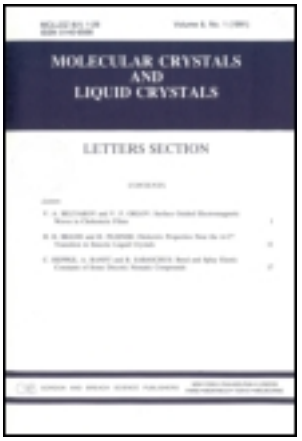
This article was downloaded by: [Chongqing University]
On: 15 February 2014, At: 04:51
Publisher: Taylor & Francis
Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

Effect of Rod Diameters on Flow Pattern and Temperature Profile in Monosilane Siemens Poly-Si Reactor

Soyoung Jeon [a], Hosub Jung [a], Jong Hoon Park [b] & Woo Kyoung Kim [a]

[a] School of Chemical Engineering, Yeungnam University, Gyeongsan, Gyeongbuk, 712-749, Republic of Korea
[b] Technical R&D Center, Semi-Materials Co. Ltd., 770-803, Republic of Korea
Published online: 08 Jan 2014.

To cite this article: Soyoung Jeon, Hosub Jung, Jong Hoon Park & Woo Kyoung Kim (2013) Effect of Rod Diameters on Flow Pattern and Temperature Profile in Monosilane Siemens Poly-Si Reactor, Molecular Crystals and Liquid Crystals, 585:1, 73-81, DOI: 10.1080/15421406.2013.849519

To link to this article: http://dx.doi.org/10.1080/15421406.2013.849519

PLEASE SCROLL DOWN FOR ARTICLE

Taylor & Francis makes every effort to ensure the accuracy of all the information (the "Content") contained in the publications on our platform. However, Taylor & Francis, our agents, and our licensors make no representations or warranties whatsoever as to the accuracy, completeness, or suitability for any purpose of the Content. Any opinions and views expressed in this publication are the opinions and views of the authors, and are not the views of or endorsed by Taylor & Francis. The accuracy of the Content should not be relied upon and should be independently verified with primary sources of information. Taylor and Francis shall not be liable for any losses, actions, claims, proceedings, demands, costs, expenses, damages, and other liabilities whatsoever or howsoever caused arising directly or indirectly in connection with, in relation to or arising out of the use of the Content.

This article may be used for research, teaching, and private study purposes. Any substantial or systematic reproduction, redistribution, reselling, loan, sub-licensing, systematic supply, or distribution in any form to anyone is expressly forbidden. Terms & Conditions of access and use can be found at http://www.tandfonline.com/page/terms-and-conditions

Mol. Cryst. Liq. Cryst., Vol. 585: pp. 73–81, 2013
Copyright © Taylor & Francis Group, LLC
ISSN: 1542-1406 print/1563-5287 online
DOI: 10.1080/15421406.2013.849519

Taylor & Francis
Taylor & Francis Group

Effect of Rod Diameters on Flow Pattern and Temperature Profile in Monosilane Siemens Poly-Si Reactor

SOYOUNG JEON,[1] HOSUB JUNG,[1] JONG HOON PARK,[2] AND WOO KYOUNG KIM[1,*]

[1]School of Chemical Engineering, Yeungnam University, Gyeongsan, Gyeongbuk 712-749, Republic of Korea.
[2]Technical R&D Center, Semi-Materials Co. Ltd. 770-803, Republic of Korea

The deposition rate of polysilicon and the temperature and concentration profiles of the reactant gases in a monosilane Siemens reactor were compared for rod diameters of 10–120 mm using the computational fluid dynamics method. It was found that the power consumption primarily depends on the Si rod diameter and the Si deposition rate. The relationship between the power consumption and the Si deposition rate at different Si rod diameters was established from the accumulated experimental data of a pilot-scale four-rod reactor, and it is incorporated into the MonoSim-S software package.

Keywords Monosilane; polysilicon; power consumption; Si deposition rate; Siemens reactor

Downloaded by [Chongqing University] at 04:51 15 February 2014

Introduction

Polycrystalline silicon (polysilicon) is used in photovoltaic cells as well as conventional semiconductor applications. One of the most widely employed methods for fabricating polysilicon involves the use of a chemical vapor deposition (CVD)-based Siemens reactor system with a mixed gas of monosilane (MS, SiH_4) or trichlorosilane (TCS, $SiHCl_3$) and hydrogen.

The Siemens process, which is considered to be an ideal method for the mass production of polysilicon, typically produces rod-shaped polysilicon in a batch-type bell-jar reactor. Many companies mostly use the TCS-Siemens process. However, owing to the high manufacturing cost, toxic by-products, equipment corrosion by Cl, and expensive by-product recycling in this process, the MS-Siemens process has been explored as an alternative process. This is mainly because MS offers many advantages such as a relatively low price, low decomposition temperature (550–800 °C), low energy consumption, less corrosiveness, and high production yield [1].

The establishment of a cost-effective Siemens process requires the appropriate design of the Siemens reactor and the optimization of its operation conditions. A reliable

*Address correspondence to Prof. Woo Kyoung Kim, School of Chemical Engineering Yeungnam University, Gyeongsan, Gyeongbuk, 712-749, Republic of Korea. Tel.: (+82)53-810-2514. E-mail: wkim@ynu.ac.kr

simulation program can allow one to adjust the reactor design (e.g., rod diameter, inlet nozzle position, etc.) and to determine the optimal operation conditions (e.g., gas flow rates, temperature profile, etc.) without performing expensive experiments. Unfortunately, no simulation program is available for the MS-Siemens process; in contrast, PolySim^{TM} is widely used for simulating the TCS-Siemens process [2]. Therefore, it is necessary to develop a simulation program for the MS-Siemens process.

Recently, we reported the results of the modeling of a four-rod MS-Siemens reactor using a computational fluid dynamics (CFD)-based ANSYS FLUENT package program [3,4], in which the kinetic parameters for the formation reaction of polysilicon were optimized and the deposition rate of polysilicon was then successfully predicted for various process conditions. In addition to the modeling of the polysilicon growth, the CFD software FLUENT is used in various disciplines. For example, Pasaogullari and Wang used it to analyze the current density effect in a fuel cell and calculate the H_2O molar concentration for models with different designs such as straight, serpentine, and interdigitated designs [5].

In this study, the temperature and gas concentration profiles were investigated using previously optimized kinetic parameters and an established reactor model. In addition, a correlation between the reactor power consumption and the process conditions was established.

Downloaded by [Chongqing University] at 04:51 15 February 2014

Modeling and Simulation

A schematic representation of the customized pilot-scale four-rod MS-Siemens reactor used in this study is shown in Fig. 1.The reactor has four cylinders, into each of which a highly pure slim Si rod (9N) is inserted. The reactor also had an exhaust system, a reactant gas nozzle, a heating jacket, an electrode, a chamber, etc. ANSYS FLUENT ver.13 was used for modeling the three-dimensional four-rod Siemens reactor with different rod diameters—10, 30, 50, 70, 90, and 120 mm. After we modeled a bell-jar-shaped reactor with four rods, we set up a one-rod section that was a part of the four-rod bell-jar reactor having periodic symmetry, as a model of the flow analysis.

Based on the above mentioned model [4], a lattice was produced in the shape of a tetrahedral prism in the entire flow field and on the wall of the reactor. A compact mesh was produced in the area of the nozzle and the rod that had a small cross-sectional shape, as compared to the entire size of the flow field. The boundary conditions were set to be suitable for the one-rod reactor model considering the actual experimental conditions of the pilot-scale MS-Siemens reactor. The flow pattern analysis was performed using a steady-state turbulence model with a realizable k-ε model. It was reported that a realizable k-ε model could be used to perform an enhanced wall treatment in the commercial CFD software [6]. The rod temperature was 800–900 °C, and the reactant gases were SiH_4 and H_2. The concentration of SiH_4 was maintained at ~2.17% by regulating the gas flow.

On the basis of our previous report [4], the overall one-step reaction model (i.e., $SiH_4 \rightarrow SiH_2 + H_2$) and the corresponding kinetic parameters were used. To correlate the power consumption with the process conditions, the experimental data collected from the pilot-scale four-rod Siemens reactor were precisely compared. Further details concerning the reactor modeling and the kinetic parameter optimization are given in our previous paper [4].

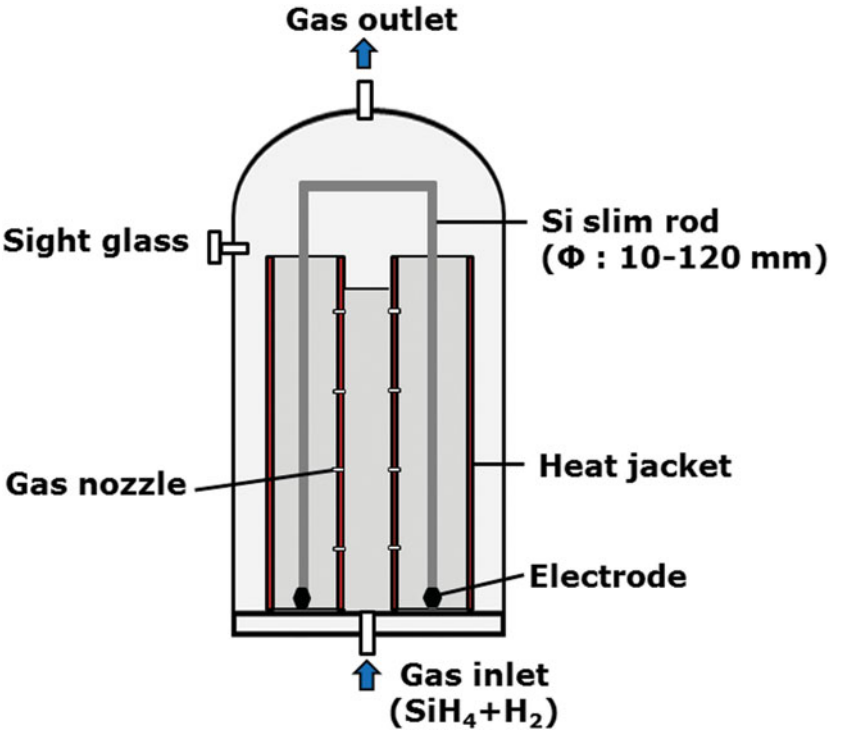


Figure 1. Schematic representation of pilot-scale four-rod MS-Siemens reactor.

Results and Discussion

The profiles of the temperature and the mass fraction of SiH_4 are shown in Figs. 2 and 3, respectively. The temperature at the surface of the rod was fixed at 800 °C (1073.15 K). If a rod's temperature profile was not uniform, it ran the risk of breaking down owing to the thermal stresses [7]. As shown in Fig. 2, the gas temperature at the outlet region (top) was higher than that at the vertical zone near the rod. The overall temperature increased with the rod diameter, probably because the formation of polysilicon from SiH_4 was an exothermic reaction and the overall gas volume was reduced by the presence of a relatively thick rod. In addition, the silicon deposition rate was proportional to the rod diameter.

It has been reported that SiH_4 gas can decompose to SiH_2 and H_2 inside a reactor and that SiH_2 gas is chemisorbed on the surface of a Si rod [4]. The chemisorbed SiH_2 is decomposed into Si and then exothermically reacts with Si atoms with dangling bonds on the surface of the Si rod. It is believed that some of the Si atoms produced from SiH_2 gases react with each other to form a Si powder. The Si powder may primarily forms near the rod and particularly around the gas inlet nozzle before moving to the top zone of the reactor. Owing to the fact that Si powder is inevitably generated from the exothermic reaction of SiH_4 in a Siemens reactor, a powder catcher system may be required [8]. A fine Si powder generated at a temperature of several hundred degree Celsius or more can degrade the crystal quality [9]. For example, the Si powder can be deposited on the wall of the reactor and then separate from the wall when its accumulated thickness reaches several millimeters. Subsequently, some of the separated Si powder will stick to the growing Si rod and then lead to the intrusion of the powder and the formation of an abnormal dendrite.

Downloaded by [Chongqing University] at 04:51 15 February 2014

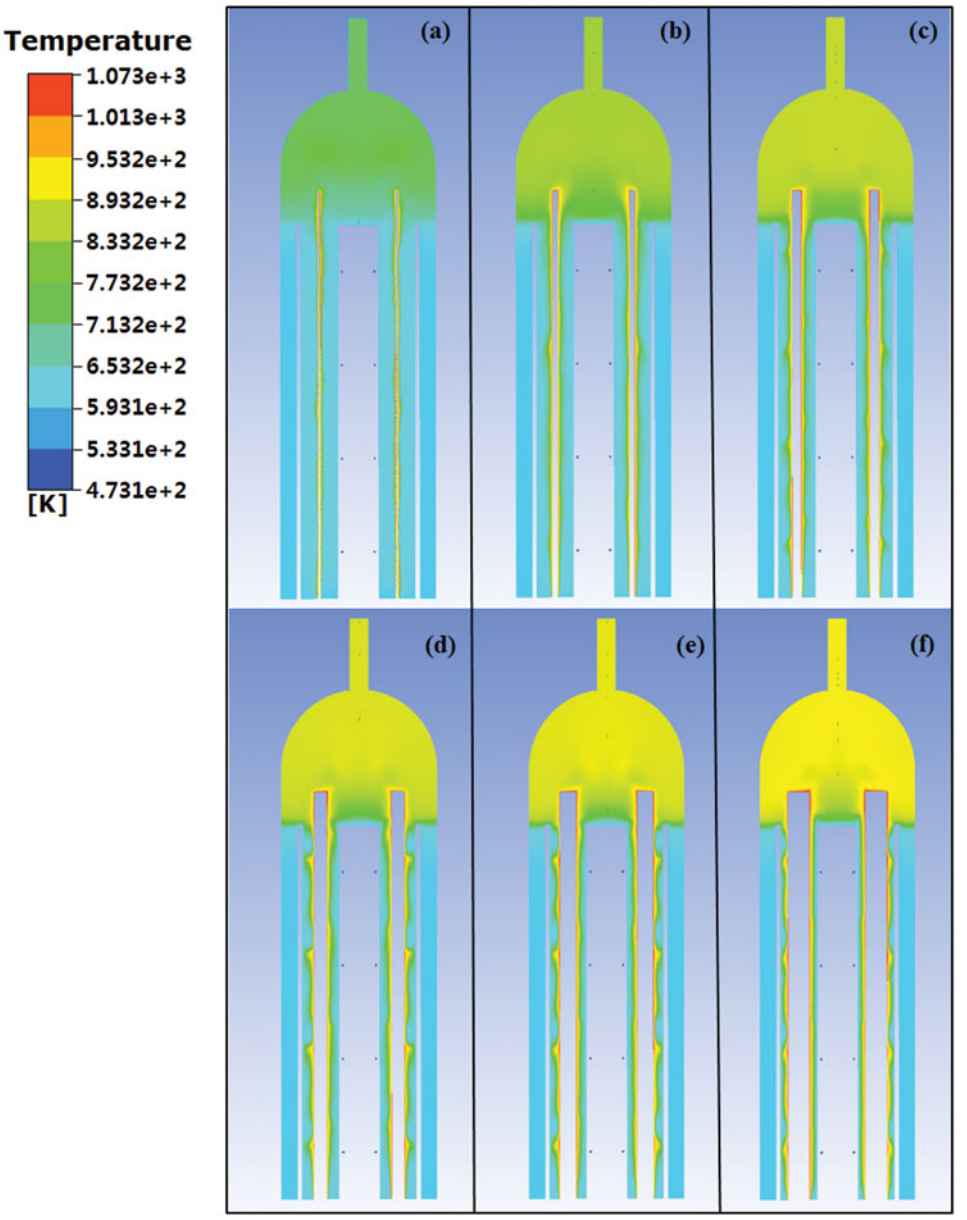


Figure 2. Contour plot of temperature at 800 °C with different rod diameters of (a) 10 mm, (b) 30 mm, (c) 50 mm, (d) 70 mm, (e) 90 mm, and (f) 120 mm.

The formation of a polysilicon powder was often experimentally observed in our customized pilot-scale four-rod MS-Siemens reactor. Because the temperature of reactant gases inside the reactor increased with the deposition of Si, the wall of the metal bell jar was cooled to around 100 °C to prevent off-rod silicon deposition. In a real Siemens reactor, the bell-jar-type reactor chamber and the base-plate are cooled down by a cooling jacket whose outside temperature is thus lower than the inside temperature. As shown in Fig. 2,

Downloaded by [Chongqing University] at 04:51 15 February 2014

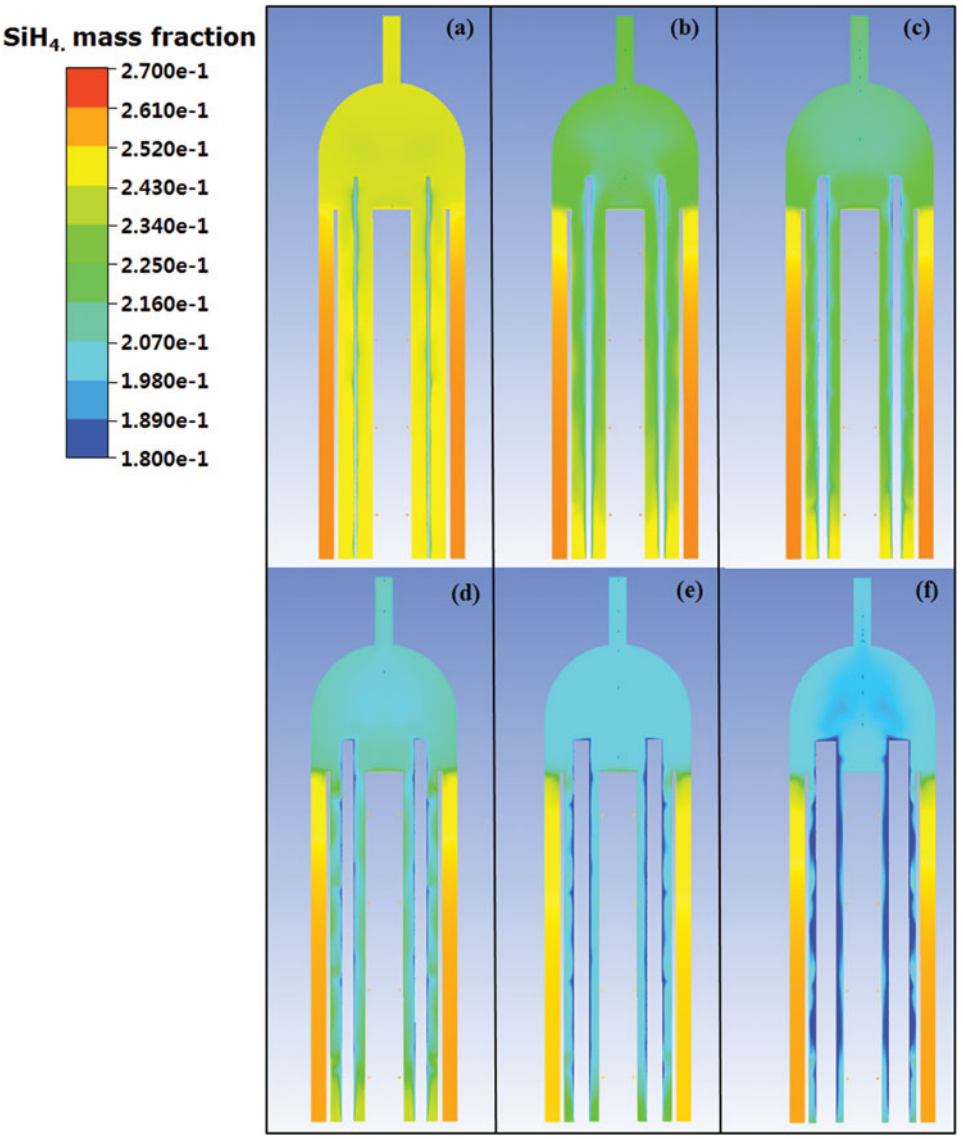


Figure 3. Contour plot of SiH_4 mass fraction with different rod diameters of (a) 10 mm, (b) 30 mm, (c) 50 mm, (d) 70 mm, (e) 90 mm, and (f) 120 mm.

the calculation suggests that the temperature near the gas nozzle is higher than at other positions, which may be attributed to the active reaction near the inlet gas nozzle.

As seen in Fig. 3, the mass fraction of SiH_4 tends to decrease because the Si deposition rate increases with the rod diameter by the rapid decomposition of SiH_4 in the reactor. The H_2 mass fraction, on the other hand, shows an opposite trend because of the reaction $SiH_4 \rightarrow Si + 2H_2$. It is also observed that the mass fraction of SiH_4 outside and at the bottom of the heat jacket is larger than that inside the heat jacket. This is likely because of the fact that the unreacted SiH_4 gases that are not discharged through the outlet port are accumulated

Downloaded by [Chongqing University] at 04:51 15 February 2014

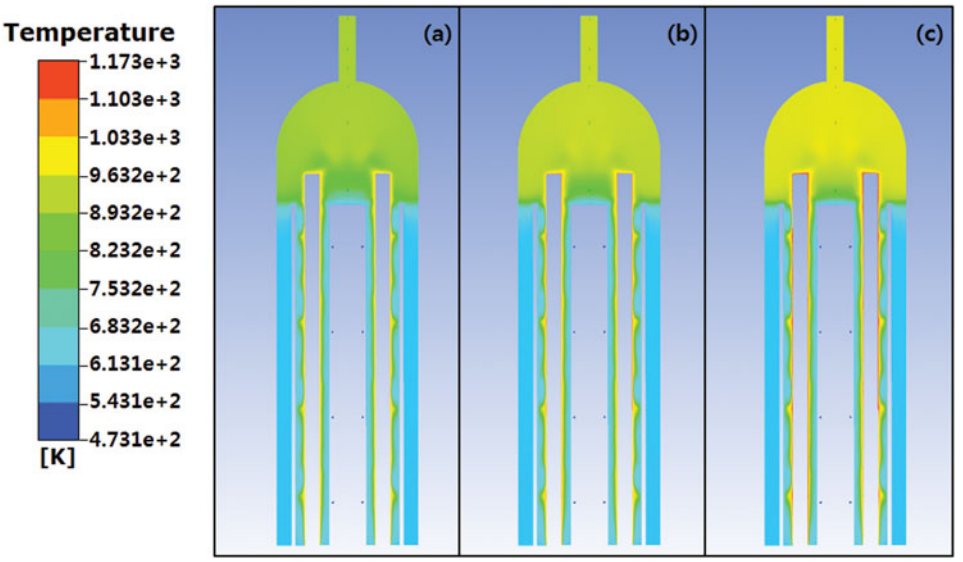


Figure 4. Contour plot of temperature at a fixed rod diameter of 90 mm with different rod surface temperatures of (a) 800 °C, (b) 850 °C, and (c) 900 °C.

outside the heat jacket. Unfortunately, it is impossible to measure the concentration of SiH_4 gas directly because of the high probability of an explosion.

The contour plots of the temperature and the SiH_4 mass fraction are illustrated in Figs. 4 and 5, respectively, when the temperature of the rod surface was varied from 800 to 900 °C with a fixed rod diameter of 90 mm. The temperature contour showed that the gas temperature in the top zone of the reactor was considerably larger than that near the

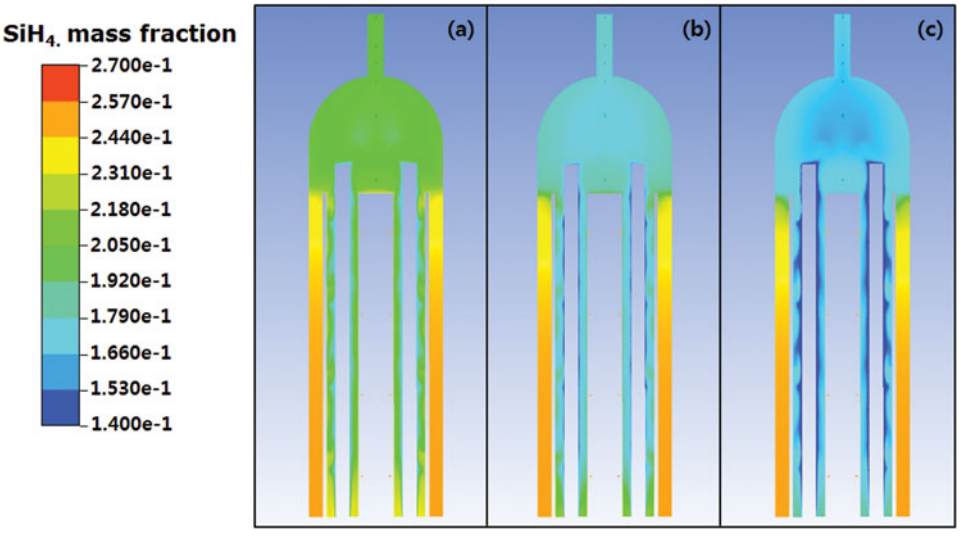


Figure 5. Contour plot of SiH_4 mass fraction with different rod surface temperatures of (a) 800 °C, (b) 850 °C, and (c) 900 °C.

Downloaded by [Chongqing University] at 04:51 15 February 2014

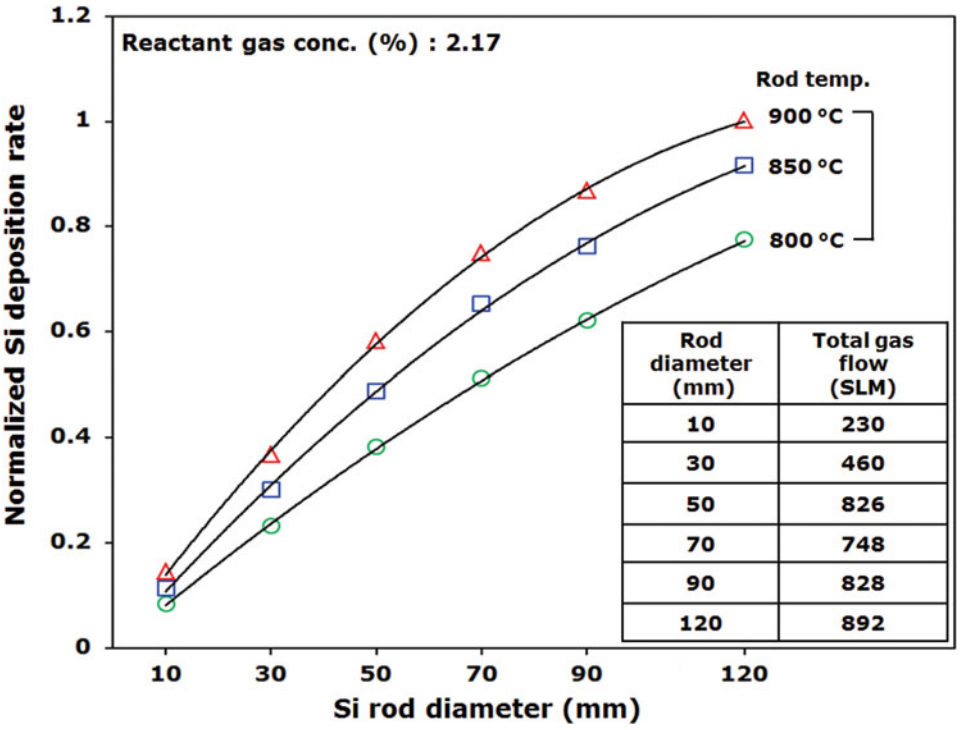


Figure 6. Si deposition rate calculated by FLUENT with respect to rod diameters.

rod, as shown in Fig. 4. The temperature difference between the top zone and the rod zone increased with the surface temperature of the rod. The SiH_4 mass fraction tended to decrease monotonically at the top of the reactor with an increase in the rod temperature (Fig. 5).

When the reactant gas concentration was maintained, the simulation results showed that the Si deposition rate increased with the rod diameter and the rod temperature. Therefore, the results for the temperature contour and SiH_4 mass fraction according to the rod surface temperature shown in Figs. 4 and 5 were also produced with an increase in the rate of Si deposition.

Following a systematic comparison of the power consumption with the process conditions, it was found that the power consumption was highly correlated with the Si deposition rate. As shown in Fig. 7, the power consumption is linearly proportional to the Si deposition rate and the slope increases with the rod diameter. The power consumption was predicted by substituting the value of the Si deposition in the equation that was obtained from the relationship between the Si deposition rate in a real MS-Siemens reactor and its power consumption.

PolySim^{TM} is a tool used for the optimization of the reactor for polysilicon deposition from TCS by the Siemens process [2]. A considerable amount of useful information regarding the reactor and the polysilicon deposition characteristics for the given process conditions, primarily the silicon deposition rate and the energy consumption, can be obtained using this tool. Similarly, a user-friendly simulation program (called "MonoSim-S") that can predict factors such as the Si deposition rate, Si deposition efficiency, power

Downloaded by [Chongqing University] at 04:51 15 February 2014

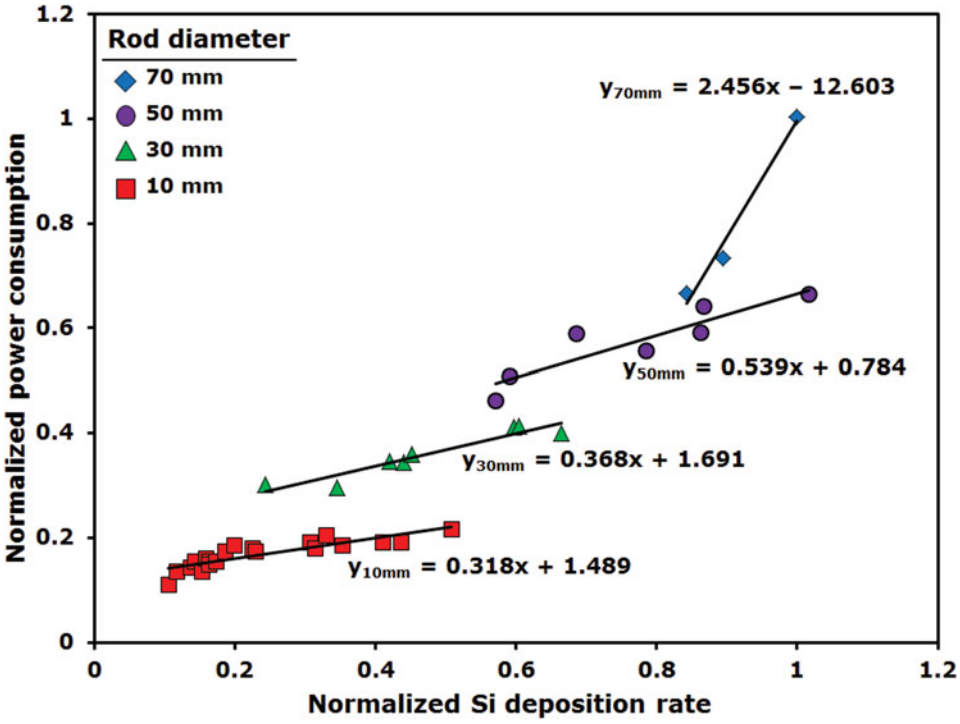


Figure 7. Si deposition rate in an actual MS-Siemens reactor vs. power consumption.

consumption, and fluid flow pattern was developed using equations and images that were derived from the values of the power consumption and various process parameters.

Conclusions

The Si rod diameter was found to affect the temperature and reactant gas profiles as well as the Si deposition rate. It was also found that the extracted relationship between the power consumption and the Si deposition rate at different Si rod diameters might be effectively used for monitoring and optimizing the design of an MS-Siemens reactor.

Acknowledgment

This research was supported by the Yeungnam University research grants in 2011, and the Human Resources Development program (No.20104010100580) of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant funded by the Korea government Ministry of Trade, Industry and Energy.

References

[1] Luque, A., & Hegedus, S. (2011). *Handbook of Photovoltaic Science and Engineering*, Wiley: New York, 2nd ed.
[2] Galyukov, A. (2009). Presented at ISTC & CSTIC, Shanghai.

Downloaded by [Chongqing University] at 04:51 15 February 2014

[3] Kang, S. O., Lee, U. J., Kim, S. H., You, H. J., Park, K., Park, S. E., & Park J. H. (2012). *Int. J. of Photoenergy*, 697653.
[4] Jung, H., Park, J. H., Kang, S. O., Jeong, J. H., Jeon, S., Jung, J. H., & Kim, W. K. (2012). *Jpn. J. Appl. Phys.*, *51*, 10NA10.
[5] Hu, M., Zhu, X., Wang, M., Gu, A., & Yu, L. (2004). *Energy Convers. Manage.*, *45*, 1883.
[6] Duran, J. E., Mohseni, M., & Taghipour, F. (2010). *Chem. Eng. Sci.*, *65*, 1201.
[7] del CoSo, G., Tobías, I., Cañizo, C., & Luque, A. (2007). *J. Cryst. Growth*, *299*, 165.
[8] Keck, D. W., Nagai, K., Yatsurugi, Y., Morihara, H., & Izawa, J. (1995). US patent No. 5,478,396.
[9] O'Mara, W. C. *et al.* (1990). *Handbook of Semiconductor Silicon Technology*, Noyes Publications: New Jersey.

Downloaded by [Chongqing University] at 04:51 15 February 2014