

# **A simulated study of temperature as a function of gas flow rate in a chemical vapor deposition reactor**

## **Abstract**

A study to further simulation research of a commercial chemical vapor deposition (CVD) reactor is presented. A simulation is created using the computational fluid dynamics software package, Fluent (version 4). The variation of gas temperature inside the reactor system, as a function of gas flow rate, is examined. Data is collected for trials of several initial flow rates and iterations. Results from Fluent are to be compared to data from other simulation techniques to test accuracy and reliability.

## **Introduction**

Commercial manufacturing is driven by the concepts of cost effectiveness and optimal performance. In order to guarantee that these conditions are met, it is necessary to understand all of the specifics of the manufacturing process. Unfortunately, under some circumstances, it is virtually impossible to monitor and understand each and every aspect of the system. There are a number of reliable ways to compensate for the inability to describe these processes with certainty. However, there is an ongoing search to determine which of these methods is the most accurate and the most efficient. One such method, which is used heavily to model the behavior of these “mysterious” systems, is the technique of simulation. There are a few different approaches to simulating a process. Research has been and continues to be conducted to determine what equations and formulas can accurately describe certain types of systems. The simulating process can be worked out by hand. However, to avoid using so much time, many of these equations and formulas have been compiled into numerous software packages, which are used primarily for simulation purposes.

One such manufacturing system, whose dynamics are not fully understood, is a chemical vapor deposition (CVD) reactor. These systems are used to develop semiconductor materials to be manufactured for processing purposes. Gases are pumped into the reactor and heated to cause certain chemical reactions. These reactions result in the deposition of a filmy layer of substances on the surface of a heated silicon wafer. It is the properties of this film that are of importance to the manufacturer. The optimal result is a wafer with a uniform layer of film across the entire surface. Additionally, the process must be duplicable so that the exact same result can be reproduced from wafer to wafer. In order for this to be accomplished, as much as possible must be known about the internal activity and conditions of the reactor, so that they can be reproduced any number of times. Since it is impossible to manually observe the CVD process, engineers rely on simulation research to imitate the behavior of the system. As a useful tool to simulation researchers, many different software packages have been introduced. These programs

come equipped with the numerous engineering equations and formulas, preventing the scientist from having to tediously work them out countless times. Simulations are often meant to model many different aspects of a particular process. These software packages make it much easier to change necessary parameters and conditions without having to redo calculations each time.

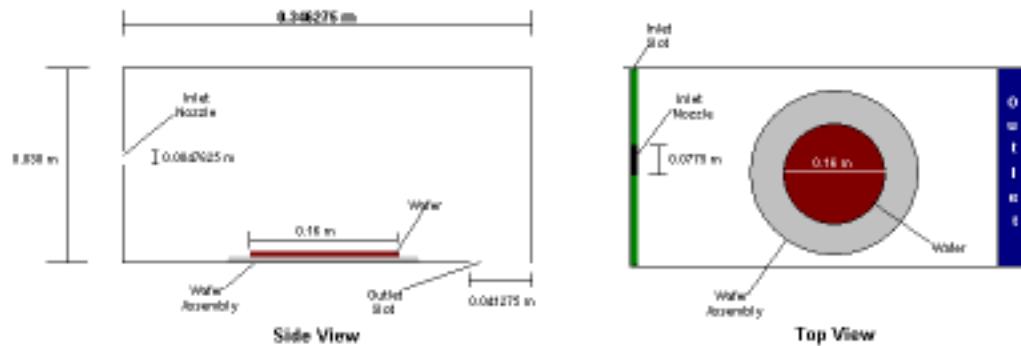
One important factor of the CVD system is the temperature of the gas inside the chamber. The observation of this temperature is essential because it affects how the film is deposited across the wafer surface. The distribution of the gas temperature can vary as a result of a few other conditions inside the reactor system. The rate at which the gas is introduced into the chamber, called the gas flow rate, is one of these conditions. Using a simulation to monitor the variation of the gas temperature, as a function of the gas flow rate, is a very convenient and reliable method. In order to accomplish this goal, a simulation software package can be very helpful. The first step in the procedure is to define the physical dimensions of the system. Then select the boundary conditions that are involved in the problem. The specified boundary conditions determine which equations the program will solve to produce the data. These can be easily changed to study other areas of the problem or to consider other situations. Once the problem is set up, the simulation can be iterated any number of times to predict the expected results from the actual system.

Using the fourth version of the computational fluid dynamics software package, Fluent, this procedure was carried out. Several initial gas flow rates were used and varied numbers of iterations were calculated. The contour plots of the gas temperature were produced in each case. Ultimately, the results from Fluent will be compared to the data calculated using simulation methods being developed by the research group to test accuracy.

### **Problem Description**

To build a simulation using Fluent, the first step is to set up the discretization grid. Version 4 was used because it appeared to be the most “user friendly” option for this project. The CVD reactor geometry includes four main walls. (Figure 1) The left wall contains the inlet slot and the inlet nozzle, which introduces the gas into the chamber. The bottom wall, or the floor of the chamber, is where the heated wafer sits and is also

the location of the outlet slot where the gas leaves the chamber. The length of the grid



**Figure 1**

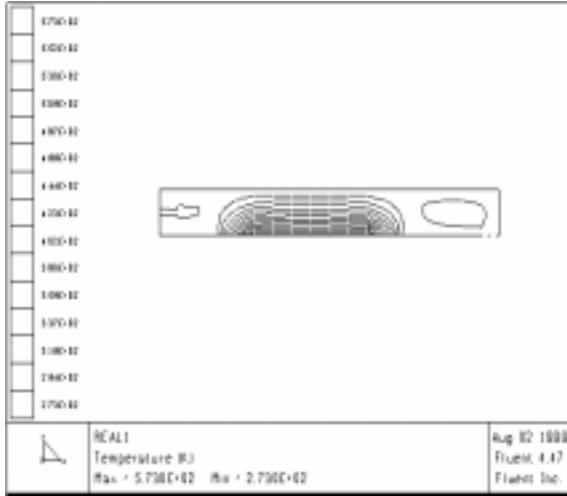
was set to 0.305 meters (m) along the bottom wall. However, a 0.16 m centered section was designated for the heated wafer assembly area and an extra 0.041275 m was added on for the outlet slot. Therefore, the total length of the top wall was 0.346275 m. The height of the grid was 0.038 m on both the left and the right walls, with an inlet slot of 0.0047625 m centered in the left wall. Both the inlet and outlet slots ran the entire width of the grid, which was 0.254 m. The inlet nozzle had a width of 0.0775 m. The actual visual display of the grid was two-dimensional. However, the width was included to ensure the accuracy of the calculations.

After the grid has been set up, the next step is to define the boundary conditions. The temperature of all of the walls and at the gas inlet was set to 298 degrees Kelvin (K). In the area designated for the heated wafer surface, the temperature was much higher, at 573 K. Other conditions to be considered included the reactor mean operating pressure (67 Pa), the density ( $0.001075 \text{ kg/m}^3$ ), thermal conductivity ( $0.017584 \text{ W/(m K)}$ ), heat capacity ( $520 \text{ J/(kg K)}$ ), and viscosity ( $2.253 \text{ e-5 kg/(m s)}$ ). The gas composition was given as Argon, with a molecular weight of 39.944 kg/kgmole, and was treated as an ideal gas. Four different simulations were run, each corresponding to a different gas flow inlet velocity. As somewhat of a control situation, the first velocity used was 0.0 m/s. There would be no reason to run the system with no inlet gas flow, but the data was collected for comparative purposes. Simulations were also run for velocities of 1.52 m/s, 15.2 m/s and 20.0 m/s. In actuality, the gas would never be introduced with an initial velocity of 20.0 m/s, but, once again, the data was collected for comparative and exploratory purposes. Each simulation was iterated 100 times and the contour plots of the temperature distribution inside the chamber were recorded.

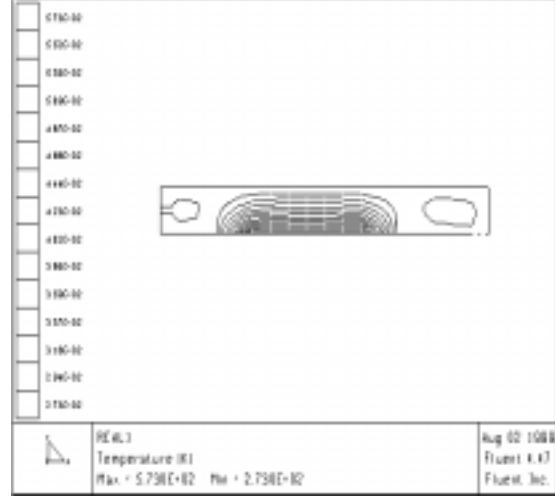
## **Results**

Using an inlet flow rate of 0.0 m/s, it should be expected that the temperature in the chamber would be fairly uniform, with no inlet stream to upset the state of the system.

As seen in Figure 2, the contours around the wafer area appear to be quite even, suggesting an even temperature distribution. However, because the gas is not entering the system, and therefore not causing the deposition of materials onto the wafer surface, this case is of no real use to us. With an inlet flow rate of 1.52 m/s, the plot (Fig. 3) does

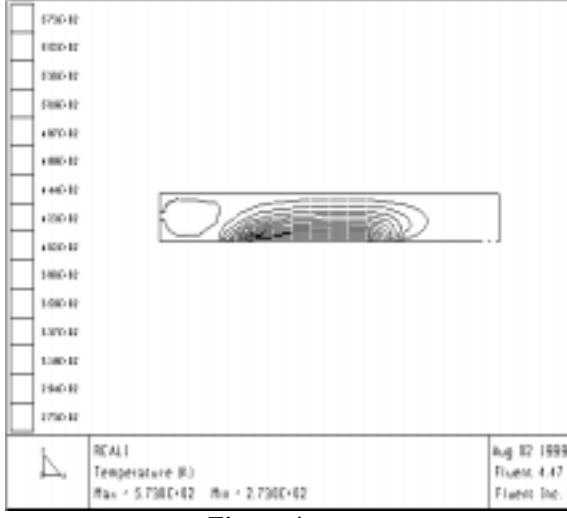


*Figure 2*

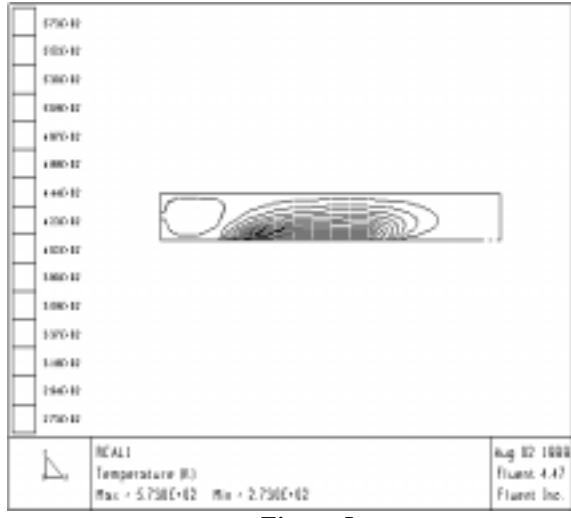


*Figure 3*

not show much difference from that of the system with no gas. The temperature is spread evenly across the surface of the wafer, suggesting that the film will be deposited evenly as well. With an elevated inlet velocity of 15.2 m/s (Fig. 4), we begin to see the shift in temperature distribution as a result of the faster inlet flow. The contours appear to be more concentrated on the left side of the wafer and more spread apart on the right.



*Figure 4*



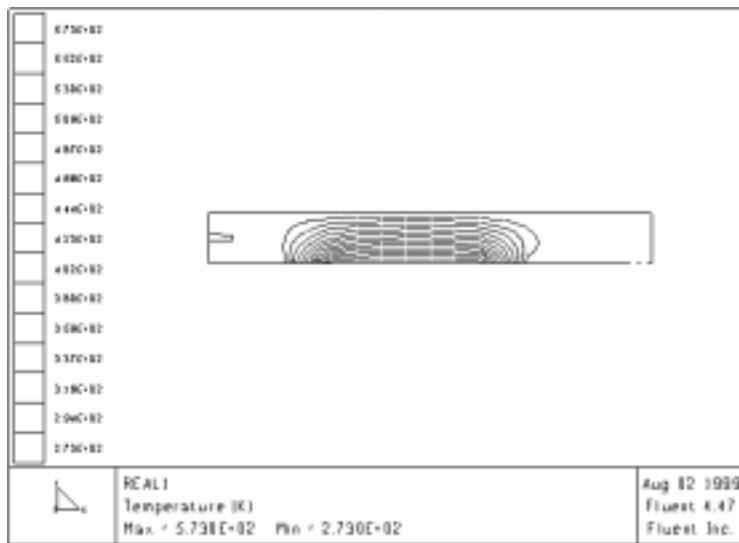
*Figure 5*

This shows the unevenness in the gas temperature and, furthermore, suggests an uneven deposition of materials onto the wafer surface. Finally, the highest simulated gas flow rate, 20.0 m/s, produces a plot that is a slight exaggeration of the previous result. (Fig. 5) However, due to the fact that this flow rate is highly unlikely to be used in the true reactor, we could simply suggest that any inlet velocity higher than 15.2 m/s would continue to show uneven temperature contours.

## **Conclusions**

One set back in the simulation process using Fluent is the way the discretization grid must be defined. Fluent allows a limited number of cells to be defined as part of the grid. When dealing with exact dimensions, obviously, each cell must represent a set portion of the total length or height of the reactor. However, if a set number of cells does not exactly define a portion of the grid, for instance the inlet nozzle or outlet slot, it is necessary to designate either too few or too many cells to define the area. This takes away from the exact dimensions of the grid and may affect the results, and therefore the accuracy.

After first beginning with simulations of 50 iterations, the data was fairly inconclusive. The temperature contours showed only very slight shifts, even with the higher two flow rates. The shifts were so slight, they could almost be considered insignificant. However, upon increasing the number of iterations to 100, the results clearly show that higher inlet gas flow rates increase the variation in temperature around the heated wafer area. Further increasing the number of iterations to 200 revealed more. As time passed, even the low flow rate of 1.52 m/s showed a very slight shift in the contours. (Fig. 6) It follows, naturally, that the plots from the higher velocities showed even larger amounts of



***Figure6***

discontinuity in the temperature distribution. A possible suggestion would be to run the reactor for as short a time as possible, to reduce the likelihood of allowing the temperature shift to take place.

The data collected using the software package Fluent gives an acceptable amount of information about the problem. The contour plots serve adequately to show the resultant temperature distributions as a result of the gas flow rate. This information gathered using the simulations created with Fluent can now be compared to the results obtained using alternate simulation techniques.

## References

- [1] Adomaitis, R. A., Y. -H. Lin, and H. -Y. Chang 1999, A computational framework for boundary-value problem based simulations. *ISR TR 98-41*.
- [2] Chang, H. -Y. and R. A. Adomaitis 1997, Analysis of heat transfer in a chemical vapor deposition reactor: An eigenfunction expansion solution approach. *Int. J. Heat and Fluid Flow*, accepted for publication; also ISR TR 97-84.
- [3] Fluent Inc. Computational Fluid Dynamics Software, Version 4. Fluent Incorporated, © 1996.