Process Engineering: Ethical and Profitable Synthesis of Polycrystalline Silicon for Solar Cell Mass Production

Christia Ellerman, Alissa Koniszewski, Ashfiha Rahman, Talia Ritchie, and Paige Wilcox
Department of Chemical and Biomolecular Engineering, University of Maryland, College Park, MD

Introduction

Polycrystalline silicon (poly-Si), also known as polysilicon or multi-crystalline silicon, is a key material in solar cells for photovoltaic (PV) modules. These cells convert sunlight into electricity via the photovoltaic effect. Due to its cost-effectiveness, durability, and environmental benefits, poly-Si is widely used in large-scale solar energy production. Chemical engineers are well-suited to design poly-Si manufacturing processes, which require precise control of complex reactions and purification steps. The standard method, the Siemens process, involves purifying metallurgical-grade silicon (Mg-Si) into trichlorosilane (TCS), which is then reacted with hydrogen to produce high-purity poly-Si. Our team seeks to develop an improved, sustainable, and cost-efficient process for poly-Si production, offering a commercially viable and eco-friendly path to solar energy generation.

Reactions

Key Reactions in Polysilicon Production:

1. Carbothermic Reduction in Submerged Arc Furnace
   a. Primary reaction:
      $SiO_{2\,(s)} + 3C_{(s)} \rightarrow SiC_{(s)} + 2CO_{(g)}$
   b. Secondary reaction (at higher temperatures):
      $SiO_{2\,(s)} + 2SiC_{(s)} \rightarrow 3Si_{(l)} + 2CO_{(g)}$
      i. Result: Metallurgical-grade silicon (MGS, ~98% purity).
1. Fluidized Bed Reactor: Trichlorosilane Synthesis Chlorination:
   b. Primary reaction:
      $Si_{(s)} + 3HCl_{(g)} \rightarrow SiHCl_{3\,(l)} + H_{2\,(g)}$
      i. Conditions: ~300 degrees Celsius, powdered MGS reacts with HCl.
1. Siemens Process: High-Purity Polysilicon Deposition Hydrogen Reduction:
   b. Primary reaction:
      $SiHCl_{3\,(l)} + H_{2\,(g)} \rightarrow Si_{(s)} + 3HCl_{(g)}$
      i. Conditions: ~700 degrees Celsius via chemical vapor deposition (CVD). Output: Electronic-grade silicon (99.99% purity)

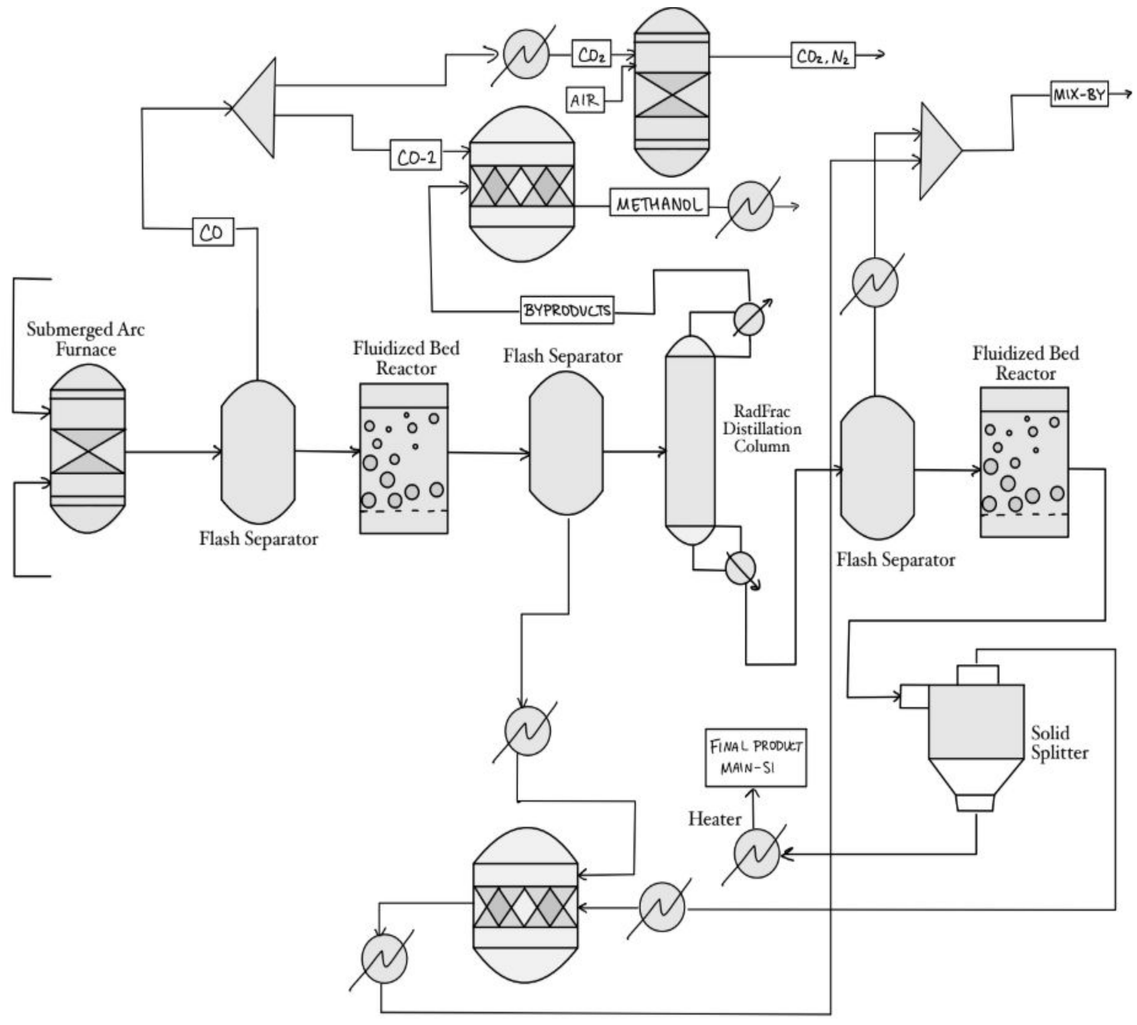

Figure 1. *Optimized Process Flow Diagram:* The process flow diagram of the optimized design for the polycrystalline process. This diagram contains the recycle streams as well as the bells and whistles that were added to optimize the design.

Process Description

Polycrystalline silicon for solar cells is produced through a multi-step process involving quartz (SiO_2), carbon (C), and hydrogen chloride (HCl) as key reactants. Quartz and carbon are reduced in a high-temperature RGibbs furnace to form metallurgical-grade silicon (Mg-Si), which undergoes purification through a series of flash separators. The Mg-Si reacts with HCl in a CSTR to form trichlorosilane ($SiHCl_3$), which is further purified via flash separation and distillation (RadFrac column) to reach 99.99% purity. The purified $SiHCl_3$ is then converted into high-purity silicon in a chemical vapor deposition reactor. A final solid-splitting step ensures separation of residual impurities, yielding polycrystalline silicon suitable for solar cell manufacturing.

Economics

The company aims to lead in manufacturing high-efficiency M10 solar cells for commercial use, operating from Arizona—a state with abundant sunlight, strong clean energy incentives, and access to skilled labor. With an initial investment of $64.8 million, the projected Net Present Value is $190.4 million, ROI is 63.64%, and the payback period is 1.56 years. The solar market's 17% CAGR and rising global demand make this a highly profitable venture. The company plans to produce 2.55 million solar cells annually, priced competitively at $0.19/cell, with methanol byproduct sales further enhancing revenue. Automation, energy-efficient equipment, and proximity to major markets like California and Texas support sustainable growth and cost savings.

Safety & Environment

The silicon production process incorporates key safety and environmental controls to manage hazardous byproducts like carbon monoxide (CO) and hydrogen chloride (HCl). CO is converted to CO_2 via controlled combustion, enhancing worker safety while maintaining emissions at 5.592 kg/hr. HCl, used in converting metallurgical-grade silicon to trichlorosilane, is recycled and fully converted to a more stable product, improving efficiency and reducing risks. Continuous monitoring, automated shutdowns, and proactive containment ensure safe operation. Environmentally, CO and H_2 are further processed into synthetic methanol, aligning with carbon capture goals, reducing Scope 1 emissions, and supporting compliance with EPA, OSHA, and clean energy regulations.

References

1. OpenAI. (2025). ChatGPT (April 8 version) [Large language model].
2. What Are the Benefits of Polycrystalline Silicon Solar Power Generation? - MJK Power- China PV Module Solar Panel Supplier. (2023, October 16).