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James M. Parker*

*CPFD Software, LLC, james.parker@cpfd-software.com
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Abstract

In this work, a CFD model for simulating industrial scale particle-fluid systems is used to model a fluidized bed reactor for the deposition of high-purity silicon from silane gas. The performance of these reactors is directly dependent on a large number of factors and parameters which make the design and optimization of the deposition reactors an engineering challenge. Using the reactor design and experimental data from work performed at the Jet Propulsion Laboratory as a basis for validation, the CFD model was found to accurately model the deposition rate, silicon fines production, and temperature distribution within a silane deposition reactor. Additionally, the CFD model is demonstrated to be an effective tool for comparing different reactor designs on the basis of fluidization mode, reaction conversion, heat transfer, and particle mixing.

KEYWORDS: silicon deposition, fluidized bed reactor, computational particle fluid dynamics, CFD

The deposition of solid silicon in a fluidized bed reactor (FBR) is an important step in the industrial production of high purity polysilicon, the primary substrate for modern electronic and photovoltaic components. In the silane-based process, a mixture of silane and hydrogen gas is forced through a gas distributor in the bottom of the reactor where it fluidizes silicon seed particles in the reactor. Upon entering the reactor, the silane gas reacts at the surface of the silicon seed particles and deposits additional silicon, resulting in the growth of the particle. After growing to the desired size, the silicon particles are removed from the reactor as product and are replaced with new seed particles.

The fluidized bed reactor performance is strongly dependent on the fluidization mode and temperature distribution within the reactor (Hsu, 1987), which are functions of the reactor dimensions, gas distributor, gas flow rates, particle size distribution, reaction kinetics, and heat transfer within the bed. Furthermore, the long-term operability of the reactor is adversely affected by erosion on reactor internals and feed systems as well as clogging and plugging due to deposition of silicon on walls and inlet areas. To design, operate, and maintain a deposition FBR, it is necessary for the engineer to understand the sources of reactor malfunction, the interaction between the reactor operating parameters, and the corresponding effect on reactor performance. Often, good information on reactor design and operation is difficult to obtain due to a lack of experimental data or reliable correlations. Fortunately, robust computational tools for modeling particle-fluid interactions are available and have been successfully used to predict the behavior of particle-fluid systems. As a result, a rigorous particle-fluid dynamics computational model is a valuable asset to an engineer for understanding experimental results and discovering opportunities for optimization of a fluidized bed reactor for polysilicon deposition.

In this work, the operation of a fluidized bed reactor for the deposition of solid silicon from silane gas is modeled with the Barracuda® commercial computational fluid dynamics (CFD) software package. Barracuda rigorously simulates fluid-particle interactions using the CPFD® numerical method (Snider, 2001; Snider, 2007; O'Rourke et al, 2009) and is an established commercial simulation software package for the study of industrial-scale fluidized bed reactors (Zhao et al, 2006; Snider et al, 2010). The geometry and operating conditions of simulation are based upon an experimental reactor that was operated at the Jet Propulsion Laboratory (JPL). After validation of the CFD model against the experimental data, the model was used to compare the performance of two inlet gas distributors: a screen mesh and a ¼" nozzle. In a deposition FBR, the fluidization through a screen mesh distributor creates a bubbling bed that leads to high conversion of silane. The use of an inlet nozzle, however, has been found to be significantly better at minimizing clogging in the reactor. Consequently, it is not surprising that current design work for deposition reactor inlets (Ege et al,

2008) have produced hybrid inlet systems that attempt to capitalize on the benefits of both types of inlet configurations. The use of CFD to explore the screen and nozzle inlets lays the foundation for the future design of stable, high performance fluidized bed reactors for silane deposition.

Operation of a Fluidized Bed Reactor for Silane Deposition

During operation, a silane deposition reactor is partially filled with high-purity silicon particles in the range of 0.1 to 1.0 mm diameter. A gas mixture, consisting of silane (SiH_4) and hydrogen (H_2), is fed to the bottom of the reactor at a velocity which ensures fluidization of the silicon particles. The resulting reaction in the system is complicated, but previous modeling efforts (Praturi et al, 1977; Lai, 1986; Hsu, 1986; Hsu et. al., 1987; Piña et. al., 2006) have established a general framework for the reaction mechanism for silane deposition. In this previous work, it has been assumed that there are two routes for solid silicon formation within the reactor: 1) the heterogeneous deposition of silane gas on a solid silicon surface and 2) the homogeneous decomposition of silane gas into a silicon dust or *fines*. Upon contact with the larger particles in the reactor, the fines will be adsorbed onto the particle surfaces and contribute to the growth of the large particles. This complicated *scavenging* phenomenon is represented in a simplified form in this work. The kinetics of these reactions will be discussed in the following section.

Reaction Kinetics of Silane Deposition

The primary silane reaction in this work is the heterogeneous deposition of silane over a silicon particle. This reaction is described stoichiometrically as

$$\mathrm{SiH_4} + \mathrm{Si(s)} \xrightarrow{k_{\mathrm{het}}} 2\mathrm{Si(s)} + 2\mathrm{H_2}. \tag{1}$$

Because the reaction occurs on the surface of a silicon particle, the reaction rate for the growth of silicon (and consumption of silicon), the heterogeneous reaction rate is

$$r_{\mathrm{het}} = \frac{dC_{\mathrm{SiH_4}}}{dt} = -k_{\mathrm{het}} \left(\frac{S_{\mathrm{Si}}}{V_R} \right) C_{\mathrm{SiH_4}} \tag{2}$$

where S_{Si}/V_R is the surface area of silicon particles per reactor volume and k_{het} is the heterogeneous reaction rate constant. Based upon deposition experiments by Iya et al. (1982) in a bed with average particle size of 1595 microns and a bulk density of 1.14 g/cm^3, k_{het} is calculated to have an Arrhenius-type dependence on temperature, *T*, given in Equation 3.

$$k_{\mathrm{het}} = 2.793 \times 10^6 \exp\left(-\frac{1.954 \times 10^4\,[\mathrm{K}]}{T} \right) \; \left[\left(\frac{\mathrm{m^3\ reactor}}{\mathrm{m^2\ Si\ surfaces}} \right) \frac{1}{s} \right] \tag{3}$$

The secondary route of silicon formation is the homogeneous decomposition of silane into silicon fines. Because this reaction occurs away from a surface in the gas, the homogeneous reaction has a distinctly different set of kinetics. Furthermore, the silicon fines produced by this reaction are undesirable because of their size and unless scavenged, these silicon fines leave the reactor as a dust. Stoichiometrically, the homogeneous reaction is given by

$$\mathrm{SiH_4} \xrightarrow{k_{\mathrm{hom}}} \mathrm{Si(s)} + 2\mathrm{H_2}. \tag{4}$$

Because there is no surface reaction, the homogeneous reaction rate, r_{hom}, can be modeled with a first order expression.

$$r_{\mathrm{hom}} = \frac{dC_{\mathrm{SiH_4}}}{dt} = -k_{\mathrm{hom}} C_{\mathrm{SiH_4}} \tag{5}$$

The value of the reaction rate constant, k_{hom}, as a function of temperature, was found experimentally by Hogness (1936) to be

$$k_{\mathrm{hom}} = 2 \times 10^{13} \exp\left(-\frac{2.604 \times 10^4\,[\mathrm{K}]}{T}\right)\ \left[\mathrm{s}^{-1}\right]. \tag{6}$$

The scavenging rate is the final rate expression in the model. This rate expression describes the growth of silicon particles (and reduction in silicon fines) due to the accumulation of silicon fines on the particle surface. The scavenging of the silicon fines is represented in this work as a function of particle surface area per volume and mass per volume of silicon fines present.

$$r_{\mathrm{scav}} = \frac{d\left(\rho_{\mathrm{fines}}\right)}{dt}\left(M_{\mathrm{Si}}\right)^{-1} = -\alpha\left(\frac{S_{\mathrm{Si}}}{V_R}\right)\frac{\rho_{\mathrm{fines}}}{M_{\mathrm{Si}}} \tag{7}$$

where the value of α is a scavenging factor determined from comparison with experimental data and ρ_{fines} is the mass density of silicon in fines in the gas phase. This simple scavenging expression is a constant velocity approximation of the equation suggested by Hsu, et al (1987). There are other factors that will affect the scavenging rate, such as diffusional and hydrodynamic effects near the particle, but for this work the scavenging rate is suitable for validation with the available experimental data. A basic search of scavenging factors was conducted through which a value of $\alpha = 2.0 \times 10^{-4}\ \left[\left(\frac{\mathrm{m^3\ reactor}}{\mathrm{m^2\ particle\ surface}}\right)\frac{1}{s}\right]$ was found to fit the experimental data reasonably well. This value of α was used in this work.

In terms of the reaction rate constants, the growth rate of a particle in the reactor is

$$\frac{\text{Change in Mass of Particles}}{(\text{Unit Reactor Volume})\,(\text{Unit time})} = -\left(r_{\mathrm{het}} M_{\mathrm{Si}} + r_{\mathrm{scav}} M_{\mathrm{Si}}\right)\left(1 - \theta_s\right) \tag{8}$$

where θ_s is the volume fraction of solids in the reactor.

Experimental Data Used for Validation

In the 1980's, a significant amount of research into silane deposition was conducted at the Jet Propulsion Laboratory. Experimental data from the operation of a 6" diameter fluidized bed reactor was reported by Hsu et al. (1984, 1986, 1987), Lutwack (1986), and Rohatgi (1986). The reactor consisted of an externally heated reaction zone (6" diameter, 48" tall), a disengagement zone (24" diameter, 24" tall), and a cooled inlet zone. Reactor heating was provided by a two-zone lower heater and a single zone upper heater.

The JPL researchers tested five different gas distributors for the reactor inlet. Four of these distributors produced a uniform gas distribution at the reactor bottom, resulting in a bubbling fluidized bed. A ¼" nozzle that created a spouted fluidized bed was also tested. As discussed by the JPL researchers, the spouted bed created by the nozzle did not provide ideal performance: "A very poor situation is one in which the fluidized bed operates in a slugging mode to favor a large amount of homogeneous decomposition and thus high fines production" (Hsu et al, 1984). Ultimately, a screen mesh distributor producing a uniform gas flow at the reactor inlet was selected for use by the JPL researchers.

From the experimental data reported by JPL researchers (Hsu et al. 1984; 1986; 1987; Rohatgi, 1986), the experimental conditions in Table 1 were selected for simulation. While the concentration of silane at the inlet is different for each run, the following conditions were consistent for all runs:

- Pressure at the top of the reactor: 5 psig
- Reactor bed temperature: 650°C
- Initial bed weight: 10 kg
- Average particle diameter: 250 microns
- Total inlet gas flow rate (SiH_4 and H_2): 3 mol/min ($u / u_{mf} \approx 5$ at inlet, as reported by Hsu et al. 1984; 1986; 1987; Rohatgi, 1986)
- Hydrogen makeup gas
- The inlet area is cooled to approximately 100°C.

Table 1. Experimental results from 6" reactor (Hsu et al. 1984; 1986; 1987; Rohatgi, 1986). Feed gas assumed be ideal (vol% ≈ mol%)

	SiH_4 Feed *(mol%)*	**Avg. Particle Diameter *(um)***		**Deposition Rate** *(kg/hr)*	**Reactor Fines** *(%)*
		Initial	Final		
1	20%	227	235.5	1.0	3.9%
2	50%	268	297.6	2.4	-
3	57%	236	251.9	3.0	9.4%
4	80%	212	241.5	3.5	11.1%

Computational Method

Traditional commercial CFD packages are designed for single-phase flow, either gas-only or liquid-only flows. Extensions over the 40 years or so that CFD has been popularized have allowed many such packages to handle some narrowly defined particle-fluid problems. The Barracuda® simulation package from CPFD Software, LLC (Albuquerque, NM), however, provides robust simulation capabilities for highly-coupled particle fluid systems at industrial scales. Furthermore, the capability to model gas-phase and surface reactions (including particle growth and shrinkage) and heat transfer in the reactor makes Barracuda an effective computational tool for modeling an FBR for polysilicon deposition.

The numerical method employed in Barracuda is called Computational Particle Fluid Dynamics (CPFD®) and offers specific advantages that were essential to the success of this modeling effort. The CPFD method solves the fluid and particle momentum equations in three dimensions. The fluid is described by the Navier-Stokes equation with strong coupling with the discrete particles. The particle momentum follows the multi-phase particle-in-cell (MP-PIC) numerical description from O'Rourke (2009), Andrews (1996), Snider (1998), and Snider (2001) which is a Lagrangian description of particle motion described by ordinary differential equations with coupling with the fluid. The CPFD solution (Snider, 2001) as applied in Barracuda is aimed at solving commercial problems, which are generally physically large systems. (Though the JPL units are relatively modest in size, full-scale commercial deposition reactors are substantially larger.) In the CPFD method, a numerical-particle is defined where particles are grouped with the same properties (species, size, density, temperature, etc.). The numerical-particle is a numerical approximation which allows a large commercial system containing billions of particles to be analyzed using millions of numerical-particles without losing the advantages of discretizing the solid phase in a Lagrangian frame of reference. As a result of CPFD's unique numerical approach, the following aspects of fluidized bed behavior are captured:

1. The ability to model full particle size distribution (PSD) for any number of solid species – critical for any fluidized process and not supported by traditional commercial CFD packages.
2. The capacity to model any solids loading from fully dilute up to close-packed (>60% solid by volume) regime in the same simulation and without prior knowledge of what the loading is likely to be.
3. Complete Lagrangian formulation for the solids, capturing mass, momentum, heat transfer, wear, etc.
4. A chemistry modeling capability allowing full gas-gas, gas-solid, and solid-solid chemistry.
5. The ability to model systems with physical particle counts over 1E16 particles.

The ability of the model to handle a wide range of particle loading in the same simulation domain was important in this work. The testing of both a uniform inlet distributor and an inlet nozzle produced different fluidization modes (bubbling and spouting) and solids loading ranging from fully dense packed to extremely dilute. While not studied in the current work, the capability of Barracuda to model the particle forces, including impact-induced wear on the internals and particle attrition would be valuable in the future for predicting long term reactor reliability and studying the production of fines due to the breakage of particles.

Setup of CFD Simulations

The deposition of polysilicon from silane gas in an FBR was simulated for two different geometries: the JPL reactor with an inlet screen (uniform gas distribution) and the JPL reactor with a ¼" inlet nozzle. The dimensions of each geometry are illustrated in Figure 1. Each reactor was simulated with a pressure boundary condition at the top equal to 135.8 kPa and total gas flow rate of 3 mol/min at the reactor inlet (bottom). In each simulation, the gas and particles were initially at rest and gas flow was ramped up to the operating rate over 5 seconds. A uniform particle size distribution from 75 micron to 425 micron diameters is assumed. The average of this distribution, 250 microns, is consistent with the particle diameter reported in the experimental data. The close pack particle volume fraction is assumed to be 0.54.

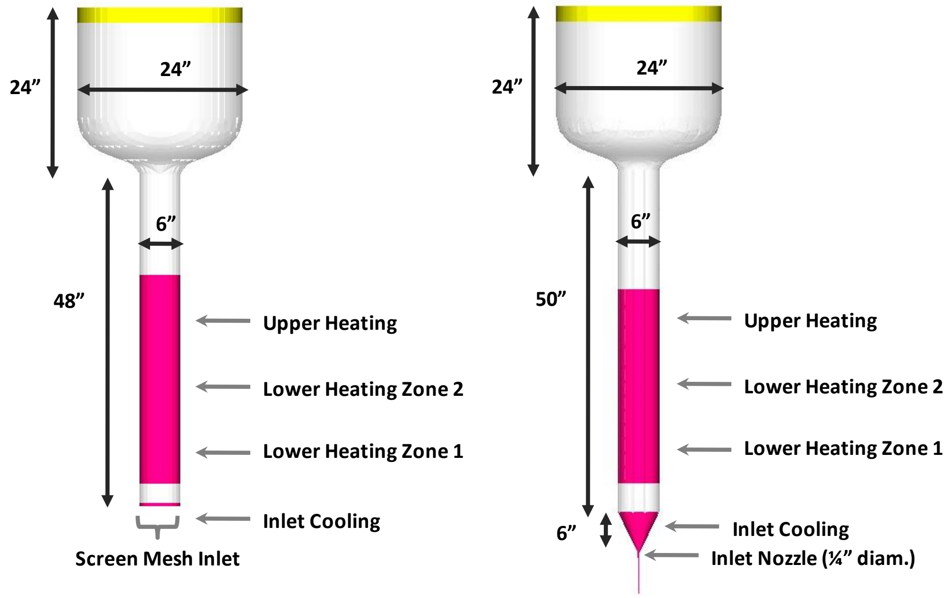

Figure 1. Geometry of Modeled Deposition Reactors. (LEFT) with Inlet Screen; (RIGHT) with Inlet Nozzle

Three sets of simulations were performed. In the first set, the deposition rate of silicon and the formation of fines were studied for the reactor with an inlet screen (bubbling bed reactor). Temperature was assumed to be isothermal at 650°C. The reactor with the inlet screen was modeled for each of the operating conditions in Table 1. In the second set of simulations, the silicon deposition rate and fines formation in the reactor were studied with the inlet nozzle at 650°C (isothermal), simulating each of the operating conditions in Table 1. The third set of simulations examined the temperature distribution and heating requirements for reactors with both inlet distributors. Convective and conductive heat transfer was considered. For this third set of simulations, total gas flow was 3 mol/min of which silane was 20 mol%. The inlet walls and inlet gas were both cooled to 100°C while the heated reactor walls were at 650°C using a temperature boundary condition. The gas and particles were initially at 640°C. For all three sets of simulations, the seed particle feed and product withdrawal systems were not considered and wall deposition reactions are not included in the reaction set.

To model the fines production within the capabilities of the CFD package, the silicon fines were treated as a gaseous species, as particulate formation through direct deposition (i.e., gas-to-solid phase change where no seed particle is present) is not yet directly supported in the software. This assumption should have a negligible effect on the fluidization behavior of the reactor due to the relatively high molecular weight of silicon compared to hydrogen and due to the relatively low levels of fines in the reactors.

Results - Validation of CFD Model

In the first set of simulations, the flow rate of silane entering and leaving the reactors and the amounts of silicon fines leaving the reactor were tracked. From this information, the deposition rate of silicon within the bed and the percentage of silicon leaving the reactor as fines were calculated. The results of the CFD model are compared with the experimental results (from Table 1) in Figure 2 and Figure 3. As the concentration of silane being fed to the reactor increases, the additional availability of reactant causes the deposition rate within the reactor to increase also. Increasing the silane concentration also leads to an increase in the percentage of silicon leaving the reactor as fines. Comparison between the computational results and the JPL data shows that the CFD results match very closely with the experimental data reported from the research conducted at JPL for both the deposition rate of polysilicon and the fines production within the reactor.

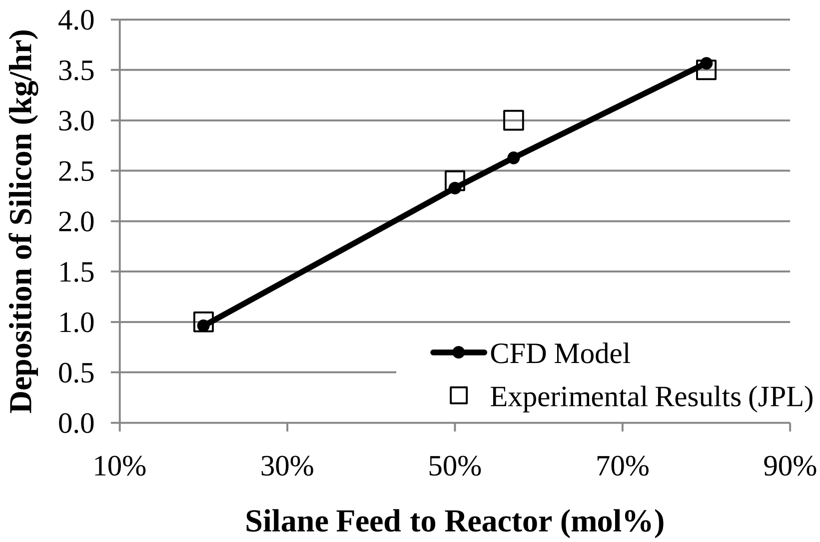

Figure 2. Comparison of Experimental Results with Barracuda Model for Polysilicon Deposition Rate in Reactor with Inlet Screen

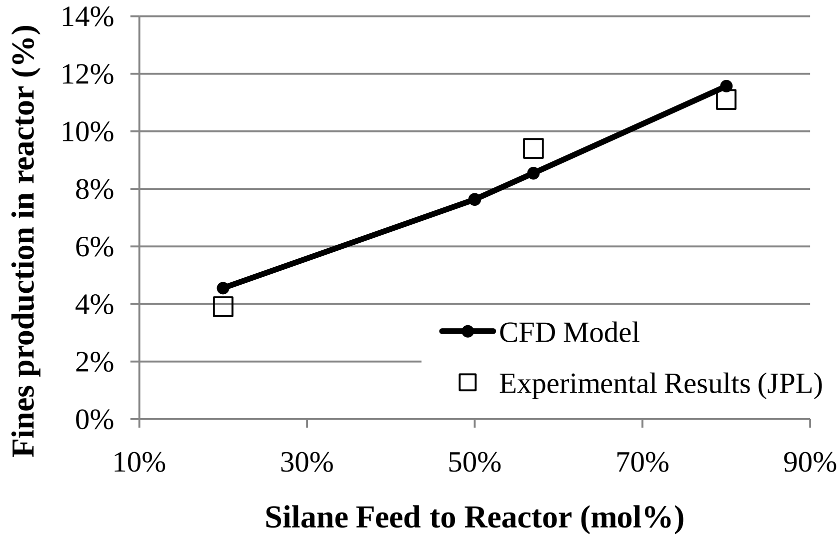

Figure 3. Comparison of Experimental Data with CFD Model for Fines Production Inside Reactor with Inlet Screen.

In the third set of simulations, the fluid temperature was determined along the centerline of the reactor with the inlet screen. A comparison of the simulated temperatures with the reported experimental data is shown in Figure 4. Both the experimental data and the CFD model show a very quick rise from the inlet temperature of ≈100°C to the bed temperature of ≈650°C and both experimental data and the model show that the operating temperature is reached within 10 cm of the reactor inlet. The comparison of the simulation results with experimental data for silicon deposition, fines production, and temperature profile demonstrates the validity of using the CPFD method to model the deposition of polysilicon in a fluidized bed reactor.

Results - Effect of Gas Distributor on Reactor Performance

The modeled behavior of the reactor was affected greatly by the type of distributor used at the reactor inlet, as the results from JPL's experiments would suggest. Consistent with the experimental observations (Hsu, 1987), the uniform gas distribution associated with a screen mesh distributor created a bubbling bed while the 1/4" nozzle created a spouted bed. The effect of the distributor type was examined for particle-fluid hydrodynamics, reactant and product distribution, temperature distribution, and particle mixing. All time averaging has been performed over 15 seconds of simulated time.

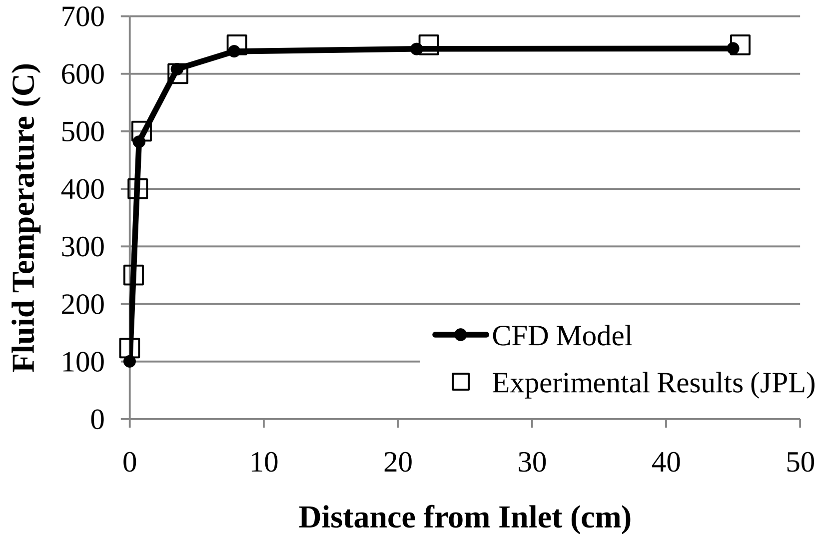

Figure 4. Temperature Distribution in FBR with Inlet Screen

Particle and Gas Flow

The instantaneous and time-averaged plots of both the particle volume fraction and fluid velocity are shown for the reactor with inlet screen in Figure 5 and for the reactor with the inlet nozzle in Figure 6. These figures illustrate the dramatically different bed behavior for each type of distributor. The uniform gas velocity created by the screen distributor creates a fairly uniform upward flow of gas throughout the bed. As a result, the time-averaged particle volume fraction varies by 10% to 20% in the bed. The nozzle distributor, however, creates a high velocity jet of gas up the center of the bed. The resulting particle volume fraction decreases to the range of 0.10 to 0.2 at the center whereas at the outside of the bed it is densely packed with a particle volume fraction of 0.54.

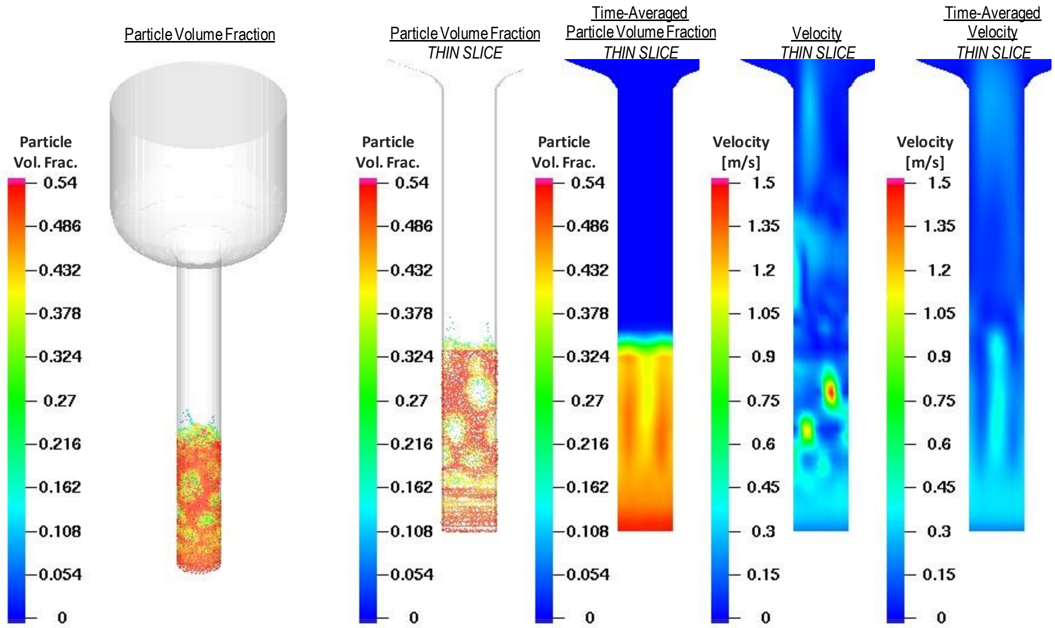

Figure 5. Particle and Gas Flow in FBR with Inlet Screen (Bubbling Bed)

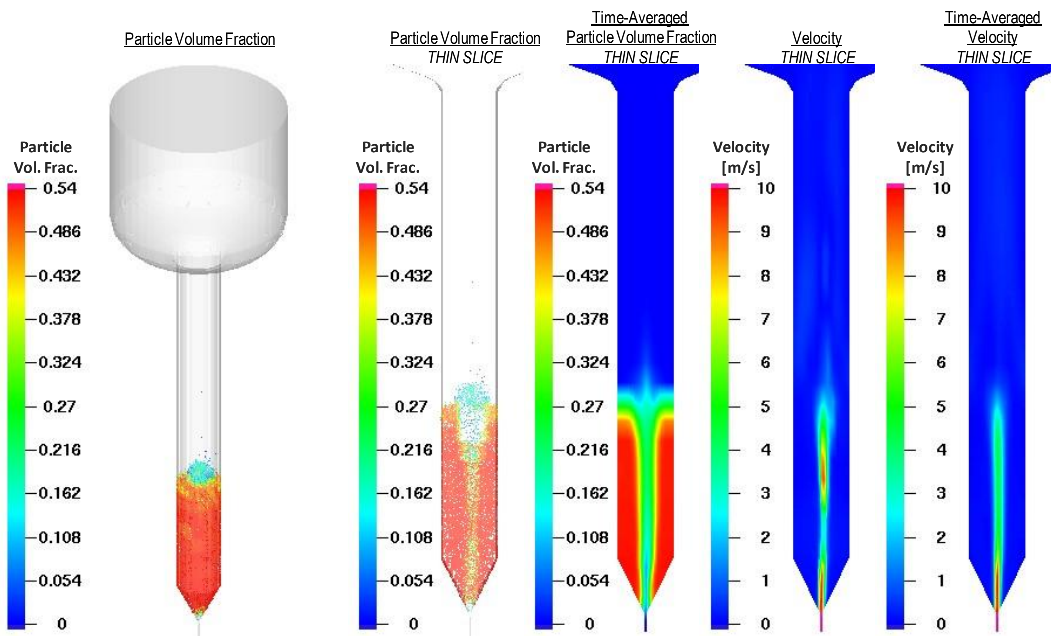

Figure 6. Particle and gas Flow in FBR with Inlet Nozzle (Spouted Bed)

Reactant and Product Distribution

The effect of the reactor inlet type and the resulting fluidization mode in the bed consequently has a significant effect on the distribution of reactants and products within the FBR. As shown in Figure 7, the screen mesh creates a distribution of reactants and products that varies mainly with height in the reactor but is fairly independent of radial location. The reactor with the nozzle, however, behaves very differently. For the nozzled reactor, there is a strong dependence on radial location, consistent with a large amount of reactant transport in the spout. For the simulated bed weight, gas flow rates, and reactor dimensions, it can be seen that a large percentage of the silane is being transported through the bed in the spout, severely reducing opportunities for the silane to deposit on a particle surface. As a result, much of the silane that enters the space above the particles homogeneously reacts to form silicon fines. Consequently, the deposition rate is lower and the fines formation is higher in the reactor with the inlet nozzle than in the reactor with the inlet screen. This is shown in Figure 8 and Figure 9.

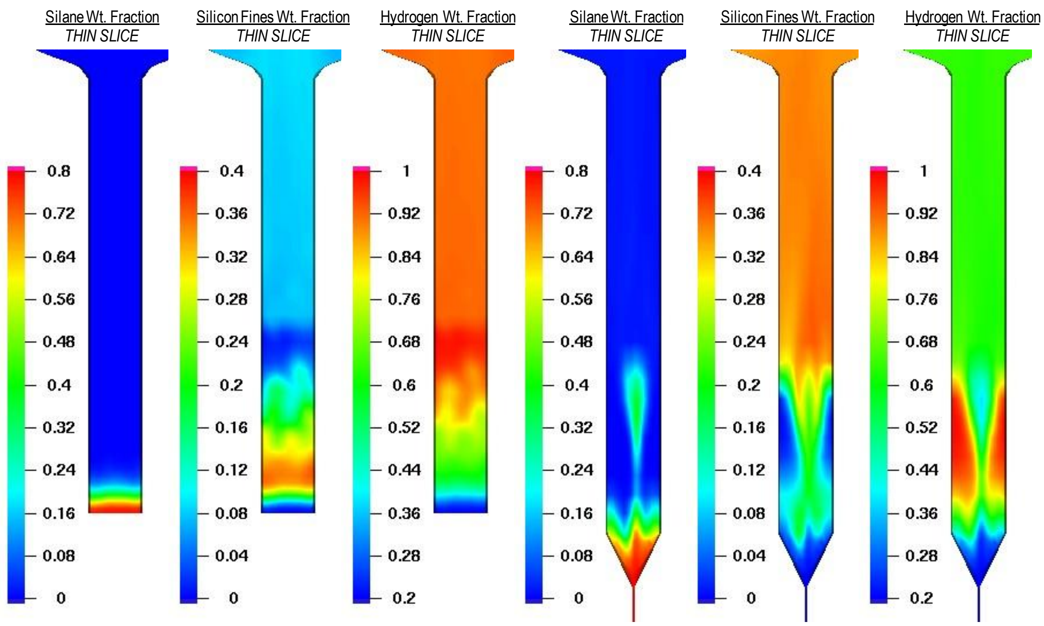

Figure 7. Reactant and Product Concentrations in FBRs; with Inlet Screen, 1-3; with Inlet Nozzle, 4 – 6

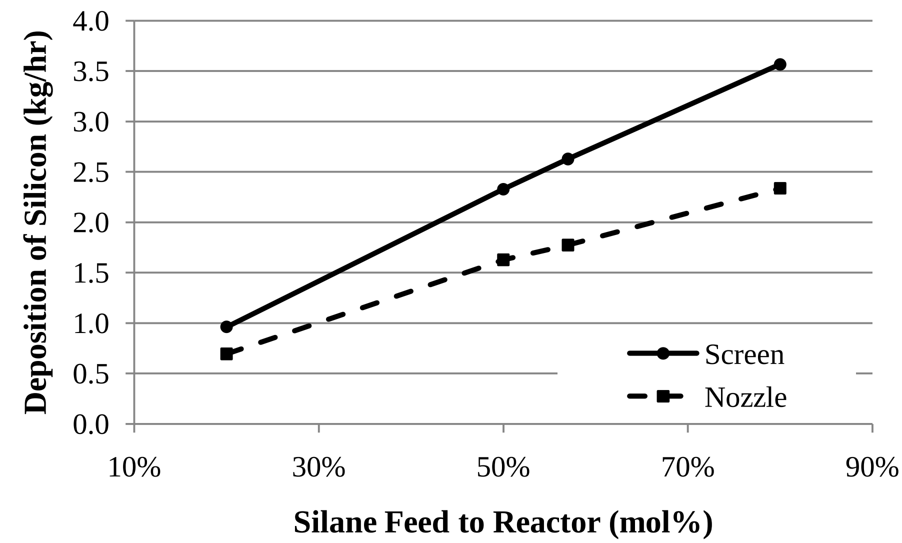

Figure 8. Modeled polysilicon deposition rate in deposition reactors

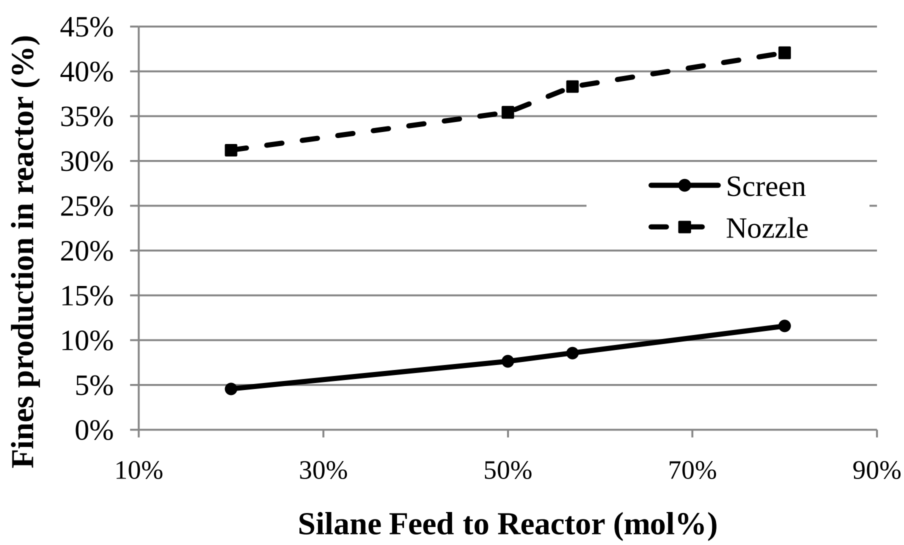

Figure 9. Simulated Production of Silicon Fines in Deposition Reactors

Temperature

Like the reactant and product distributions, the type of gas distributor also has an effect on the temperature within the reactor. Temperature is very important in the inlet areas of the reactors as it is necessary to cool the inlet areas to prevent deposition at the inlets which can lead to clogging, while maintaining a constant bed temperature to optimize the deposition on silicon particles. Figure 10 shows that the inlet nozzle provided better cooling due to the increased wall area and jetting of cold gas from the bottom minimizes the local recirculation of gases from the bed.

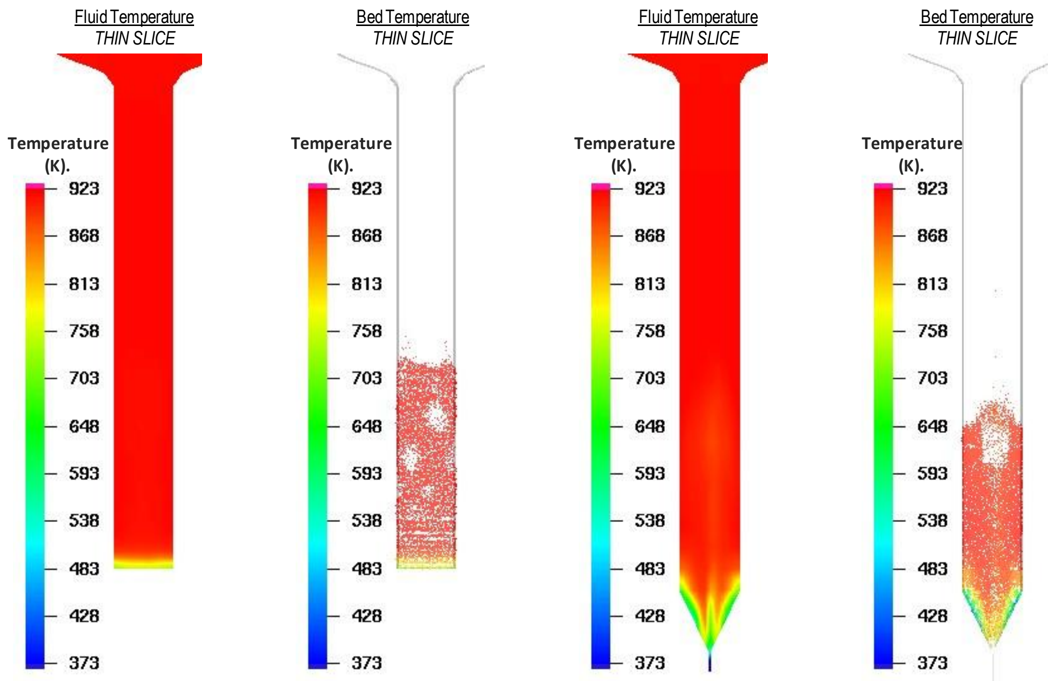

Figure 10. Temperature Distribution in FBRs; with inlet screen, 1-2; with inlet nozzle, 3-4

Particle Mixing

To examine the effect of each distributor type on the particle mixing on the bed, the particles that were initially in the top of the part of the bed (colored red in Figure 11 and Figure 12) were distinguished from the those particles that were initially located in the bottom half of the fluidized bed (colored blue in Figure 11 and Figure 12). The time series for the screen distributor is shown in Figure 11 whereas Figure 12 shows the mixing resulting from the nozzle distributor.

In these simulations, the nozzle distributor creates a very ordered mixing whereas the mixing created by the screen distributor is somewhat more random. Nevertheless, it appears that both distributor types are able to adequately mix the bed within a short period of time.

Summary and Conclusions

In this work, the operation of a fluidized bed reactor for the deposition of solid silicon from silane gas was modeled with the Barracuda CFD package. From this analysis, the ability of the simulation to closely fit the experimental data for silane deposition was demonstrated by comparing the CFD results with published experimental data. The CFD model was then used to explore the effects of inlet feed system on the FBR performance, specifically looking at fluidization and hydrodynamic behaviors, reactant and product distribution within the reactor, temperature profiles, and particle mixing within the bed.

Fluidized bed reactors for silicon deposition have complex interactions between the reactor geometry, gas flow rates, particle size distribution, and bed heat transfer and therefore can be challenging to design and optimize. The Barracuda software, using the CPFD method to model particle-fluid interactions, can provide valuable information to an engineer on the effect that operating parameters have on the fluidization mode, temperature distribution, silicon deposition, and unwanted side reactions. Furthermore, simulations of fluidized bed reactors can provide information on the wear of internal reactor structures as well as sites of likely deposition and clogging. Simulations based upon the CFD method were shown in this study to be valuable and effective tools for design and optimization of silicon deposition reactors.

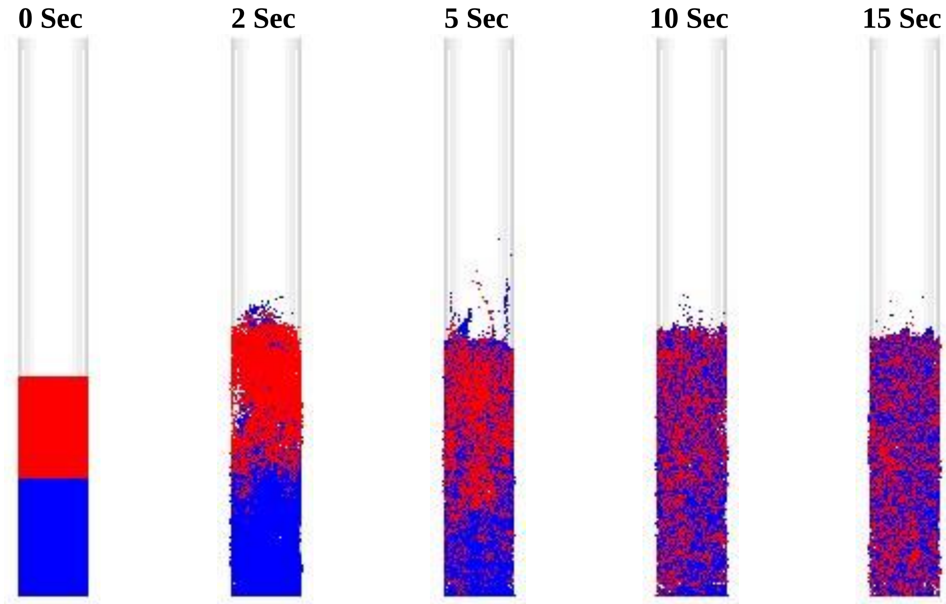

Figure 11. Mixing in Bed With Screen Distributor

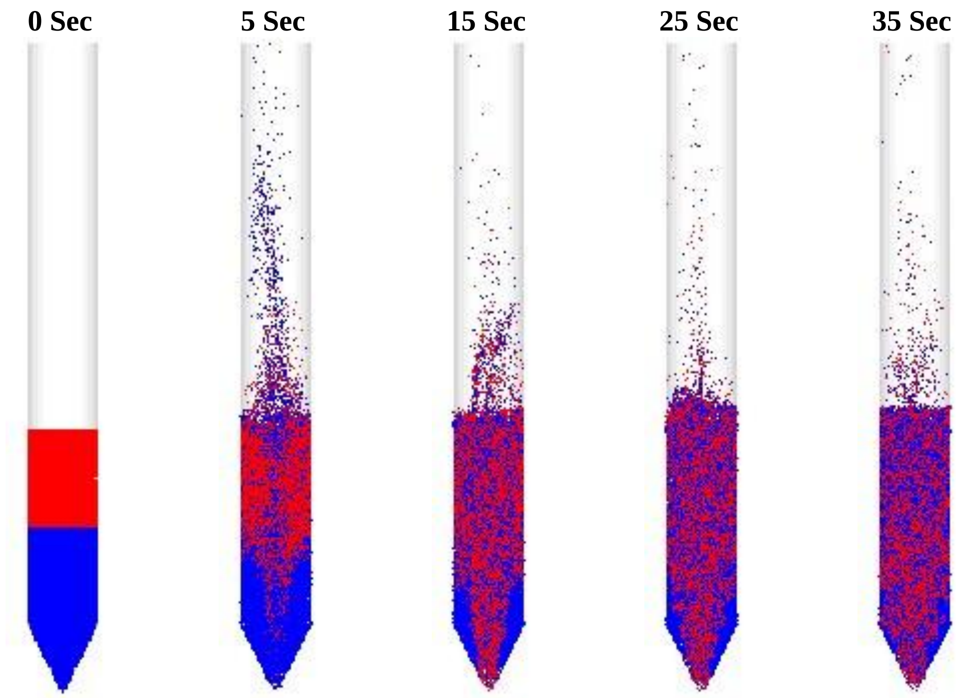

Figure 12. Mixing in Bed with Nozzle Distributor

Notation

k_{het}	heterogeneous reaction rate constant, [(m^3/m^2) s^{-1}]
k_{hom}	homogeneous reaction rate constant, [s^{-1}]
M_{Si}	molecular weight of silicon, [g/mol]
r_{het}	heterogeneous reaction rate, [mol/m^3/s]
r_{hom}	homogeneous reaction rate, [mol/m^3/s]
r_{scav}	scavenging rate, [mol/m^3/s]
S_{Si}/V_R	surface area of silicon particles per reactor volume , [m^2/m^3]
T	temperature, [K]
u	superficial velocity entering reactor, [m/s]
u_{mf}	minimum fluidization velocity, [m/s]

Greek letters

α	scavenging constant, [(m^3/m^2) s^{-1}]
ρ_{fines}	mass density of silicon fines, [kg/m^3]
θ_{s}	volume fraction of solids in reactor, [m^3/m^3]

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