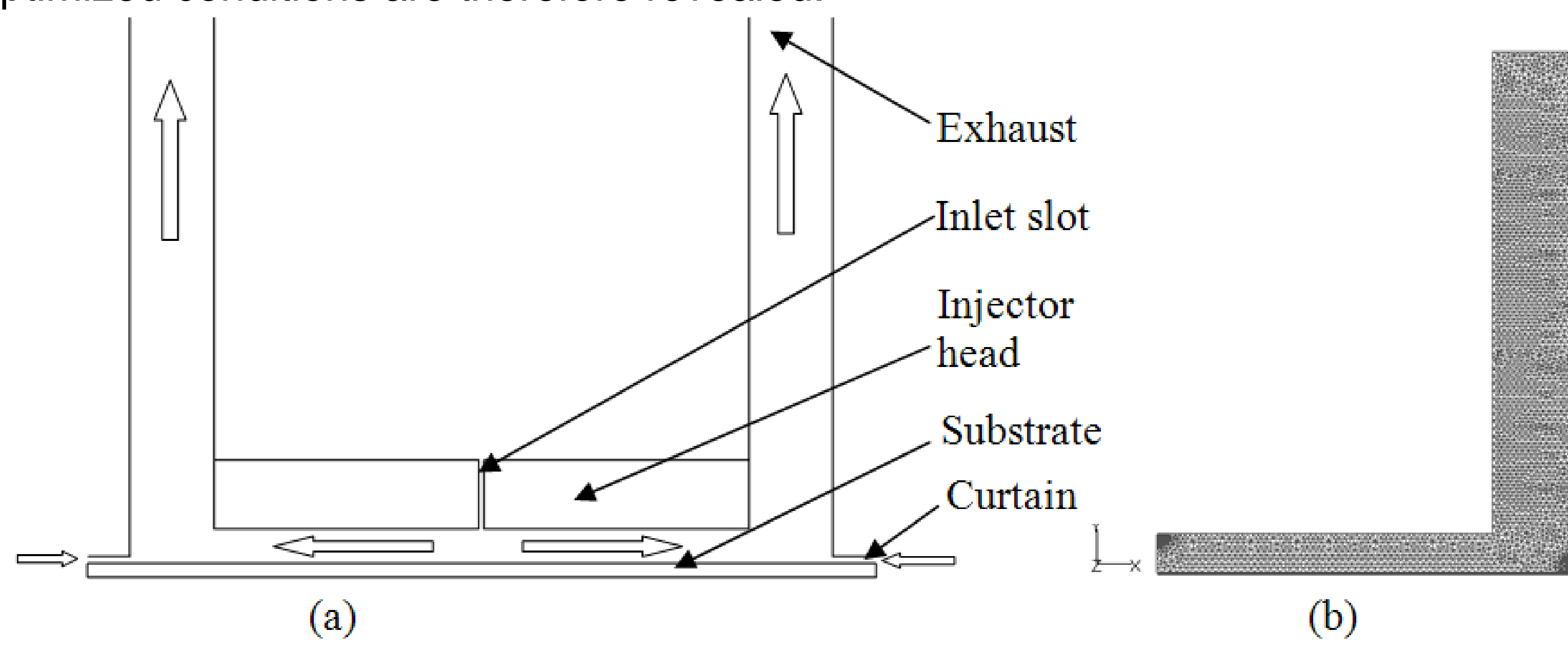


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ABSTRACT

Atmospheric Pressure Chemical Vapor Deposition (APCVD) thin film coating is one of the most cost efficient large area thin film coating solutions presently available on the market. It can be as much as 2-2.5X lower in cost than a low pressure sputtering system. Advanced materials such as transparent conductive oxides (TCO), used for solar panel manufacturing and for energy saving (Low-E) windows, have already been deposited by APCVD. These films have been developed by incorporating one or more modules, each depositing a film such as SiO₂, TiO₂ and F:SnO₂, etc. onto a glass sheet. However, further improvement in material efficiencies, and operational cost reductions, are needed to satisfy the growing demand for such highly customized materials. In the future, it will also be desirable to have the capability to deposit other material films, with targeted properties. These newer films, such as ZnO must be developed in a cost efficient manner as well.

The purpose of this work is to perform a parametric Computational Fluid Dynamics (CFD) study to investigate the improvement potential for a traditional APCVD deposition module. In the model, all of the transport phenomena mentioned above are considered in order to predict SiO₂ deposition rate and rate distribution. A commercially available APCVD deposition module design, originally developed by Watkins-Johnson for SiO₂ deposition, has been selected as a base case. We incorporated the same operating conditions as these earlier experiments, and the simulation results are compared with the published experiment data. Significant agreement is achieved between the resulting data sets. Based on this, geometric and operating conditions are modified systematically in order to identify their effect upon the final deposition rate and quality. Optimized conditions are therefore revealed.



Assumption: (i) steady state; (ii) laminar flow; (iii) chemical reaction is finite rate;

Continuity

$$\nabla \cdot (\rho \vec{u}) = 0$$

Momentum

$$\nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \mu \nabla^2 \vec{u} + \rho \vec{g}$$

Energy

$$\nabla \cdot (\rho C_p T \vec{u}) = \nabla \cdot (k \nabla T) + S$$

Species

$$\nabla \cdot (\rho \vec{u} Y_i) = -\nabla \cdot \vec{J}_i + R_i$$

Chemical Reaction Mechanism

Gas phase reactions: BTW (Britten-Tong-Westbrook) model is used; 70 reversible elementary reactions are included;

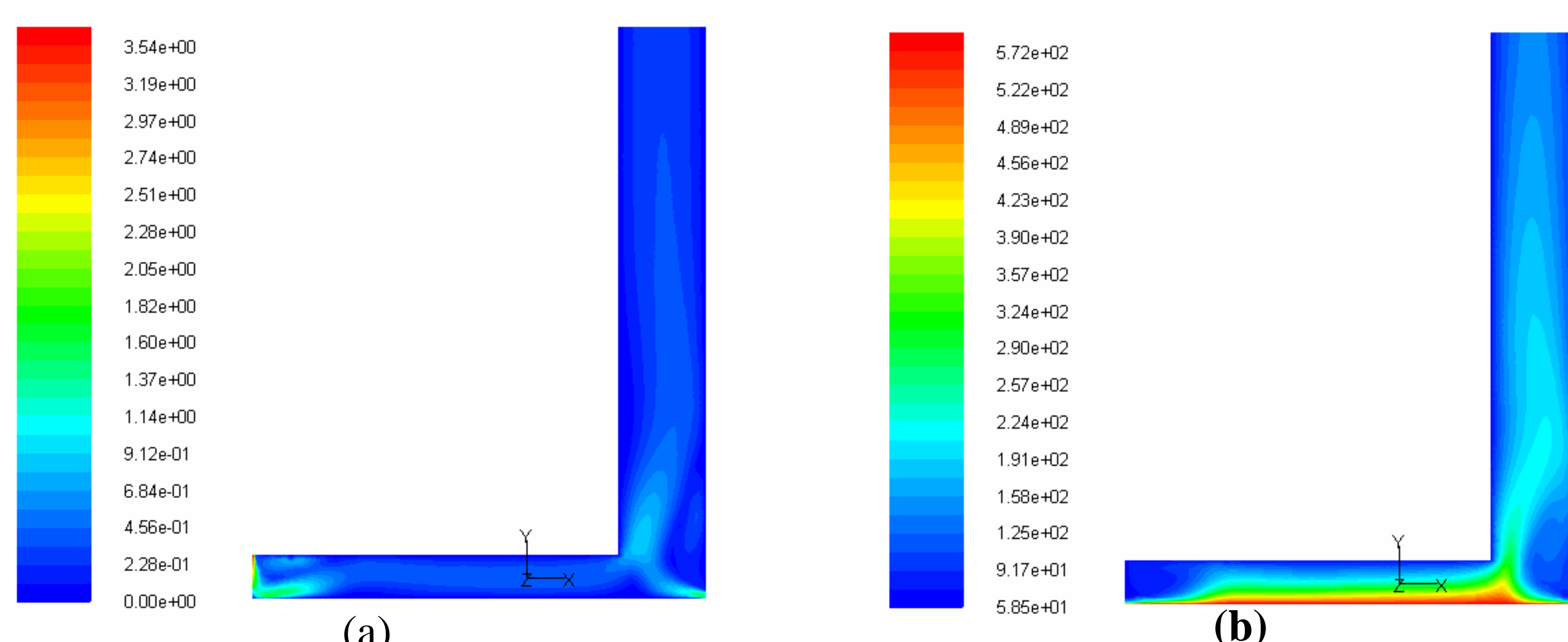
Surface reactions: sticking coefficient method is applied; It is assumed that all silicon-containing species except Silane will deposit a certain amount of SiO₂ based on the specified sticking coefficient

$$R_s = g_i C_i \sqrt{\frac{RT_s}{2pM_i}}$$

RESULTS & DISCUSSION

Velocity Field and Temperature Distribution

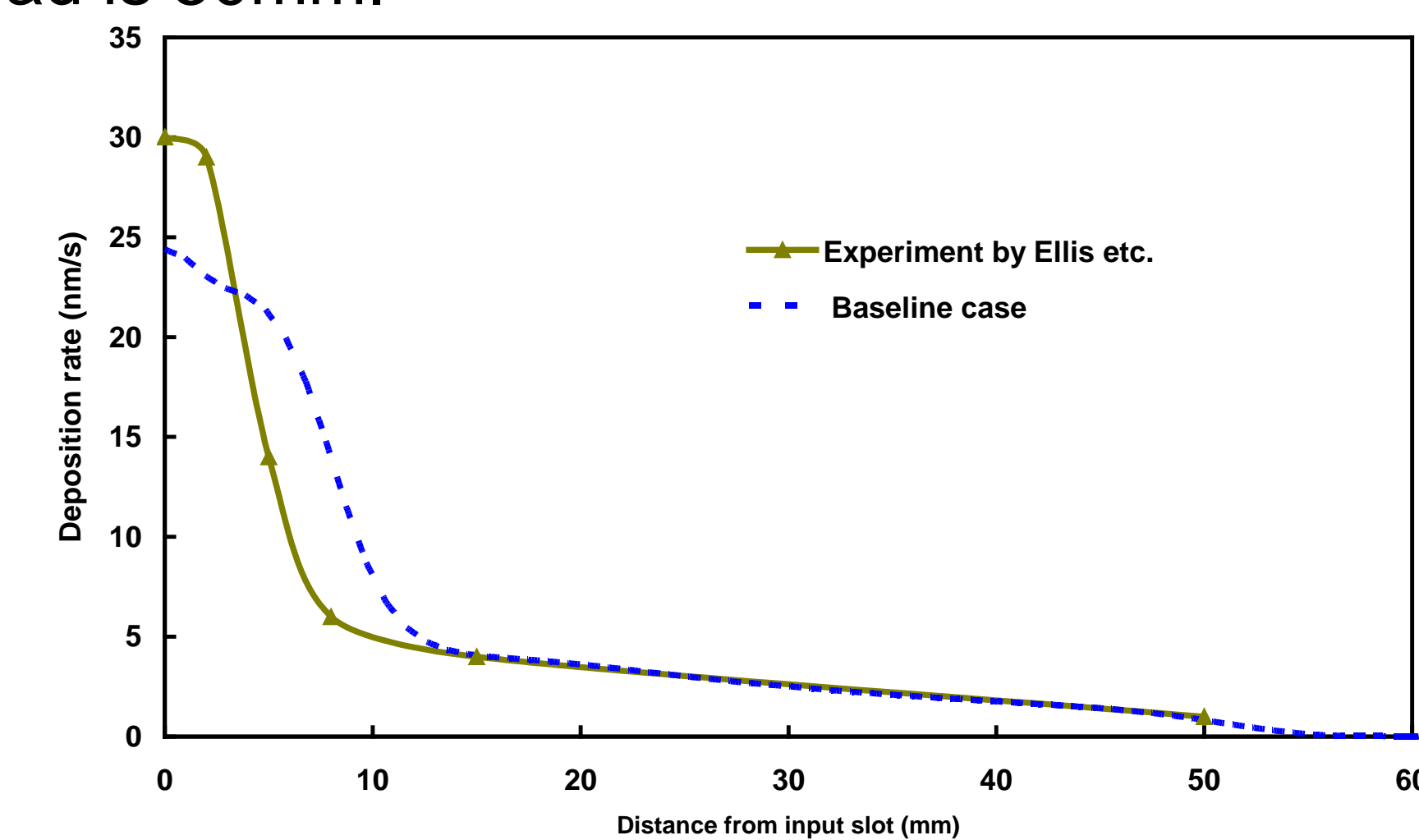
Highest velocity occurs in the inlet slot because of the small gap. After a certain distance from the inlet slot, gas flow is well developed. Recirculation is formed near the gas inlet regions. It is clearly seen that the gas is heated up by the hot substrate. In the region where gas flow is well developed, temperature profile along gas moving direction is very uniform.



(a) Contours of velocity magnitude, m/s and (b) Temperature distribution of baseline case, °C.

Comparison of Simulation Result to Experimental Data

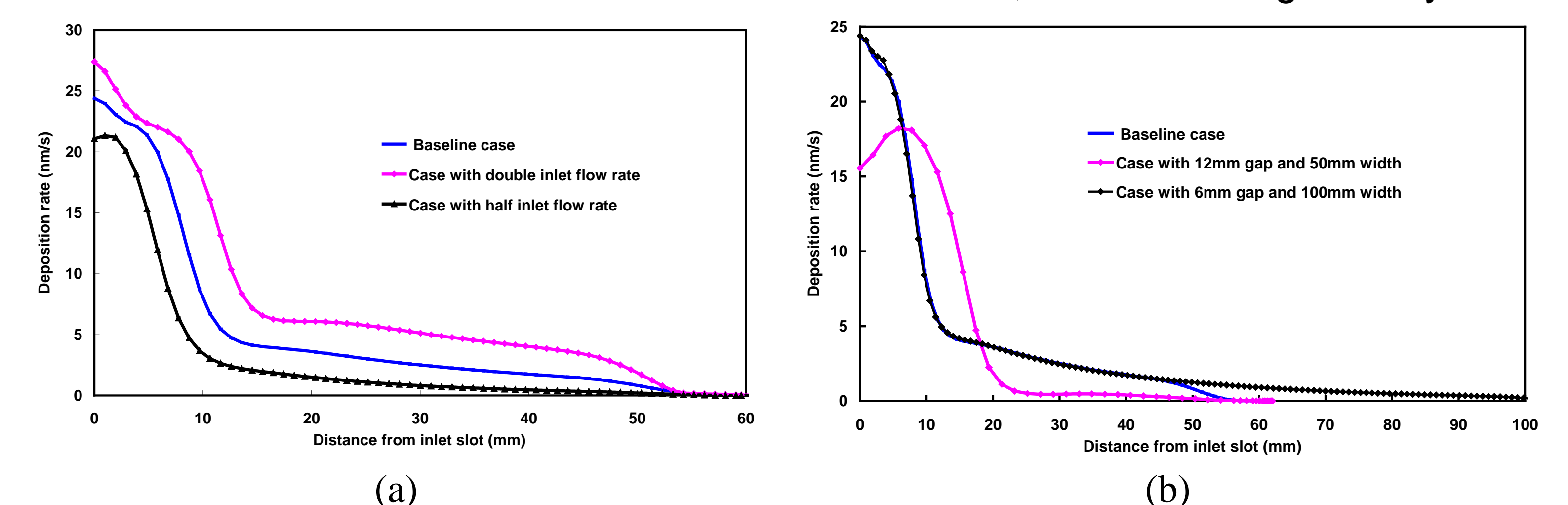
In our 2D CFD modeling, the same experiment conditions are used. Two profiles of deposition rates obtained by simulation and experiment match well, with the exception of the region near the inlet. This might be caused by the difference of flow condition and the temperature boundary condition between CFD modeling and experiment. In the baseline case, the width between the injector head roof and the glass is 6mm, and the length of injector head is 50mm.



Effect of Inlet Flow Rate and Reactor Geometry Variation on Deposition

Two more cases with half or double inlet flow rate were run. With the increase of inlet flow rate, the maximum and average deposition rate is increased correspondingly. The conversion efficiency of Silane to silicon dioxide for the three cases are 12.8%, 17.2% and 20.6%, respectively. Therefore, the efficiency is reduced with an increase of inlet flow rate. This indicates that the increase of deposition rate is achieved by the sacrifice of conversion efficiency when a larger inlet flow rate is used.

Another two cases, with double width (12mm) or double length (100mm), were run. It is observed that the maximum deposition rate is shifted to the right for the case with double width. After a 20mm distance from the gas injection port, the deposition rate decreases rapidly. For the case with doubled length, the deposition rate within 50mm is almost the same as that of baseline case. After 50mm, it is reduced gradually.

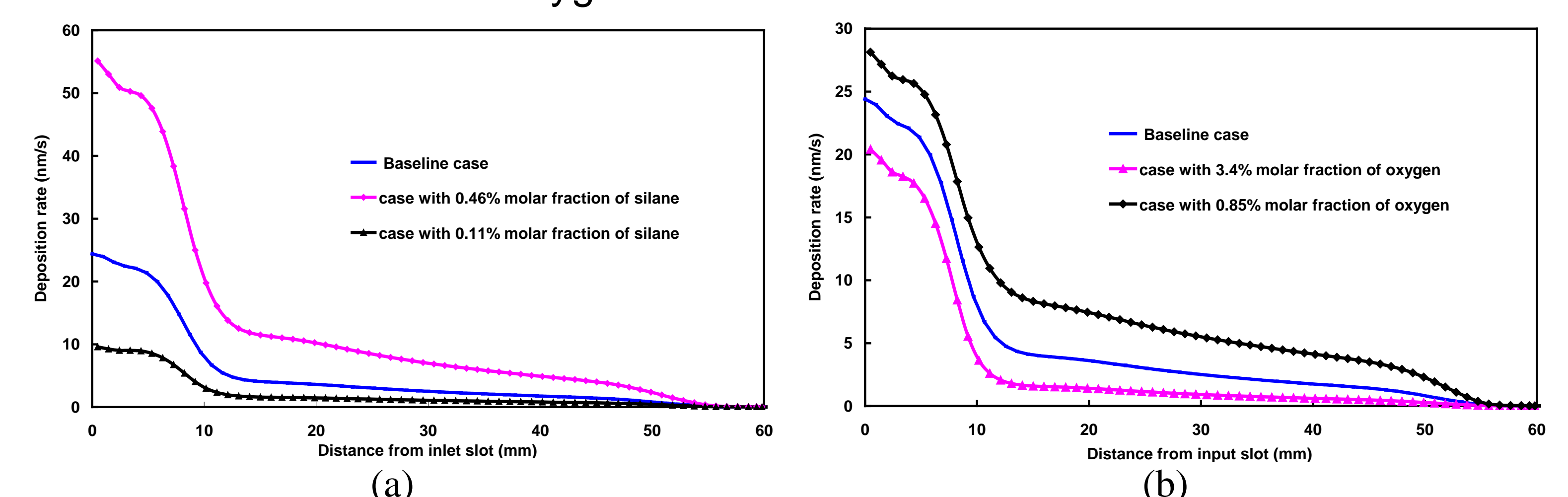


(a) Comparison of deposition rate for three cases with different inlet flow rates, (b) Change of deposition rate when width between injector roof and substrate, and length of injector head are modified

Effect of Silane and Oxygen Molar Fraction

Two more cases are conducted in which the molar fraction of Silane is doubled and then reduced to half, respectively. It was found that both the average and maximum deposition rate is increased with the increase of molar fraction of Silane.

In another two cases, molar fraction of Oxygen is doubled or decreased to half. It was observed that both maximum and average deposition rates decrease with the increase of molar fraction of Oxygen.



(a) Comparison of deposition rate for cases with different molar fraction of Silane, (b) Comparison of deposition rate with different molar fraction of Oxygen

Summary of Conversion Efficiency for All Cases

The conversion efficiency obtained for all of the run cases is summarized. It was found that the case with double molar fraction of Oxygen has the lowest conversion efficiency and the case with half molar fraction of Oxygen resulted of the highest conversion efficiency of all cases studied.

Case description	Conversion efficiency	Ratio to baseline case
Baseline case	17.2%	
Double inlet flow rate	12.8%	74.4%
Half inlet flow rate	20.6%	120.3%
Double molar fraction of Oxygen	10.6%	61.7%
Half molar fraction of Oxygen	25.2%	146.5%
Double molar fraction of Silane	20.8%	121.5%
Half molar fraction of Silane	13.8%	80.2%

CONCLUSIONS

This work performed parametric CFD modeling of SiO₂ by an APCVD process using Silane and Oxygen as CVD precursors. The spatial varying deposition rate distribution matches the experimental data well when a suitable sticking coefficient is chosen. Effects of inlet gas flow rate, the gap between the injector roof and substrate, width of injector head, molar fraction of Silane and Oxygen on the deposition rate and conversion efficiency were investigated. We observed that the most effective way to increase conversion efficiency was to decrease the molar fraction of Oxygen and to increase the deposition head width. The results obtained by current CFD modeling can be used to optimize the next generation offline and online CVDgCoat™ APCVD platform.