature (°C)	Pressure (Pa)	Bed Mass (g)	HCl Conversion (%)
1	208	3.2	321	101325	56	53
2	160	1.9	321	101325	56	60
3	124	1.9	321	101325	56	74
4	88	1.6	321	101325	56	78

Model Setup

In Barracuda, each model was set up with geometry and operating conditions listed in Table 1. Since a particle size distribution is unknown, the particles were assumed to be of uniform size. To determine a kinetic expression from the rate reported by Jain et al, it was assumed that the fixed bed had a packing fraction of 0.63. In the model, the kinetic expression shown below was used, where θ_P is the volume fraction of silicon particles and $[\mathrm{HCl}]$ is the molar concentration of HCl. Due to the simple reaction kinetics provided, it is assumed that TCS is the only reaction product.

$$\frac{d\mathrm{Si}}{dt} = -\frac{\left(0.767\ \mathrm{s}^{-1}\right)}{0.63}\theta_P\,[\mathrm{HCl}] = -\left(1.217\ \mathrm{s}^{-1}\right)\theta_P\,[\mathrm{HCl}] \tag{2}$$

In the Barracuda models, isothermal conditions were assumed due to the small diameter of the reactor. For the simulation of larger reactor systems, the modeling of heat transfer in the system along with the inclusion of side reactions would be necessary. The production of TCS is highly exothermic and Barracuda can provide valuable insight into reactor inefficiencies caused by inadequate heat removal or maldistribution of gas flow. Furthermore, Barracuda can be used to study wear and erosion of reactor internals caused by the motion of the silicon particles. Previous simulations of polysilicon systems (Parker 2011) have shown that Barracuda can be an effective tool for studying larger reactors with thermal considerations.

Simulation Results

For each run, the Barracuda model was run until reactor output equilibrated. In Figure 1, the HCl conversion predicted by the Barracuda simulations is compared with the experimental results collected by Jain et al. A very close match between the Barracuda simulations and the experimental data was obtained.

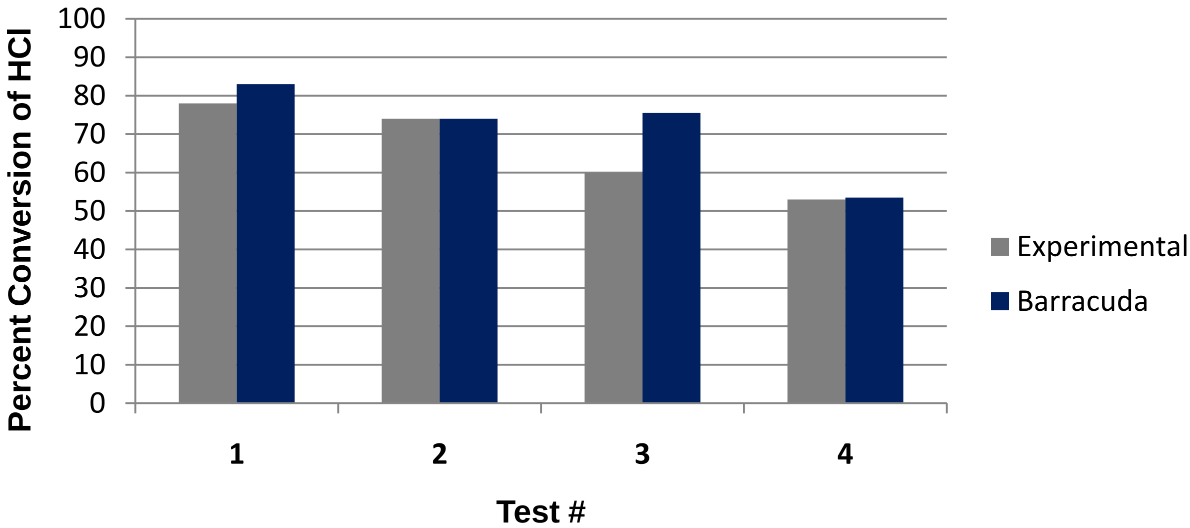

Figure 1 - HCl conversion in TCS reactor. Comparison between Barracuda simulations and experimental results

References

Jain, M., Sathiyamoorthy, D., and Rao, V. (2009). Studies on Hydrochlorination of Silicon in a Fluidised Bed Reactor. *Indian Chemical Engineer*. 51 (4) : 272 – 280.

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