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Numerical investigation of Polysilicon Particle Growth in a Fluidized Bed Reactor

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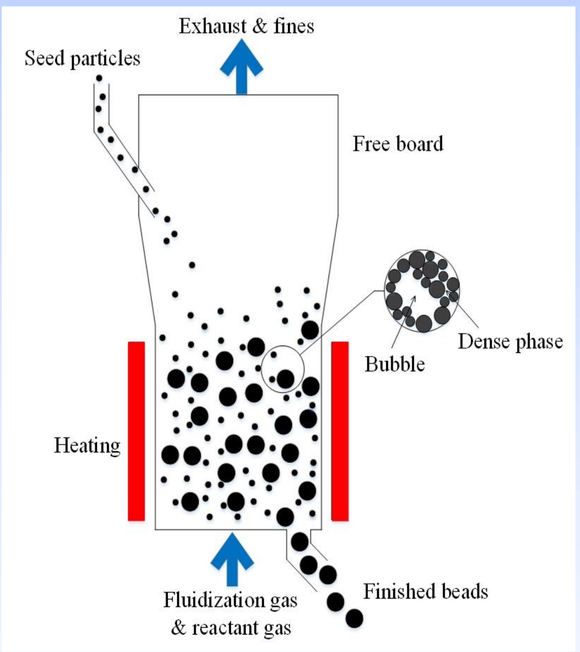
Background

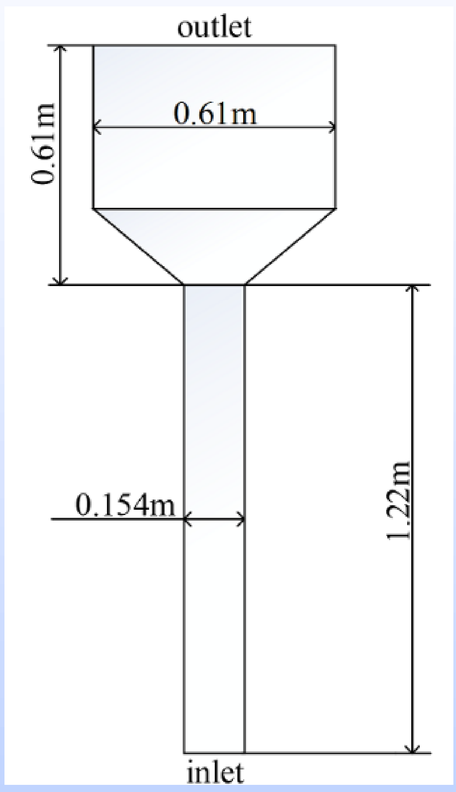


The fluidized bed reactor (FBR) method, using silane as the reactant gas, has attracted much attention due to efficient heat and mass transfer capacities, relatively low energy consumption, and high silane conversion. In a polysilicon FBR, the silicon seeds are loaded into the reactor, then they are fluidized by the gas mixture of silane and carrier gas.

In FBR, the complex silane pyrolysis reaction occurs in gas phase and the surface of the silicon seeds during the chemical vapor deposition (CVD) process. The silane homogeneous pyrolysis in gas phase leads to the unwanted formation of silicon fines. The silicon fines can also be captured by the seed particles, which is known as the scavenging mechanism. The scavenging mechanism is related to the seed diameter, the silicon fines concentration, and the velocity difference between the seed particle and silicon fines. However, previous studies only consider the seed diameter and the silicon fines concentration, the velocity difference of silicon seeds and silicon fines is neglected.

Modelling

➢ Geometry

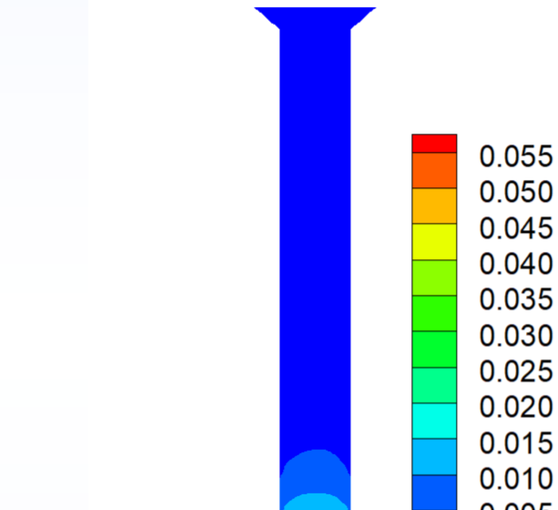


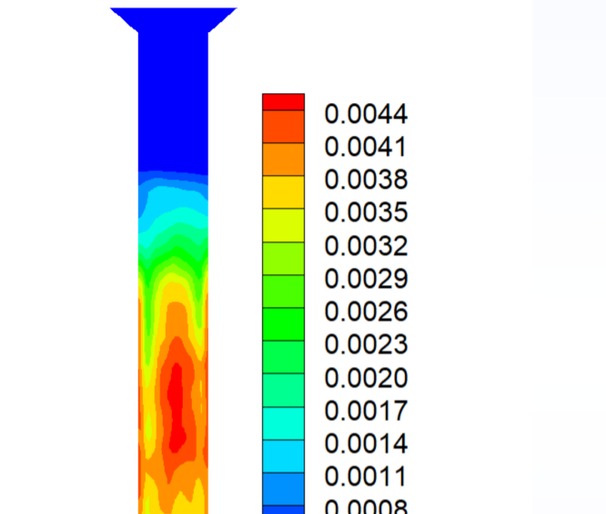
➢ Simulation setting

- **Two-fluid model**
- **Gidaspow drag model**
- ***k-ε* turbulence model**
- **Initial particle diameter:** 236μm
- **Inlet gas velocity:** 0.6m/s
- **Silane density:** 0.42kg/m^3
- **Hydrogen density:** 0.027kg/m^3
- **Particle density:** 2330kg/m^3
- **Initial bed height:** 0.61m

Results

➢ Model validation & gas concentration





The simulation matches the experimental data well. A reverse mass fraction distributions of silane and silicon fines appear along the reactor height, indicating the heterogeneous deposition mainly occurs at the bed bottom.

➢ Instantaneous distributions of the increment of polysilicon particle diameter

a) Mean hetergeneous reaction mass transfer rate (kg/m^3·s)

b) Mean scavenging mass transfer rate (kg/m^3·s)

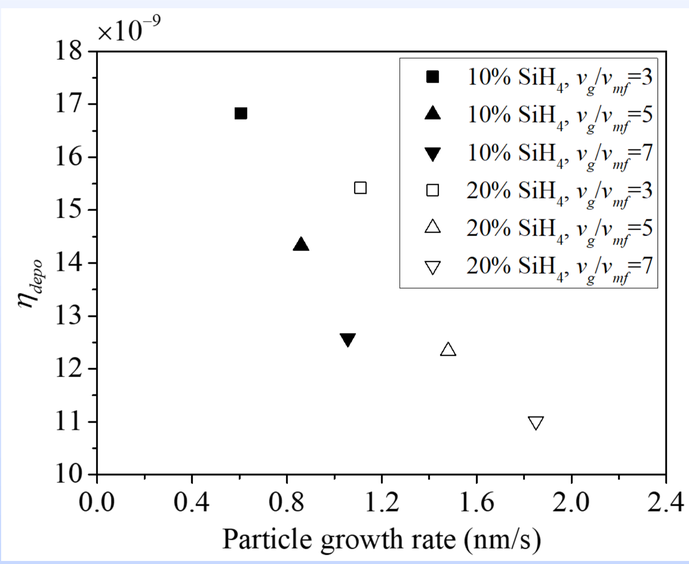
Silicon fines scavenging occurs in almost the whole solid phase, especially in central and near-wall regions.

➢ Effect of operating condition on particle growth process

Silicon deposition efficiency (η_{depo}) is proposed as following:

$$\eta_{depo} = \frac{G(L)}{v_g \times C_{SiH_4}}$$

$G(L)$, v_g and C_{SiH4} are the particle growth rate, gas velocity and silane mole fraction at the reactor inlet.



Increases of operating velocity and silane mole fraction lead to the decrease of deposition efficiency

Conclusions

1. The heterogeneous reaction mainly occurs at the bed bottom.

2. The scavenging mass transfer rate is low near the bottom and upper surface, and it shows a "W" shape distribution in radial.

3. The increases of operating velocity and silane mole fraction lead to the increase of particle growth rate, while the silicon deposition efficiency decreases.