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Chapter 3. Modeling and Simulation Part II: 
2D and 3D Flow and 1D Plasma Discharge*

3.1. Introduction

In this chapter we follow the same modeling approach for coupling the models as in previous chapters: The plasma model is applied in the discharge zone and the reactive flow model is used in the entire reactor volume (see Section 2.1). To study the influence of the reactor configuration on the flow field and on the deposition homogeneity, we develop a 2D reactive flow model suitable for simulating axisymmetric reactors. For the asymmetric geometries, a 3D flow model is also developed as an extension of 2D. The purpose of this Chapter is to investigate only the influence of the flow dynamics, and not the spatial effects of plasma, so we keep the 1D plasma model as in the previous chapter.

3.2. 2D and 3D flow models

The model presented in this section is an extension of the one-dimensional model [9,10] previously developed by the authors. In the whole reactor domain we solved the two- or three-dimensional Navier-Stokes equations for the flow of a viscous compressible multi-component chemically active gas mixture. More details on the models are given below.

3.2.1. Governing equations for reactive flow

We use computational fluid dynamics to simulate the physical and chemical processes that occur in PECVD reactors. The governing Navier-Stokes equations for an unsteady laminar flow of viscous compressible multi-component mixture of chemically reacting gases can be written as [11]:

\[
\frac{d}{dt} \int_V U \, dV + \int_S (F + G) \cdot dS = \int_S H dV ,
\]

(3.1)

where \( t \) is time and \( U = (\rho, \rho u_x, \rho u_y, \rho u_z, \rho e, \rho f_1, ..., \rho f_{N+1}) \) is a vector of conservative variables (here \( \rho \) is the gas density, \( u_x, u_y, u_z \) are the velocity vector components, \( e = e_{\text{int}} + \left( u_x^2 + u_y^2 + u_z^2 \right)/2 \) is the total energy per mass unit and \( f_i \) is the mass fraction of the \( i \)-th species, \( \sum_{i=1}^{N+1} f_i = 1 \)), \( V \) is the arbitrary gas volume enclosed by the surface \( S \), and \( dS \) is the unit vector perpendicular to the surface element, pointing outward. The internal energy is given by \( e_{\text{int}} = \sum_{i=1}^{N} f_i e_{\text{int}_i} \), \( e_{\text{int}_i} = h_0 + \frac{T}{n_0} \int_{n_0}^{T} \frac{C_p}{T} \, dT - R_i T \). Here \( h_0 \) is the heat of

* Parts of this chapter were published in [1-8]
formation at $T_0 = 293$ K, $C_p$ is the heat capacity at constant pressure $p$, and $R_i$ is the gas constant of the $i^{th}$ species.

The flux vector $\mathbf{F} = F_x \mathbf{i} + F_y \mathbf{j} + F_z \mathbf{k}$ is associated with the inviscid gas transfer, and $\mathbf{G} = G_x \mathbf{i} + G_y \mathbf{j} + G_z \mathbf{k}$ describes viscous transfer, energy dissipation, heat conductivity and diffusion:

$$
\begin{align*}
F_x &= 
\begin{bmatrix}
\rho u_x \\
\rho u_x^2 + p \\
\rho u_x u_y \\
\rho u_x u_z \\
\rho u_x f \mathbf{i}_x \\
&\cdots \\
\rho u_x f \mathbf{i}_{N-1x} 
\end{bmatrix}, \\
G_x &= 
\begin{bmatrix}
0 \\
-\sigma_{xx} \\
-\tau_{xy} \\
-\tau_{xz} \\
J_{xx} \\
&\cdots \\
J_{(N-1)x} 
\end{bmatrix}
\end{align*}
$$

Similar expressions hold for $F_y, F_z, G_y, G_z$.

The viscous stress tensor elements are given by $\sigma_{ij} = 2\mu \left( \frac{\partial u_i}{\partial x_j} - \frac{1}{3} \frac{\partial}{\partial x} \text{div} \mathbf{u} \right)$, $\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial y_j} + \frac{\partial u_j}{\partial x_i} \right)$. The heat flux vector is $\mathbf{q} = -\lambda \cdot \text{grad}(T) + \sum_{i=1}^{N} \mathbf{j}_i h_i$, where $h_i$ is the enthalpy of the $i^{th}$ species per mass unit and $\lambda = \mu C_p / Pr$ is the mixture heat conductivity, and $Pr$ is the Prandtl number. The diffusive flux vector is given by $\mathbf{j}_i = -\rho D_i \cdot \text{grad}(f_i)$. The transport coefficients, dynamic viscosity $\mu$ and diffusion coefficients $D_i$, are calculated from the molecular kinetic theory of gases using the Lennard-Jones 6-12 potential [10,12].

The source term $H = (0,...,0,H_1,...,H_N)^T$ in eq. (1) describes the species production due to the chemical reactions, with $H_i = \frac{M_i}{N_A} \left( B_i - A_i n_i \right)$, $A_i = \sum_{j=1}^{N} \left( n_j k_{ij} + \sum_{\beta=1}^{N} K_{\beta j} n_\beta \right)$, $B_i = \sum_{j=1}^{N} n_j \left( n_j k_{ij} + \sum_{\beta=1}^{N} K_{\beta j} n_\beta \right)$, where $k_{ij}$ and $K_{\beta j}$ are reaction rate constants for electron-induced reactions and neutral-neutral reactions respectively, $N_A$ is the Avogadro number, $n_i$ is the number density and $M_i$ is the molar mass of the $i^{th}$ species.

### 3.2.2. Boundary conditions for the reactive flow model

Under the low gas densities involved in the reactor (of order of $10^{-3}$-10$^{-4}$ kg/m$^3$), the Knudsen number (ratio of the mean free path of the radicals to the inter-electrode distance) is of the order of 0.01, at which the continuum approach starts to fail. To take into account this effect, a slip velocity and temperature jump boundary conditions at the wall should be applied. The effect of the velocity slip is probably negligible under most of the conditions for which simulations were done. But the effect of thermal accommodation is definitely important, since the accommodation coefficients for the diluent hydrogen are known to be small, particularly for SiC [13,14]. It was shown that at low pressures (near or below 100
3.3 Numerical methods and algorithms

Pa), the gas can be substantially colder than the surface at a distance less than one mean free path from that surface. This drastically lowers the rate of chemical reactions in the reactor volume with respect to the case where accommodation would be complete [15].

In the local 2D coordinate system x'-y' with the axis y', perpendicular to the wall (see Fig. 3.1) the velocity slip boundary condition is given by [16]:

\[ u'_x = \frac{2 - \theta}{\theta} \frac{\partial u'_y}{\partial y'} \frac{\mu}{\rho} \sqrt{\frac{\pi}{2 R_e T}} \sum_{j=1}^{N} \left( \frac{f_j}{M_j} \right)^{1/2}, \quad u'_y = 0. \]

Here \( R_u \) is the universal gas constant and \( \theta \) is an accommodation coefficient (close to 1).

The temperature jump boundary condition at the wall is given by:

\[ T = T_w + \frac{T_w}{T} \frac{\partial T}{\partial y'} \frac{1}{2 R_e} \sqrt{\frac{\pi}{2 R_e T}} \frac{2 - \theta}{\theta} \lambda \rho \sum_{j=1}^{N} \left( \frac{f_j}{M_j} \right)^{1/2}, \]

where \( T_w \) is the wall temperature.

The boundary condition for the species concentration at the wall was derived in [9]:

\[ \frac{\partial \rho f_j}{\partial y'} = \frac{s_i}{(2 - s_i) D_i} \rho f_i, \]

where \( s_i = 0.0 \) for the molecules SiH_{2n+2}, \( s_i = 0.15 \) for the radicals with one free bond SiH_{2n+1} and \( s_i = 1 \) for the radicals with more than one free bond.

The deposition rate is calculated as follows [10]:

\[ \dot{R}_j = - N_v \sum_{i=1}^{N} \frac{q_i D_i}{M_i} \frac{\partial \rho f_i}{\partial y'}, \]

where \( v = 2.195 \times 10^{-20} \text{ m}^3 \) is the silicon atom volume, and \( q_i \) is the number of silicon atoms in a depositing radical.

For the inlet boundary conditions, the flow rate, temperature and mixture composition need to be specified. The outlet pressure is set equal to the gas pressure inside the reactor chamber, and for all the other variables a "soft" boundary condition is used: \( \partial / \partial y' = 0 \).

3.3. Numerical methods and algorithms

3.3.1. Numerical scheme

To solve the set of equations (3.1) we used the operator splitting technique, decoupling the physical processes [17]. According to this method the problem can be split into inviscid and viscous "steps":

\[ \frac{\partial}{\partial t} \int_U \mathbf{U} \cdot dV + \int_S \mathbf{G} \cdot dS = \int_S H \cdot dV, \quad \mathbf{U}^{*\#}(t) = \mathbf{U}(t + \Delta t) \]

\[ \frac{\partial}{\partial t} \int_U \mathbf{U} \cdot dV + \int_S \mathbf{F} \cdot dS = 0, \quad \mathbf{U}^{*}(t) = \mathbf{U}(t) \]

The stiffness of the system is resolved by implicit numerical schemes. At the first step, an implicit ENO-scheme [18] is used in combination with a bi-diagonal algorithm [19].
for implicit increment calculation. For solving the "viscous" part, an implicit finite-difference scheme [20] is used. Given these finite-difference schemes we need to define the actual computational mesh.

### 3.3.2. Multi-block mesh generation

Since a PECVD reactor has a complex shape, a multi-block mesh generation algorithm is used, where the complete computational domain is divided into simple blocks, and in each block a regular mesh is generated. A mechanical analogy with deformed bodies [4] is applied for generation of non-uniform meshes in non-rectangular blocks, see Fig. 3.2. An irregular block connection was used for blocks with non-coinciding mesh vertices.

![Fig. 3.2. A mechanical analogy with deformed bodies for generation of non-uniform meshes in non-rectangular blocks](image)

### 3.3.3. Parallelization

Two levels of parallelization have been applied to solve the problem efficiently on computer clusters: job-level parallelization (parameter sweeps) and task-level parallelization (domain decomposition). The task-level parallel algorithm used beam distribution among the processors. A detailed description of parallelization methods will be given in Section 5.2.

### 3.4. Implementation and Problem Solving Environment components

For implementation of the numerical scheme and parallel algorithms, the MPI message passing interface was used in combination with a computational C++ core. The graphical user interface (GUI) was designed with the use of C/C++ programming languages, widespread platform independent GTK+ graphics library (glib, gdk, gtk) [21] and the Glade user interface builder [22]. The developed application provides users with an intuitive interface that allows them to interactively control the simulation processes, to visualize numerical results in real-time (or postponed) mode, and to access chemical components data or the archives of results. All modules of the Virtual Reactor problem
solving environment are platform-independent and were tested on Unix-like and Microsoft Windows operating systems.

To provide access to the Virtual Reactor, an interface for remote use was developed based upon Web technology, using a client-server model. For this interface, we created HTML pages, Java applets, JavaScript and CGI scripts. This system, like a local GUI, provides control over simulations and graphical representation of physical parameters, and was integrated into the Migrating Desktop.

To utilize the advantages of the parameter-sweep approach, a task Manager system was developed, looking after cluster processor idleness and loading them with new jobs. When one of the processors finished its job, the Manager initiates a process with new initial data set, running over the values of parameters studied. The jobs are submitted through the Migrating Desktop Grid-portal and the job management is done by the Resource Manager of the Grid environment. More details on the Virtual Reactor PSE are given in Chapter 6.

### 3.5. 2D Simulation Results

#### 3.5.1. Comparison with experiment and investigating possible causes of mismatch

The simulations of 2D flow with 1D plasma (where the 1D electron distribution is simply extrapolated along the 2D electrodes) predict a "convex" shape of film thickness, with maximum in the center and minimum at the edges (see for instance Fig. 3.3). The experimentally observed film thickness distribution however, was "concave, with a minimum in the center and a maximum near the edges [23].

![Figure 3.3. Simulation results of deposition rate distribution along the substrate.](image)

A number of test experiments were performed to find out which parameters can be responsible for this mismatch in the film distribution. A little non-uniformity in substrate temperature distribution (actually measured in experiments) does not influence the deposition rate too much: the dip in the middle is only of 1-2% (see Fig. 3.4, left). The electron density non-uniformity (artificially introduced in the simulation) does influence the deposition significantly (see Fig. 3.4, right). This is a clear indication that a 2D plasma model is needed to correctly predict the film distribution along the substrate.
3.5.2. Influence of the flow rate, temperature and discharge power

In the following experiments the inter-electrode spacing is 5 cm, gas temperature inside the chamber and at the inlet 300 K, substrate temperature 523 K, pressure 0.15 Torr (20 Pa), power supplied to the electrode 5 W and the discharge frequency 50 MHz. Equal molar fractions of SiH₄ and H₂ are injected, with a nominal total flow rate of 20 sccm [4]. The gas mixture enters the chamber at the left side of the simplified chamber geometry shown in Fig. 3.5.

Fig. 3.5. Simplified design of a 2D reactor chamber.

The simulation showed that tripling the flow rate (from 20 sccm to 60 sccm) reduces the film growth rate, and the deposited film becomes essentially asymmetric, with a noticeably higher growth rate at the downwind side of the substrate (see Fig. 3.6). Another remarkable observation is that the contribution of higher silanes (SiₓHᵧ) to deposition decreases when flow rate increases. This is explained by the relatively low reactivity and high diffusion-reaction length of this species (four times as large as that of SiH₄), which
makes it travel over long distances without chemical transformations and be removed from the volume above the substrate. Decreasing the flow rate leads to a more uniform and symmetrical film profile and a higher contribution of Si$_3$H$_4$ into the resulting film.

![Graph showing deposition rate and species contribution](image1)

**Fig. 3.6.** Contribution of different species into deposition. Pressure $p=0.15$ Torr, discharge power $W=0.05$ W/cm$^2$. Flow rate is 20 sccm (left) and 60 sccm (right).

Influence of pressure on the deposition rate is demonstrated in Fig. 3.7 for two different surface temperatures. Increasing the pressure significantly slows down the deposition process, keeping the relative contribution of different species to the deposition approximately constant. The same trend is observed in real experiments for pressures up to 1.5-2 Torr. This can be explained by the fact that pressure most strongly influences the plasma discharge and electron concentration, which in turn affects the radical production in electron-impact reactions R1-R7 and in reactions with atomic hydrogen (see Table 3-1).

![Graph showing deposition rate vs. pressure](image2)

**Fig. 3.7.** Influence of pressure on the deposition rate. Discharge power $W=0.05$ W/cm$^2$.

- **Left:** Deposition in the middle of the hot substrate ($T=520$ K).
- **Right:** Deposition in the middle of the cold electrode ($T=300$ K).
Table 3-1. List of chemical reactions and reaction constants used in simulations in this Section. Data for electron-impact reaction rates are given for the same reference conditions as in Table 2-2.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Reference reaction rate, cm³/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1 SiH₄ + e → SiH₃ + H + e</td>
<td>3.00e-11</td>
</tr>
<tr>
<td>R2 SiH₄ + e → SiH₂ + 2H + e</td>
<td>1.50e-10</td>
</tr>
<tr>
<td>R3 SiH₄ + e → SiH + H + H₂ + e</td>
<td>9.34e-12</td>
</tr>
<tr>
<td>R4 SiH₄ + e → SiH₂ + H₂ + e</td>
<td>7.19e-12</td>
</tr>
<tr>
<td>R5 H₂ + e → 2H + e</td>
<td>4.49e-12</td>
</tr>
<tr>
<td>R6 Si₂H₆ + e → SiH₃ + SiH₂ + H + e</td>
<td>3.72e-10</td>
</tr>
<tr>
<td>R7 Si₂H₆ + e → Si₂H₄ + 2H + e</td>
<td>3.70e-11</td>
</tr>
<tr>
<td>R8 SiH₄ + H → SiH₃ + H₂</td>
<td>2.53e-12</td>
</tr>
<tr>
<td>R9 SiH₄ + SiH₃ → Si₂H₅ + H₂</td>
<td>1.78e-15</td>
</tr>
<tr>
<td>R10 SiH₄ + SiH₂ → Si₂H₆*</td>
<td>1.00e-11</td>
</tr>
<tr>
<td>R11 SiH₄ + SiH → Si₂H₃ + H₂</td>
<td>1.70e-12</td>
</tr>
<tr>
<td>R12 SiH₄ + SiH → Si₂H₅</td>
<td>2.50e-12</td>
</tr>
<tr>
<td>R13 SiH₃ + H → SiH₂ + H₂</td>
<td>1.00e-10</td>
</tr>
<tr>
<td>R14 SiH₃ + SiH₃ → SiH₄ + SiH₂</td>
<td>1.50e-10</td>
</tr>
<tr>
<td>R15 SiH₃ + SiH₃ → Si₂H₆**</td>
<td>1.00e-11</td>
</tr>
<tr>
<td>R16 SiH₃ + SiH₂ → Si₂H₅</td>
<td>3.77e-13</td>
</tr>
<tr>
<td>R17 SiH₂ + H → SiH + H₂</td>
<td>7.96e-13</td>
</tr>
<tr>
<td>R18 SiH₂ + H → SiH₃</td>
<td>1.11e-12</td>
</tr>
<tr>
<td>R19 SiH₂ + H₂ → SiH₄</td>
<td>2.00e-13</td>
</tr>
<tr>
<td>R20 SiH₂ + SiH → Si₂H₃</td>
<td>7.22e-13</td>
</tr>
<tr>
<td>R21 SiH + H₂ → SiH₃</td>
<td>1.98e-12</td>
</tr>
<tr>
<td>R22 Si₂H₆ + H → SiH₄ + SiH₃</td>
<td>7.16e-12</td>
</tr>
<tr>
<td>R23 Si₂H₆ + H → Si₂H₅ + H₂</td>
<td>1.43e-11</td>
</tr>
<tr>
<td>R24 Si₂H₆ + SiH₃ → Si₂H₅ + SiH₄</td>
<td>3.27e-12</td>
</tr>
<tr>
<td>R25 Si₂H₆ + SiH₂ → Si₃H₈</td>
<td>1.20e-10</td>
</tr>
<tr>
<td>R26 Si₂H₆ + SiH → Si₃H₇</td>
<td>1.00e-11</td>
</tr>
<tr>
<td>R27 Si₂H₆ + Si₂H₄ → Si₄H₁₀</td>
<td>1.00e-10</td>
</tr>
<tr>
<td>R28 Si₂H₆* + M → Si₂H₆ + M</td>
<td>1.00e-10</td>
</tr>
<tr>
<td>R29 Si₂H₆* → Si₂H₄ + H₂</td>
<td>5.00e6 c-1</td>
</tr>
<tr>
<td>R30 Si₂H₆** → Si₄H₄ + SiH₂</td>
<td>2.30e7 c-1</td>
</tr>
<tr>
<td>R31 Si₂H₆** → Si₂H₄ + H₂</td>
<td>2.30e7 c-1</td>
</tr>
<tr>
<td>R32 Si₂H₆** + M → Si₂H₆ + M</td>
<td>2.00e-10</td>
</tr>
<tr>
<td>R33 Si₂H₅ + H → Si₂H₄ + H₂</td>
<td>1.00e-10</td>
</tr>
<tr>
<td>R34 Si₂H₅ + SiH₄ → Si₂H₆ + SiH₃</td>
<td>5.00e-13</td>
</tr>
<tr>
<td>R35 Si₂H₅ + SiH₃ → Si₂H₄ + SiH₄</td>
<td>1.00e-10</td>
</tr>
<tr>
<td>R36 Si₂H₅ + SiH₃ → Si₃H₈</td>
<td>1.00e-11</td>
</tr>
<tr>
<td>R37 Si₂H₅ + Si₂H₅ → Si₄H₁₀</td>
<td>1.00e-11</td>
</tr>
<tr>
<td>R38 Si₂H₄ + H₂ → SiH₄ + SiH₂</td>
<td>1.00e-10</td>
</tr>
<tr>
<td>R39 Si₂H₄ + H₂ → Si₂H₆</td>
<td>5.33e-13</td>
</tr>
</tbody>
</table>
R40  Si2H₄ + SiH₄ → Si₃H₈  1.00e-10  
R41  Si2H₃ + H₂ → Si2H₅  1.70e-12  
R42  Si3H₈ + H → Si2H₅ + SiH₄  2.17e-11  
R43  Si3H₈ + SiH₃ → Si₃H₇ + SiH₄  3.30e-12  
R44  Si3H₈ + SiH₂ → Si4H₁₀  1.00e-11  
R45  Si3H₈ + SiH → Si4H₉  1.00e-11  
R46  Si3H₈ + Si2H₄ → Si₅H₁₂  1.00e-10  
R47  Si3H₇ + H → Si3H₈  1.00e-11  
R48  Si3H₇ + SiH₃ → Si₃H₆ + SiH₄  3.30e-12  
R49  Si3H₇ + SiH → Si₄H₁₀  1.00e-11  
R50  Si3H₆ + SiH₃ → Si₄H₉  2.00e-11  
R51  Si₄H₁₀ + SiH₃ → Si₄H₉ + SiH₄  3.30e-12  
R52  Si₄H₁₀ + SiH₂ → Si₅H₁₂  1.00e-11  
R53  Si₄H₁₀ + SiH → Si₅H₁₁  1.00e-11  
R54  Si₄H₉ + H → Si₄H₁₀  1.00e-11  
R55  Si₄H₉ + SiH₃ → Si₄H₈ + SiH₄  3.30e-12  
R56  Si₄H₉ + SiH₃ → Si₅H₁₂  1.00e-11  
R57  Si₄H₉ + SiH₂ → Si₅H₁₁  1.00e-11  
R58  Si₄H₈ + SiH₃ → Si₅H₁₁  2.00e-11  
R59  Si₅H₁₁ + H → Si₅H₁₂  1.00e-11  
R60  Si₅H₁₁ + SiH₃ → Si₅H₁₀ + SiH₄  3.30e-12  
R61  Si₅H₁₂ + SiH₃ → Si₅H₁₁ + SiH₄  3.30e-12

The influence of discharge power is illustrated in Fig. 3.8. One can see that increasing the discharge power (and consequently the electron concentrations) increases the deposition rate. Moreover, the relative contribution of higher silanes (Si₃H₇) into the deposition grows with increasing power.

![Fig. 3.8. Influence of discharge power W on the deposition rate. P=0.5 Torr. W=0.05 W/cm²](image)

(a): W=0.025 W/cm²; (b): W=0.05 W/cm²; (c): W=0.075 W/cm²

3.5.3. Influence of reactor geometry

Here, the influence of reactor geometry and the pumping path was investigated. In the first case (Fig. 3.9a), a gas mixture was pumped into the reactor chamber through the
inlets located outside the discharge area, while in the second case (Fig. 3.9b) the mixture enters through a hole in the middle of one of the electrodes (left electrode in Fig. 3.9b).

Fig. 3.9a,b shows the distribution of silyl (SiH₃) and higher silane (Si₃H₆) concentrations. Silyl is the main component that contributes to the film growth. One can see that in the second case (Fig. 3.9a) its distribution along the substrate (that is marked with a bold red line) is more homogeneous, that provides a better homogeneity of the film. However, it grows slightly slower in this case, since the absolute concentration of silyl near the substrate is less. Concentration of Si₃H₆, that triggers dust production, is less in the first case (Fig. 3.9a, right), thus in terms of chemical composition, the film quality is better here.

![Simulation results: concentration fields of silyl (left), higher silanes (right) and stream lines of the flow (black lines). a, b - different geometrical configuration of reactors. 2D axisymmetric configurations.](image)

Many industrial PECVD reactor configurations are essentially asymmetric and cannot be studied by axisymmetric models. To study the influence of the flow in such chambers, we performed simulations in 2D planar configurations shown in Fig. 3.10. The simulation results showed for instance that adding a small sub-chamber before the pump outlet (Fig. 3.10, B) completely changes the flow pattern: in this case the flow of the source mixture goes from the inlet located at the opposite side through the inter-electrode spacing,
whereas without this side-chamber the flow almost does not penetrate the discharge zone (Fig. 3.10, A).

![Image of flow behavior with and without side-chamber](image)

Fig. 3.10. Influence of geometry (location of pumping tube) on the flow behaviour. 2D planar configurations.

### 3.5.4. Deposition dynamics in the final stages of the PECVD cycle

One of the least studied questions in PECVD film deposition is what happens at the end of the production cycle, when the plasma is ‘switched off’, the inflow of the source gases is stopped, and pressure is increased to atmospheric value. These abrupt changes in the process conditions cause significant changes in the deposition dynamics. Experimental analysis of the processes occurring at this stage is very difficult if not impossible, because the processes of plasma recombination, radicals’ diffusion towards the surface and their attachment to the film, are much faster than the time needed for film characterization. Moreover, the measurements of the composition and homogeneity are usually done ‘off-line’, after the film is taken out of the reactive chamber. In order to study computationally the finishing stages of the PECVD cycle, we carried out a series of simulation experiments varying the basic physical and chemical parameters, as well as the moments in time when these final stages occur (plasma switch-off, gas inflow and heating shut-down) [1]. Some of the results are presented in Fig. 3.11-Fig. 3.13. When the discharge is switched off, we observe not only a rapid decrease in the absolute values of the deposition rate, but also a
strong shift in the film composition, with a noticeable decrease of a relative contribution of silyl and sililyl and increased relative contribution of long-living higher silane radicals (see Fig. 3.11). Another example is stopping the inflow of the source gas mixture into the chamber (with pumping also stopped to keep the pressure constant). It causes not only the obvious decrease in deposition rate due to silane depletion, but also an increased inhomogeneity of film distribution (larger difference between the minimal and maximal deposition rates in Fig. 3.12) and accumulation of higher silanes (see Fig. 3.13), which can form dust particles and stick to the film surface, dramatically changing film properties and causing defects. To avoid this and remove the dusty particles from the reactor volume, a chamber "cleaning" stage is essential with a silane-free gas mixture after the plasma is switched off and before the flow is stopped, without interruption of the production cycle.

Fig. 3.11. Degradation of film deposition: RF discharge switched off.

Fig. 3.12. Decrease of the deposition rate after the flow shut-down. Maximum deposition rate in the center and minimal deposition rate at the edges are traced separately.
3.6 3D Simulation Results: Flow in Complex Reactor Configurations

The previous section shows that the flow can have a strong influence on the PECVD processes. In industrial reactors this effect can even be more pronounced, due to the essentially asymmetric (3D) geometrical configurations of the reactor chambers. In this section we study the flow in different reactor configurations, without taking into account the plasma and chemical processes.

Four different reactor chamber configurations have been simulated (type A, B, C, D). The models designed accounted for the main features of typical industrial chambers used in plasma doping technology. Small parts such as Langmuir probes and rudimentary side dead-ends were neglected for their effect on the flow dynamics is considered to be insignificant. Fig. 3.14 shows the sketches of the simulated chambers with the generated computational meshes.

[1] Our estimation that SiH₃ concentration is approximately constant in the discharge is correct.
[2] SiH₃ concentration in the case without flow is almost four times larger than with flow, therefore SiH₃ in this case will effectively disappear due to reaction with SiH₂: SiH₂ + SiH₃ → SiH₄ + H₂.

Fig. 3.13. Accumulation of higher silanes in a closed chamber (no inflow and outflow).
Two inflow rates were simulated: 200 sccm and 500 sccm, and three gas mixtures were considered: <1> 0.05% B\textsubscript{2}H\textsubscript{6}, 99.95% He, <2> 5% B\textsubscript{2}H\textsubscript{6}, 95% He, and <3> 0.05% B\textsubscript{2}H\textsubscript{6}, 98.95% He, 1% Ar. The percentage was counted as a mole fraction; therefore for instance 5% of B\textsubscript{2}H\textsubscript{6} in case <2> means that the mass fraction of B\textsubscript{2}H\textsubscript{6} is 25.5%.

The pressure was fixed to 0.9 Pa, the mixture in the inflow and the initial gas mixture inside the chamber were assumed to be at room temperature (298 K), and the substrate temperature was fixed to 100 deg C (373 K). Sticking coefficient \( s_i \) in the boundary condition for species concentration, see eq. (2.11), was assumed to be 1.0 for B\textsubscript{2}H\textsubscript{6} on the substrate surface (all molecules that reach this wall stick to it), and 0.0 for other species. This is a very rough model that helps understanding the major trends in species distribution.
without going into detail of simulating plasma-chemistry that causes diborane decomposition and sticking of individual radical species.

In the sequel we will only present the simulation results for the A-type chamber at 200 scem inflow rate and mixture composition case <2>. The results for the other 3 types showed similar trends (data not shown). Fig. 3.15 clearly shows the zone with lower density of the gas above the “hot” substrate. Gas temperature distribution is illustrated in Fig. 3.16.

![Fig. 3.15. Mixture density distribution in the shell planes (left) and in the horizontal parallel cross-section slices (right).](image1)

![Fig. 3.16. Gas temperature distribution in the shell planes (left) and in the horizontal parallel cross-section slices (right).](image2)

The specificity of the chamber design causes high velocities in the area with a relatively narrow flow way between the electrode cylinder and the outer chamber walls. This effect is shown in Fig. 3.17 and Fig. 3.18 with the absolute values and vectors of the flow velocity. Due to this effect, a region with high vorticity appears right behind the edge of the electrode downstream on the way of the main flow path (see Fig. 3.19).
Fig. 3.17. Flow velocity distribution in the shell planes (left) and in the horizontal parallel cross-section slices (right).

Fig. 3.18. Flow velocity vectors in the horizontal parallel cross-section slices, left and right parts of the chamber.

Fig. 3.19. Vorticity distribution in the horizontal parallel cross-section slices, whole chamber (left) and zoom-in in the area with high vorticity.
A detailed study of the dynamics of the spatial distribution of chemical components revealed that convection does not influence the homogeneity of B$_2$H$_6$ concentration along the substrate at a 200 sccm flow rate, but causes a slight asymmetry at 500 sccm. As can be seen from Fig. 3.20, diffusion plays a major role in the dynamics of the diborane concentration, which swiftly smooths throughout the reactor chamber. It is worth mentioning that the concentration of B$_2$H$_6$ in the cross-section slice far above the substrate (and close to the inlet) becomes 5 times lower at the time step N=100000 (see the last picture in Fig. 3.20) compared to the initial value (see the first picture in Fig. 3.20). This shows how efficient the diffusion transport is for the conditions simulated.

![Fig. 3.20. B$_2$H$_6$ mass fraction distribution in the horizontal parallel cross-section slices at different time steps N.](image)

These experiments indicate that the homogeneity of the species spatial distribution is mainly defined by diffusive transport and not by convection; therefore the inflow rate can be reduced to the minimal required values just to supply enough of source mixture to the reactive chamber.
3.6.1. Comparison of 3D and 2D Simulation of Gas Flow

To explore a wide range of parameters influencing the flow process and to tune the model, a very large number of simulation runs shall be performed. Full 3D simulations are very time consuming, so we decided to perform 2D simulations for faster analysis. The results of 3D simulations were very encouraging in this respect: there was basically no asymmetry in the radial distribution of the main variables in the geometry of the type B chamber, and the contribution of the third dimension in the type A and Type C configurations was not significant.

To test the accuracy of 2D simulations we chose the Type A chamber geometry. The Type B configuration is almost axisymmetric, and the Type C features a relatively homogeneous flow radial distribution near the wafer because the inflow is organized far from the substrate. Type A is the most asymmetric in the part near the wafer, because the gas enters the chamber relatively close to the electrode.

The configuration of the 2D chamber design was taken equivalent to the geometry of the main plane of symmetry slice used in 3D simulations to cut one half of the computational domain. Fig. 3.21 shows the sketches of the simulated 3D and 2D chambers with the generated computational meshes.

![Simulated reactor chambers and the generated computational meshes for the 3D (left) and 2D (right) models of the Type A configuration](image)

Fig. 3.21. Simulated reactor chambers and the generated computational meshes for the 3D (left) and 2D (right) models of the Type A configuration

Initial and boundary conditions for 2D simulations were the same as for the 3D simulations. Below we show comparison of some of the 2D reactor chamber simulation results with those of 3D configuration. Fig. 3.22 and Fig. 3.23 show the distributions of gas mixture density and temperature, respectively.

![Density](image)

![Temperature](image)
Fig. 3.22. Gas mixture density distribution for the 3D (left) and 2D (right) simulations

Fig. 3.23. Gas temperature distribution for the 3D (left) and 2D (right) simulations

These spatial distributions in the 2D configuration show nearly no difference compared to those in the median plane of the 3D chamber. A slight difference in absolute value of the maximum temperature in Fig. 3.23 is explained by a different mesh size in 2D and 3D simulations. The visualizer shows the values of the variables in the cell centers, thus the distance from the wall to the center of the first computational cell influences the way the fields are visualized, which is especially noticeable near the heated walls with large parameter gradients.

Fig. 3.24 shows the comparison of the flow velocity distributions. As it was noted earlier, the specificity of the chamber design causes high flow rates in the area with a relatively narrow flow way between the electrode cylinder and the outer chamber walls. This effect is even more pronounced in the 2D simulation since the area, which the current has to squeeze through, is smaller than in 3D simulation. Except for this difference, the overall picture of the flow stays very similar to that predicted by the 3D simulation.

Fig. 3.24. Flow velocity distribution for the 3D (left) and 2D (right) simulations

The same goes for the spatial distribution of $\text{B}_3\text{H}_6$ predicted by 2D and 3D simulations. As it can be seen from Fig. 3.25, two-dimensional simulation only slightly underestimates the concentration of diborane in the right lower “sleeve” of the chamber, which in 3D is connected to the main chamber through a ring around the electrode, while in 2D it is blockaded. Taking into consideration this fact, we stress once again that this
negligible difference confirms our conclusion that diffusion plays the major role in the dynamics of diborane concentration under the conditions simulated.

Fig. 3.25. $\text{B}_2\text{H}_6$ mass fraction distribution for the 3D (left) and 2D (right) simulations at two different time steps.

Fig. 3.25 also shows that the distribution of $\text{B}_2\text{H}_6$ along the wafer near the wall can be considered symmetrical in both 2D and 3D cases, thus bringing us to another conclusion, that the gas dynamic transport cannot significantly influence the characteristics of homogeneity of the doping process. We expect that it will be mainly affected by the plasma discharge distribution and electro-magnetic fields not simulated in the framework of this project.

### 3.7. Conclusions

Comparison of the results of 2D and 3D simulations shows that all the main characteristics of the flow and, more importantly, the spatial distribution of the chemical species are well captured by the 2D simulations, thus for series simulations and for studying trends it is more efficient to use 2D modeling. Both 3D and 2D simulations showed that the radial distribution of the main parameters affecting the doping process (temperature and species concentrations) along the wafer is almost ideally symmetrical with the axis of symmetry in the center of the wafer. It indicates that the homogeneity of these parameters near the wafer is mainly defined by diffusive transport and not by convection.

Since the gas dynamic transport cannot significantly influence the characteristics of homogeneity of the doping process, the latter will be affected mostly by the plasma discharge distribution and electro-magnetic fields, which were not studied in this chapter.
The Virtual Reactor allowed us to study the film degradation processes and to find the featuring trends in system response to the variation of physical and chemical parameters and the operating actions. We were able to indicate the mechanisms responsible for the layer composition at the finishing stage of the film production cycle.

We have observed a mismatch between the experimental and simulated distribution of the film thickness along the substrate. Additional computational experiments revealed that the correct (experimental) shape can be recovered by adjusting the electron density distribution rather than gas flow parameters like temperature. We therefore conclude that a 2D discharge simulation is needed. This is discussed in the next chapter.

3.8 References

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