



# Numerical modeling of deposition kinetics in the MCVD process for silica-based optical fibers

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## ABSTRACT

This study presents a numerical approach for modeling the kinetics of the Modified Chemical Vapor Deposition (MCVD) process under laminar flow conditions, aiming at controlling the refractive index profile in silica-based optical fibers for high-power laser applications. The model couples the steady-state energy and mass transport equations, solved using the Finite Volume Method (FVM) through a commercial CFD package, and the Finite Difference Method (FDM). Simulations yielded velocity and temperature fields of the carrier gas ( $O_2$ ), as well as concentration fields of reactants and oxidation products. Deposition efficiency was estimated by combining thermophoretic velocity and local species concentrations, revealing a slightly higher efficiency for  $SiO_2$  compared to  $GeO_2$  across all tested scenarios. A parametric analysis was conducted to assess the influence of peak torch temperature and mass flow rate on deposition behavior. Particle trajectories were obtained via a Lagrangian approach using Euler's integration method, showing that particles closer to the tube wall exhibited greater deposition tendencies due to stronger thermal gradients.

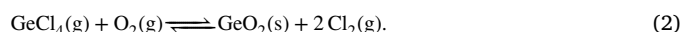
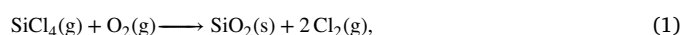
## 1. Introduction

Silica-based optical fibers are fundamental components of modern photonic systems, enabling low-loss transmission over long distances and wide power ranges. Their performance depends critically on the uniformity, purity, and spatial distribution of dopants in the glass matrix, which directly affect optical attenuation, dispersion, and power-handling capability. Consequently, fabrication techniques offering precise control of material composition and deposition kinetics are essential.

Among the available manufacturing routes, the Modified Chemical Vapor Deposition (MCVD) process remains one of the most widely adopted methods for producing high-purity optical fiber preforms. Originally developed at Bell Laboratories [1], MCVD relies on the oxidation of halide precursors inside a rotating silica tube externally heated by a moving flame, enabling controlled deposition and sintering of silica-based layers along the tube inner wall.

The optical properties of silica fibers are commonly tailored through dopant oxides, particularly germanium dioxide. As shown by [2],  $GeO_2$ -doped cores exhibit reduced optical losses due to decreased Rayleigh scattering, especially at longer wavelengths. As a result, controlling the deposition efficiency and spatial distribution of  $SiO_2$  and  $GeO_2$  during MCVD is a central technological challenge.

Despite its industrial maturity, MCVD involves a complex coupling between fluid flow, heat transfer, chemical reactions, and particle transport (Fig. 1). Halide precursors such as  $SiCl_4$  and  $GeCl_4$  are transported by an oxygen-rich carrier gas and oxidized in the high-temperature region generated by the external flame, leading to oxide formation according to



The oxide species generated in the reaction zone are transported by the carrier gas and may deposit onto the tube wall. Deposition is primarily driven by thermophoretic forces arising from steep radial temperature gradients near the heated wall, while part of the material is lost through the exhaust flow [4]. Deposition efficiency therefore plays a decisive role in material utilization, process reproducibility, and cost.

### 1.1. Objective

The objective of this work is to develop a steady-state numerical framework for analyzing deposition kinetics in the MCVD process. The

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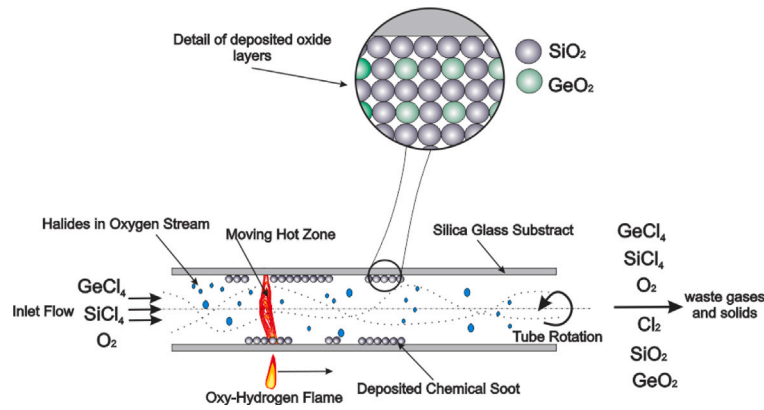


Fig. 1. Schematic diagram of the MCVD process.  
Source: Adapted from [3].

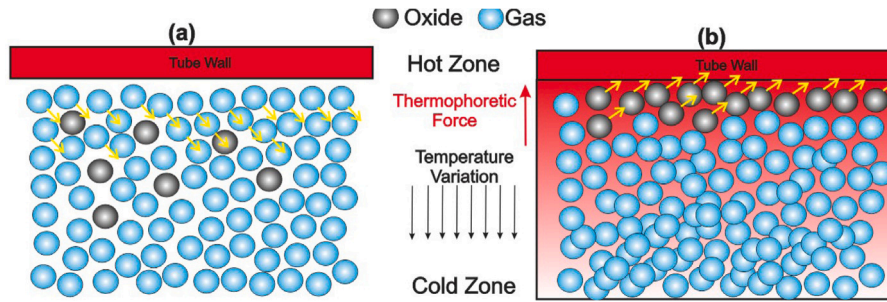


Fig. 2. Thermophoresis mechanism in a domain with a heated wall. (a) Gas molecules migrate toward cooler regions; (b) Oxide particles are driven toward the hot wall by thermophoretic forces.

model resolves the coupled transport of momentum, energy, and chemical species in a rotating silica tube, with emphasis on oxide formation, transport, and wall deposition under laminar flow conditions.

Two complementary numerical approaches are employed: a finite volume method (FVM) implemented in a commercial CFD solver and an in-house finite difference method (FDM). Their combined use enables cross-validation of numerical predictions and assessment of the influence of discretization strategies on key quantities relevant to deposition.

### 1.2. Thermophoresis

Thermophoresis refers to the migration of suspended particles in a gaseous medium induced by temperature gradients, resulting from non-uniform momentum transfer between gas molecules and particles [5]. In MCVD, characterized by strong thermal gradients imposed by an external moving torch, thermophoretic forces dominate particle transport normal to the tube wall.

Gas molecules in hotter regions possess higher thermal velocities and impart greater momentum to particles than those in cooler regions, producing a net force that drives particles toward lower-temperature zones [6]. In MCVD, this mechanism results in oxide particles migrating toward the tube wall, where deposition occurs, as schematically illustrated in Fig. 2.

Classical studies [7,8] established the dependence of thermophoretic transport on particle size, gas properties, and temperature gradients. In MCVD, thermophoresis is widely recognized as the dominant deposition mechanism for oxide particles with diameters in the range of 0.1–1.0  $\mu\text{m}$ , allowing gravitational and inertial effects to be neglected [9].

The magnitude of the thermophoretic force depends strongly on the Knudsen number. To account for the continuum-to-free-molecule

regimes encountered in MCVD, the present work adopts the formulation proposed by [10], as recommended by [3], which provides a continuous description of thermophoretic transport across multiple regimes.

## 2. Mathematical modeling

The numerical model developed in this work is structured into two complementary approaches: the Eulerian approach, which calculates the flow field of the carrier gas — such as temperature, velocity, pressure, and density — as well as the species concentrations through the transport equations; and the Lagrangian approach, which is used to track the trajectories of the oxide particles formed during the MCVD process.

### 2.1. Assumptions

To enable the solution of the proposed model and ensure consistency with the underlying physics, the following simplifying assumptions were adopted:

- The process is modeled under steady-state conditions in a translating reference frame attached to the moving torch;
- The carrier gas ( $\text{O}_2$ ) is treated as a Newtonian, continuous, and ideal gas, with laminar flow inside the tube ( $\text{Re} \approx 900$ ); density variations arise solely from temperature effects;
- The silica tube is modeled as a cylindrical domain with negligible wall thickness, and heat conduction within the solid wall is neglected;
- Due to the low concentration of metal halides relative to the carrier gas, the velocity, pressure, and temperature fields are computed from the carrier gas flow and used unchanged in the species transport equations;

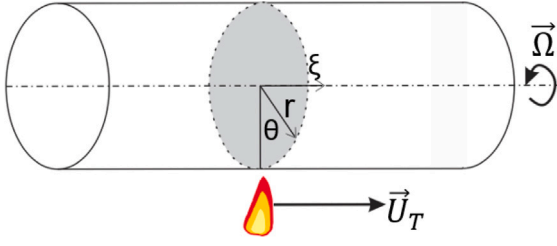


Fig. 3. Cylindrical coordinate system adopted in the numerical model. Source: [11](Adapted).

- In the Eulerian framework, metal halides and oxide products are treated as gaseous species, while in the Lagrangian framework oxide particles are assumed spherical with constant diameter;
- The oxidation of  $\text{GeCl}_4$  is treated as irreversible, and gravitational effects on particle motion are neglected.

## 2.2. Governing equations

The governing equations are formulated in a cylindrical coordinate system  $(\xi, \theta, r)$  attached to the rotating quartz tube, as shown in Fig. 3. To account for the axial motion of the external heating torch while retaining a steady-state formulation, a translating reference frame moving at constant velocity  $U_T$  is adopted, with the axial coordinate defined as

$$\xi = x - U_T t, \quad (3)$$

where  $x$  is the axial coordinate in the laboratory frame and  $U_T$  represents the axial translation velocity of the external torch.

In this torch-attached frame, statistically steady fields satisfy  $\partial\phi/\partial t = -U_T \partial\phi/\partial\xi$ , leading to stationary governing equations with an effective axial convection velocity  $(u_x - U_T)$ . This transformation exploits the fact that the dominant thermal gradients, chemical reactions, and particle formation processes remain localized near the moving heat source and exhibit invariant spatial structure in the translating frame. Under these assumptions, Eqs. (8)–(17) are solved as steady-state equations in the moving reference frame.

The conservation equations for mass, momentum, and energy are solved for the flow of the carrier gas ( $\text{O}_2$ ). The solution yields the velocity field components  $(u, v, w)$ , pressure  $(p)$ , and temperature  $(T)$ . Given that the concentration of the carrier gas is significantly higher than that of the reactive halides, the same field variables obtained from the carrier gas flow are used in the species conservation equations.

The governing equations for the three-dimensional, steady-state, laminar flow, including chemical reactions and involved species, are expressed according to the study of [11]:

### (i) Continuity equation:

$$\frac{1}{r} \frac{\partial(\rho v)}{\partial r} + \frac{1}{r} \frac{\partial(\rho w)}{\partial \theta} + \frac{\partial(\rho u)}{\partial \xi} = 0 \quad (4)$$

where  $\rho(r, \theta, \xi)$  is the density of the carrier gas  $\text{O}_2$ .

### (ii) Momentum conservation equations:

$$\rho v \frac{\partial u}{\partial r} + \rho \frac{w}{r} \frac{\partial u}{\partial \theta} + \rho(u - U_T) \frac{\partial u}{\partial \xi} = -\frac{\partial p}{\partial \xi} + \nabla \cdot (\mu \nabla u) \quad (5)$$

$$\rho v \frac{\partial v}{\partial r} + \rho \frac{w}{r} \frac{\partial v}{\partial \theta} + \rho(u - U_T) \frac{\partial v}{\partial \xi} - \rho \frac{w^2}{r} = -\frac{\partial p}{\partial r} + \rho g \cos \theta + \nabla \cdot (\mu \nabla v) - \mu \frac{v}{r^2} - \mu \frac{2}{r^2} \frac{\partial w}{\partial \theta} \quad (6)$$

$$\rho v \frac{\partial w}{\partial r} + \rho \frac{w}{r} \frac{\partial w}{\partial \theta} + \rho(u - U_T) \frac{\partial w}{\partial \xi} - \rho \frac{v w}{r} = -\frac{1}{r} \frac{\partial p}{\partial \theta} + \rho g \sin \theta + \nabla \cdot (\mu \nabla w) - \mu \frac{v}{r^2} - \mu \frac{w}{r^2} \frac{\partial v}{\partial \theta} \quad (7)$$

where  $p(r, \theta, \xi)$  is the pressure,  $\mu$  is the dynamic viscosity, and  $g$  is gravitational acceleration.

### (iii) Energy equation for the gas temperature $T(r, \theta, \xi)$ :

$$\rho c_p v \frac{\partial T}{\partial r} + \rho c_p \frac{w}{r} \frac{\partial T}{\partial \theta} + \rho c_p (u - U_T) \frac{\partial T}{\partial \xi} = \nabla \cdot (k \nabla T) + \Delta H_{\text{SiCl}_4} r_{\text{SiCl}_4} + \Delta H_{\text{GeCl}_4} r_{\text{GeCl}_4} \quad (8)$$

where  $c_p$  is the specific heat,  $k$  the thermal conductivity of  $\text{O}_2$ ,  $\Delta H$  the reaction enthalpies (251 and 46 kJ/mol for  $\text{SiCl}_4$  and  $\text{GeCl}_4$ , respectively), and  $r_i$  the oxidation reaction rates.

### (iv) Species mass fraction equations (gas phase):

$$\rho v \frac{\partial Y_{\text{SiCl}_4}}{\partial r} + \rho \frac{w}{r} \frac{\partial Y_{\text{SiCl}_4}}{\partial \theta} + \rho (u - U_T) \frac{\partial Y_{\text{SiCl}_4}}{\partial \xi} = \nabla \cdot (\rho D_{\text{SiCl}_4} \nabla Y_{\text{SiCl}_4}) - r_{\text{SiCl}_4} \quad (9)$$

$$\rho v \frac{\partial Y_{\text{GeCl}_4}}{\partial r} + \rho \frac{w}{r} \frac{\partial Y_{\text{GeCl}_4}}{\partial \theta} + \rho (u - U_T) \frac{\partial Y_{\text{GeCl}_4}}{\partial \xi} = \nabla \cdot (\rho D_{\text{GeCl}_4} \nabla Y_{\text{GeCl}_4}) - r_{\text{GeCl}_4} \quad (10)$$

$$\rho v \frac{\partial Y_{\text{O}_2}}{\partial r} + \rho \frac{w}{r} \frac{\partial Y_{\text{O}_2}}{\partial \theta} + \rho (u - U_T) \frac{\partial Y_{\text{O}_2}}{\partial \xi} = \nabla \cdot (\rho D_{\text{O}_2} \nabla Y_{\text{O}_2}) - 2r_{\text{SiCl}_4} \frac{M_{\text{O}_2}}{M_{\text{SiCl}_4}} - 2r_{\text{GeCl}_4} \frac{M_{\text{O}_2}}{M_{\text{GeCl}_4}} \quad (11)$$

$$\rho v \frac{\partial Y_{\text{Cl}_2}}{\partial r} + \rho \frac{w}{r} \frac{\partial Y_{\text{Cl}_2}}{\partial \theta} + \rho (u - U_T) \frac{\partial Y_{\text{Cl}_2}}{\partial \xi} = \nabla \cdot (\rho D_{\text{Cl}_2} \nabla Y_{\text{Cl}_2}) + 2r_{\text{SiCl}_4} \frac{M_{\text{Cl}_2}}{M_{\text{SiCl}_4}} + 2r_{\text{GeCl}_4} \frac{M_{\text{Cl}_2}}{M_{\text{GeCl}_4}} \quad (12)$$

where  $Y(r, \theta, \xi)_i$ ,  $D_i$  and  $M_i$  are the mass fractions, the diffusion coefficients and the molecular weight for each element  $i = \{\text{SiCl}_4, \text{GeCl}_4, \text{O}_2, \text{Cl}_2\}$ .

### (v) Species mass fraction equations (solid phase):

$$\rho v \frac{\partial Y_{\text{SiO}_2}}{\partial r} + \rho \frac{w}{r} \frac{\partial Y_{\text{SiO}_2}}{\partial \theta} + \rho (u - U_T) \frac{\partial Y_{\text{SiO}_2}}{\partial \xi} = \nabla \cdot (\rho D_{\text{SiO}_2} \nabla Y_{\text{SiO}_2}) - \frac{1}{r} \frac{\partial}{\partial r} (r \rho Y_{\text{SiO}_2} v_T) - \frac{1}{r} \frac{\partial}{\partial \theta} (\rho Y_{\text{SiO}_2} w_T) + \frac{\partial}{\partial \xi} (\rho Y_{\text{SiO}_2} u_T) + r_{\text{SiCl}_4} \frac{M_{\text{SiO}_2}}{M_{\text{SiCl}_4}} \quad (13)$$

$$\rho v \frac{\partial Y_{\text{GeO}_2}}{\partial r} + \rho \frac{w}{r} \frac{\partial Y_{\text{GeO}_2}}{\partial \theta} + \rho (u - U_T) \frac{\partial Y_{\text{GeO}_2}}{\partial \xi} = \nabla \cdot (\rho D_{\text{GeO}_2} \nabla Y_{\text{GeO}_2}) - \frac{1}{r} \frac{\partial}{\partial r} (r \rho Y_{\text{GeO}_2} v_T) - \frac{1}{r} \frac{\partial}{\partial \theta} (\rho Y_{\text{GeO}_2} w_T) + \frac{\partial}{\partial \xi} (\rho Y_{\text{GeO}_2} u_T) + r_{\text{GeCl}_4} \frac{M_{\text{GeO}_2}}{M_{\text{GeCl}_4}} \quad (14)$$

where the radial, azimuthal, and axial components of the thermophoretic velocity are expressed, respectively, according to the semi-empirical formulation proposed by [8]:

$$v_T = -\frac{K v}{T} \frac{\partial T}{\partial r}, \quad w_T = -\frac{K v}{T} \frac{1}{r} \frac{\partial T}{\partial \theta}, \quad u_T = -\frac{K v}{T} \frac{\partial T}{\partial \xi} \quad (15)$$

where  $v$  is the kinematic viscosity and  $K$  the thermophoretic coefficient, defined according to [8,12]:

$$K = \frac{C_s \left( \frac{\kappa_g}{\kappa_p} + C_t \text{Kn} \right)}{(1 + 3C_m \text{Kn})(1 + 2\frac{\kappa_g}{\kappa_p} + 2C_t \text{Kn})} \quad (16)$$

with  $\text{Kn} = \lambda/d_p$  being the Knudsen number, defined as the ratio between the mean free path of the gas molecules and the particle diameter;  $C_s = 1.17$ ,  $C_t = 2.18$ ,  $C_m = 1.14$ , and  $\kappa$  the thermal conductivity of gas ( $\kappa_g$ ) and particle ( $\kappa_p$ ), respectively. In this formulation, the Knudsen number falls within the continuum-to-transition regime, i.e.,  $0.01 \leq \text{Kn} \leq 10$  [8].

**Table 1**  
Transport properties of chemical species [11].

| Property                                                                     | Unit               |
|------------------------------------------------------------------------------|--------------------|
| $\nu = \frac{\mu}{\rho} = 1.39 \times 10^{-5} T^{1.64374}$                   | cm <sup>2</sup> /s |
| $k = 1.08 \times 10^{-5} + 1.82 \times 10^{-7} T - 2.34 \times 10^{-11} T^2$ | W/cm K             |
| $D_{\text{SiCl}_4} = 6.32 \times 10^{-6} T^{1.6561}$                         | cm <sup>2</sup> /s |
| $D_{\text{GeCl}_4} = 6.0 \times 10^{-6} T^{1.6561}$                          | cm <sup>2</sup> /s |
| $D_{\text{SiO}_2} = 1.0 \times 10^{-10} T^{1.6561}$                          | cm <sup>2</sup> /s |
| $D_{\text{GeO}_2} = 1.0 \times 10^{-10} T^{1.6561}$                          | cm <sup>2</sup> /s |
| $D_{\text{Cl}_2} = 1.12 \times 10^{-5} T^{1.6561}$                           | cm <sup>2</sup> /s |
| $D_{\text{O}_2} = 1.76 \times 10^{-5} T^{1.6561}$                            | cm <sup>2</sup> /s |
| $c_p = 1.09$                                                                 | J/g K              |

The thermal conductivity is given by:

$$\kappa = \frac{2\mu}{\rho\bar{c}}, \quad \text{where } \bar{c} = \sqrt{\frac{8k_B T}{\pi m}}, \quad m = \frac{1}{N_A} \sum_j MW_j \left( \frac{n_j}{\sum_j n_j} \right) \quad (17)$$

where  $k_B$  is Boltzmann's constant,  $N_A$  Avogadro's number,  $MW_j$  the molar mass of species  $j$ , and  $n_j$  the mole count.

Oxidation reaction rates follow Arrhenius-type expressions [13]:

$$r_{\text{SiCl}_4} = \left( k_{\text{SiCl}_4,0} - k_{\text{SiCl}_4,1} \rho \frac{Y_{\text{O}_2}}{M_{\text{O}_2}} \right) e^{-E/RT} \rho \frac{Y_{\text{SiCl}_4}}{M_{\text{SiCl}_4}} \quad (18)$$

$$r_{\text{GeCl}_4} = k_{\text{GeCl}_4,0} e^{-E/RT} \rho^2 \left( \frac{Y_{\text{O}_2}}{M_{\text{O}_2}} \frac{Y_{\text{GeCl}_4}}{M_{\text{GeCl}_4}} - \gamma \frac{Y_{\text{GeO}_2}}{K_{eq}} \frac{Y_{\text{Cl}_2}^2}{M_{\text{Cl}_2}^2} \right) \quad (19)$$

where  $k_i$  are pre-exponential factors:  $1.7 \times 10^{14} \text{ s}^{-1}$ ,  $3.1 \times 10^{19} \text{ cm}^3/\text{mol}$ , and  $2.3 \times 10^{15} \text{ cm}^3/\text{mol}$  for  $k_{\text{SiCl}_4,0}$ ,  $k_{\text{SiCl}_4,1}$ , and  $k_{\text{GeCl}_4,0}$ , respectively;  $E$  are activation energies: 402 and 263 kJ/mol for  $\text{SiCl}_4$  and  $\text{GeCl}_4$  (see Table 1).

It is important to note that the source terms  $+r_{\text{SiCl}_4}$  and  $+r_{\text{GeCl}_4}$  in the equations for reaction products act as particle generators, while the  $-r_{\text{SiCl}_4}$  and  $-r_{\text{GeCl}_4}$  terms in the reactant equations act as mass sinks, removing species from the equations that represent the chemical reactants.

Fig. 4 illustrates the modeling of oxidation reactions across two adjacent control volumes of the computational mesh. In the upstream cell, at a local temperature  $T_1(r, \theta, \xi)$ , the chemical precursors (metal halides) and the carrier gas are assumed to be in thermal equilibrium. Upon reaching the neighboring downstream cell — at temperature  $T_2(r, \theta, \xi)$  — the oxidation reactions are triggered, leading to the consumption of reactants and formation of products as described below.

The consumption of metal halides is represented by the negative source terms  $-r_{\text{SiCl}_4}$  and  $-r_{\text{GeCl}_4}$  in Eqs. (9) and (10), respectively. Simultaneously, oxygen is consumed in proportion to:

$$-2r_{\text{SiCl}_4} \frac{M_{\text{O}_2}}{M_{\text{SiCl}_4}} - 2r_{\text{GeCl}_4} \frac{M_{\text{O}_2}}{M_{\text{GeCl}_4}}$$

as shown in Eq. (11).

The formation of oxides is modeled by positive source terms in the mass fraction equations of the products:

$$+r_{\text{SiCl}_4} \frac{M_{\text{SiO}_2}}{M_{\text{SiCl}_4}}$$

in Eq. (13), and

$$+r_{\text{GeCl}_4} \frac{M_{\text{GeO}_2}}{M_{\text{GeCl}_4}}$$

as presented in Eq. (14)

Likewise, the generation of chlorine gas is expressed by:

$$+2r_{\text{SiCl}_4} \frac{M_{\text{Cl}_2}}{M_{\text{SiCl}_4}} + 2r_{\text{GeCl}_4} \frac{M_{\text{Cl}_2}}{M_{\text{GeCl}_4}}$$

in Eq. (12).

This formulation ensures the conservation of mass and reflects the local thermochemical behavior within the porous deposition zone.

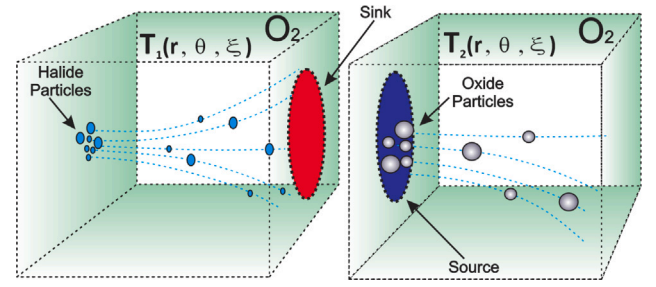


**Fig. 4.** Schematic representation of oxidation modeling in two adjacent control volumes.

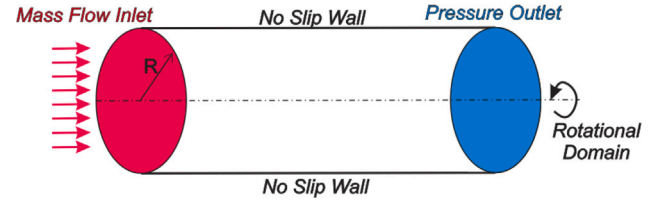


**Fig. 5.** Boundary conditions applied to the computational domain in the MCVD simulations.

### 2.3. Boundary conditions

The boundary conditions for the numerical model are defined based on the governing equations and the physical characteristics of the MCVD process. The computational domain consists of a circular tube with radius  $R$ , rotating around its longitudinal axis at an angular velocity  $\Omega$ . As a result, the velocity components vary with the radial position  $r$ , and the boundary conditions are established as follows:

(i) At  $r = R$ :

$$\omega = R\Omega, v = 0, u = 0 \quad (20)$$

$$\frac{\partial Y_{\text{SiCl}_4}}{\partial r} = \frac{\partial Y_{\text{GeCl}_4}}{\partial r} = \frac{\partial Y_{\text{O}_2}}{\partial r} = \frac{\partial Y_{\text{SiO}_2}}{\partial r} = \frac{\partial Y_{\text{GeO}_2}}{\partial r} = 0 \quad (21)$$

(ii) At  $r = 0$ : All dependent variables ( $u, v, w, Y_{\text{SiCl}_4}, Y_{\text{GeCl}_4}, Y_{\text{O}_2}, Y_{\text{SiO}_2}, Y_{\text{GeO}_2}$ ) are required to remain finite at the centerline.

Fig. 5 summarizes additional boundary conditions applied to the computational domain, as described below:

- **Inlet mass flow:** Uniform axial velocity for the reactive species introduced at the tube entrance.
- **Outlet pressure:** Gauge pressure set to zero at the tube exit.
- **No-slip tube wall:** Zero velocity imposed at the inner wall, including a temperature profile to account for heating from the external torch.
- **Tube rotation:** The effect of rotation is modeled using a moving reference frame, applied to all computational cells to simulate the rotating motion of the tube.

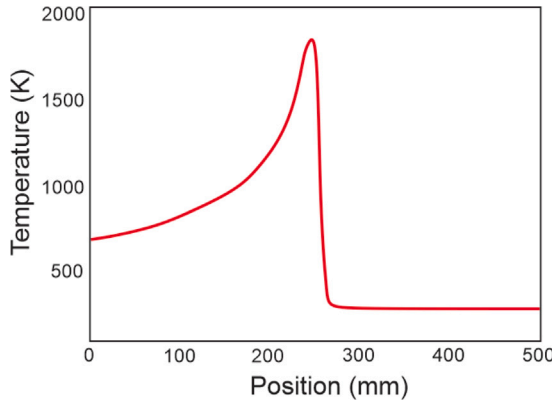
Table 2 presents the parameters adopted in the simulations. Selected parameters, such as the inlet mass flow rate and the maximum torch temperature, were varied to assess their influence on deposition efficiency.

During the MCVD process, an oxy-hydrogen torch is used to heat the rotating quartz tube, establishing a non-uniform wall temperature profile (Fig. 6). This thermal gradient is a key driver of the oxidation reaction rate and its axial distribution.

**Table 2**

Parameters used in the numerical simulations of the MCVD process [11].

| Parameter                                    | Value                                    |
|----------------------------------------------|------------------------------------------|
| SiCl <sub>4</sub> concentration at the inlet | $3.0 \times 10^{-6} \text{ mol cm}^{-3}$ |
| GeCl <sub>4</sub> concentration at the inlet | $1.9 \times 10^{-6} \text{ mol cm}^{-3}$ |
| Inlet mass flow rate                         | 2 L/min                                  |
| Maximum wall temperature                     | 1800 K                                   |
| Inner tube radius                            | 0.012 m                                  |
| Tube length                                  | 0.05 m                                   |
| Torch axial position                         | 0.025 m                                  |
| Tube rotation speed                          | 45 rpm                                   |
| Inlet Gas temperature                        | 300 K                                    |
| Torch speed                                  | 20 cm/min                                |

**Fig. 6.** Temperature profile along the inner wall of the quartz tube due to external heating.

Source: Adapted from [14].

### 3. Numerical procedure

#### 3.1. Domain discretization

The partial differential equations governing mass, momentum, energy, and chemical species transport are discretized using second-order schemes. The solution is carried out in a coupled manner using two numerical approaches: the Finite Volume Method (FVM), implemented via the CFD code StarCCM+, and the Finite Difference Method (FDM), implemented in MATLAB. It is important to note that the transport equations for the chemical species are solved using the thermodynamic properties computed for the carrier gas, that is, the velocity, pressure, temperature, and density fields.

One of the key differences between these numerical schemes lies in the discretization strategy: FVM integrates the conservation equations over control volumes centered around the mesh cells, whereas FDM approximates derivatives at discrete mesh points.

#### 3.2. Computational meshes

The computational grids used to describe the physical domain and solve the governing equations are shown in Fig. 7. The mesh used for the Finite Volume Method (FVM) was generated using StarCCM+, consisting of approximately 980,000 hexahedral cells, with characteristic sizes ranging from  $10^{-5}$  m to  $10^{-3}$  m. To accurately capture near-wall effects, 30 prism layers were adopted along the wall of the tube to resolve the boundary layer dynamics. In contrast, the mesh adopted for the Finite Difference Method (FDM) was generated in MATLAB using a structured discretization of  $100 \times 50 \times 50$  points, resulting in a regular hexahedral grid.

In order to improve the accuracy of the numerical predictions, particularly in the presence of coupled hydrodynamic and thermal effects,

the height of the first prism layer adjacent to the wall was defined to ensure a non-dimensional wall distance ( $y^+$ ) close to unity. This parameter, widely employed in CFD studies, is essential to adequately resolve the viscous and thermal boundary layers, and can be expressed as:

$$y^+ = \frac{yu_\tau}{\nu} \quad (22)$$

where  $y$  is the distance from the wall,  $\nu$  is the kinematic viscosity, and  $u_\tau$  is the friction velocity, defined by:

$$u_\tau = \sqrt{\frac{\tau_w}{\rho}} \quad (23)$$

in which  $\tau_w$  is the wall shear stress and  $\rho$  is the fluid density.

Although the flow regime is laminar, thermal gradients require accurate resolution of the wall region, where heat transfer takes place.

#### 3.3. CFD simulation setup

The CFD simulations were performed in StarCCM+ using the following physical models:

- *Steady*: Steady-state flow regime;
- *Ideal Gas*: Governing equation of state based on the ideal gas law;
- *Coupled Flow*: Coupled solution of the momentum and energy equations;
- *Multi-Component Gas*: Treatment of all chemical species as gas-phase components;
- *Reacting*: Chemical reaction model applied to the oxidation of halides;
- *Eddy Break-Up*: Turbulence-chemistry interaction model introducing a source term for reaction rate modeling;
- *Discrete Element Method*: Model for Lagrangian tracking of particle trajectories;
- *Lagrangian Multiphase*: Model used to simulate the transport and interaction of oxide particles with the carrier gas;

#### 3.4. Solution of the flow and chemical species transport equations

The conservation equations for mass, momentum, energy, and chemical species were solved sequentially. First, the continuity and momentum equations were solved to obtain the carrier gas velocity and pressure fields. The energy equation was then resolved to compute the temperature distribution within the tube.

The temperature field was subsequently used to evaluate the thermophoretic velocity, which was superimposed onto the carrier gas velocity to form the total transport velocity. This combined velocity field was employed both for Lagrangian particle tracking and for solving the species transport equations, allowing the prediction of particle trajectories and reactant/product concentration fields.

Particle motion was modeled using a one-way coupled Lagrangian approach, accounting for thermophoretic and hydrodynamic drag forces. The thermophoretic force  $F_T$  was evaluated using the model proposed by [8]:

$$F_T = -12 \frac{\pi \mu^2 r_p}{\rho} K \frac{\nabla T}{T} \quad (24)$$

where  $r_p$  is the particle radius,  $\mu$  the gas dynamic viscosity,  $\rho$  the gas density,  $T$  the local temperature, and  $K$  the thermophoretic coefficient defined in Eq. (16).

The drag force  $F_D$  was computed using the Stokes formulation with Millikan slip correction:

$$F_D = \frac{6\pi\mu r_p(v_p - v_g)}{\left[1 + \frac{\lambda}{r_p} \left(A + Be^{-\frac{Cr_p}{\lambda}}\right)\right]} \quad (25)$$

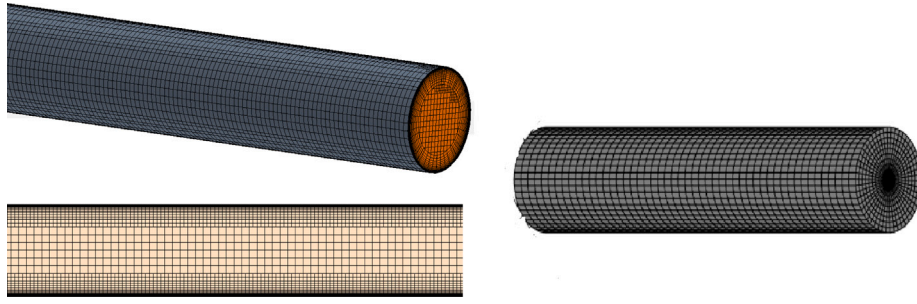


Fig. 7. Computational meshes generated using StarCCM+ (left) and MATLAB (right).

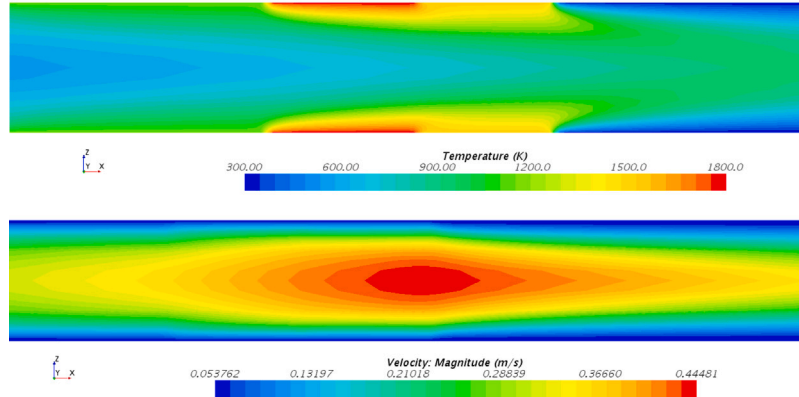


Fig. 8. Temperature (top) and axial velocity (bottom) fields of the carrier gas computed using the Finite Volume Method (FVM).

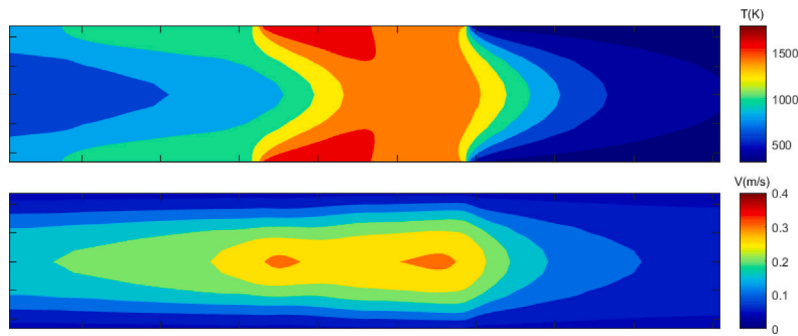


Fig. 9. Velocity and temperature fields computed using the Finite Difference Method (FDM).

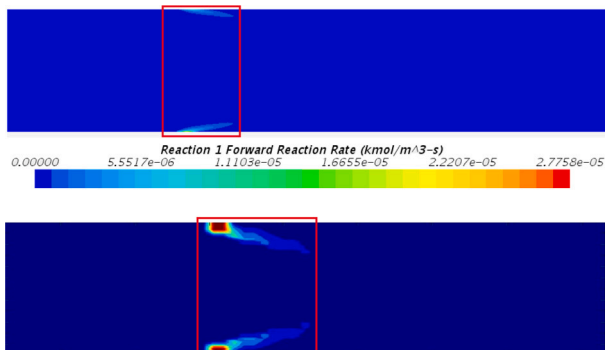


Fig. 10. Oxidation reaction rate of  $\text{SiCl}_4$  obtained by CFD (top) and FDM (bottom). The red rectangles indicate the primary oxidation zones.

where  $v_p$  and  $v_g$  denote the particle and gas velocities, respectively,  $\lambda$  is the gas mean free path, and  $A$ ,  $B$ , and  $C$  are empirical constants.

The particle velocity was obtained by integrating Newton's second law:

$$m \frac{dv_p}{dt} = F_T + F_D \quad (26)$$

Once the flow and temperature fields were established, particle trajectories and deposition patterns along the inner tube wall were computed. Combined with the predicted species concentration fields, this framework enables the estimation of deposition efficiency and the identification of preferential deposition regions.

## 4. Results

### 4.1. Velocity and temperature fields

The velocity and temperature fields of the carrier gas inside the tube were obtained by solving the governing Eqs. (4), (5)–(7), and

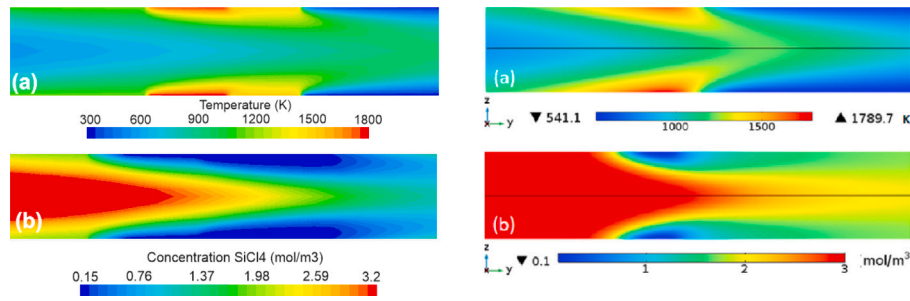


Fig. 11. Qualitative comparison of spatial field structures between the present CFD results (left) and those reported by [14] (right) for (a) temperature field and (b)  $\text{SiCl}_4$  concentration distribution.

(8). Figs. 8 and 9 show the results obtained using the Finite Volume Method (FVM) and the in-house Finite Difference Method (FDM), respectively.

Both numerical approaches predict the same global structure of the flow and thermal fields. The temperature distributions reveal a localized high-temperature region induced by the external burner, with similar axial and radial spreading in both solutions. Minor differences are observed in the sharpness of the axial temperature gradient, with the FDM solution exhibiting a slightly more confined thermal front, which can be attributed to differences in discretization schemes, numerical diffusion, and wall boundary treatment.

The velocity fields exhibit the expected parabolic laminar profile in a cylindrical duct, with maximum axial velocity along the centerline. Although the FVM predicts slightly higher peak velocities near the axis, both methods produce velocity magnitudes of the same order and capture the same qualitative flow features.

Since the subsequent particle transport and deposition analyses depend primarily on integrated flow behavior and dominant force balances, these local differences between FVM and FDM do not affect the physical interpretations presented in this study.

#### 4.2. Halide oxidation

Halide oxidation was analyzed using both FVM and FDM, with emphasis on the identification of oxidation zones and qualitative trends in oxide formation rather than strict quantitative agreement. The approaches predict a localized oxidation region associated with the high-temperature zone imposed by the external burner, which defines the onset of oxide particle formation and serves as the basis for subsequent Lagrangian particle-tracking analysis.

As shown in Fig. 10,  $\text{SiCl}_4$  oxidation occurs in comparable axial locations for both methods, although the FDM solution exhibits a slightly downstream-shifted reaction zone and higher peak reaction rates.

These discrepancies are primarily attributed to numerical effects, including differences in discretization, convective treatment, and numerical diffusion. While the CFD solver employs higher-order schemes and enhanced stabilization near steep gradients, the in-house FDM relies on a structured grid with fixed resolution, which may lead to sharper and displaced reaction fronts.

Fig. 11 presents a qualitative comparison of the predicted temperature and  $\text{SiCl}_4$  concentration fields with results reported by [14]. Despite differences in numerical formulation, boundary conditions, and parameter ranges, the temperature field shows similar spatial topology and axial localization of the reaction zone. Larger deviations observed in near-wall  $\text{SiCl}_4$  concentration are attributed to differences in chemical kinetics modeling and numerical implementation.

Figs. 12 and 13 show the spatial distributions of  $\text{GeO}_2$  and  $\text{SiO}_2$  concentrations, respectively. In both cases, higher oxide concentrations are observed near the tube wall and in the vicinity of the burner, consistent with elevated local temperatures. Cross-sectional profiles

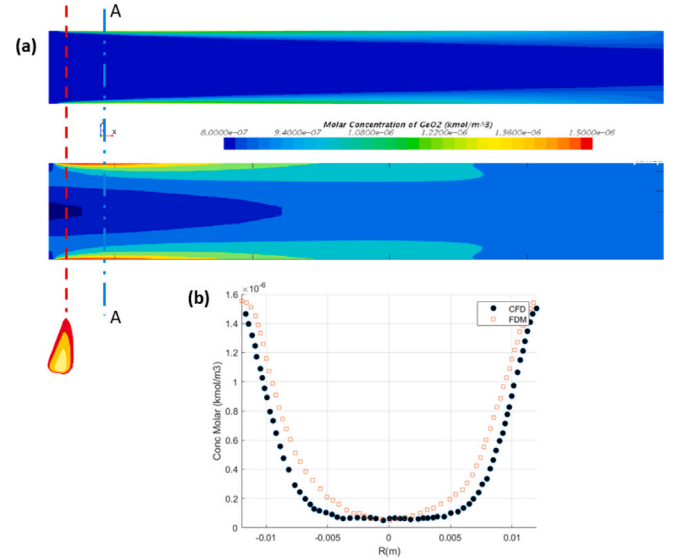


Fig. 12. (a)  $\text{GeO}_2$  concentration field obtained by CFD (top) and FDM (bottom); (b) comparison along cross-section AA. The red dashed line denotes the burner position.

along plane AA indicate higher peak concentrations predicted by the FDM approach.

The higher oxide concentrations predicted by the FDM are mainly associated with the downstream-shifted oxidation zone and reduced numerical diffusion, which preserves sharper concentration gradients. In contrast, the FVM solution yields smoother profiles due to stronger numerical stabilization and tighter coupling between flow, heat transfer, and species transport. Overall, oxide formation initiates at the leading edge of the oxidation zone and is subsequently transported downstream by the carrier gas flow, highlighting the coupled nature of reaction kinetics and convective-diffusive transport.

#### 4.3. Deposition efficiency

The deposition efficiency was evaluated following the approach proposed by [5], based on species mass conservation and the thermophoretic transport of oxide particles toward the tube wall. The deposition efficiency is defined as the ratio between the cumulative mass flux of deposited oxides and the inlet mass flux of halide precursors.

The inlet mass flux of halides is given by

$$\Phi = \rho u_0 Y_0 \pi R^2, \quad (27)$$

where  $u_0$  is the axial velocity,  $Y_0$  is the inlet halide mass fraction,  $\rho$  is the gas density, and  $R$  is the tube radius.

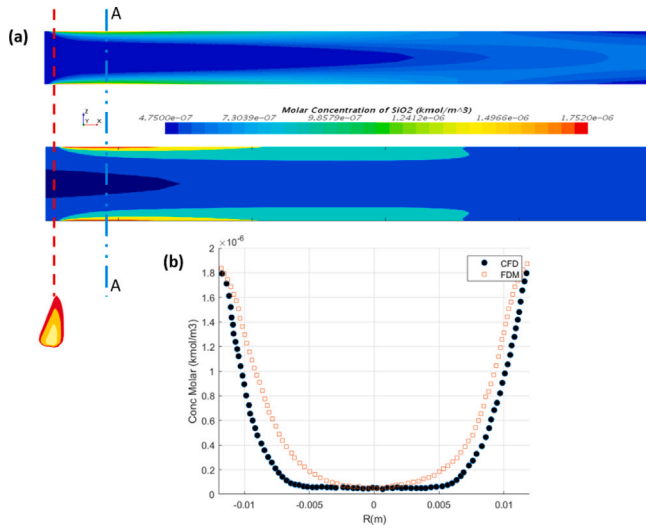


**Fig. 13.** (a) SiO<sub>2</sub> concentration field obtained by CFD (top) and FDM (bottom); (b) comparison along cross-section AA. The red dashed line indicates the burner position.

The local deposited mass flux is computed considering only the positive radial component of the thermophoretic velocity near the wall (Fig. 14). The infinitesimal deposited flux over a wall element  $2\pi R d\xi$  is expressed as

$$d\Phi = \begin{cases} 2\pi R \rho v_T(\xi, R) Y(\xi, R) d\xi, & \vec{v}_T \cdot \vec{r} > 0, \\ 0, & \vec{v}_T \cdot \vec{r} \leq 0. \end{cases} \quad (28)$$

The cumulative deposition efficiency up to an axial position  $\xi$  is defined as

$$E(\xi) = \frac{1}{\rho u_0 Y_0 \pi R^2} \int_0^\xi d\Phi. \quad (29)$$

The thermophoretic velocity field required for this evaluation was computed from the local temperature gradients according to Eq. (15). The resulting radial thermophoretic velocity field, expressed in SI units

(m s<sup>-1</sup>), is shown in Fig. 15. Maximum values are observed near the wall in the burner region, while thermophoretic effects are negligible in the tube core.

Using the computed thermophoretic velocity and species concentration fields, the deposition efficiencies of SiO<sub>2</sub> and GeO<sub>2</sub> were evaluated. Fig. 16 presents the cumulative deposition efficiency as a function of the dimensionless axial coordinate  $\xi = x/L$ . The results show consistently higher efficiencies for SiO<sub>2</sub> compared to GeO<sub>2</sub>, reflecting differences in oxidation kinetics and precursor conversion. CFD-based predictions yield slightly higher efficiencies than FDM, which may be attributed to differences in numerical discretization and spatial resolution.

Deposition efficiency increases markedly around  $\xi \approx 0.4$ , indicating the onset of deposition slightly upstream of the burner position. The predicted efficiency levels are consistent with values reported in the literature for MCVD processes [15].

#### 4.4. Effect of torch temperature on deposition efficiency

The influence of the peak external torch temperature on the cumulative deposition efficiency of SiO<sub>2</sub> and GeO<sub>2</sub> was investigated for a constant inlet mass flow rate ( $\Phi = 2 \text{ L}\cdot\text{min}^{-1}$ ). Three peak temperatures were considered: 1600 K, 1800 K, and 1900 K. The resulting temperature distributions along the longitudinal mid-plane are shown in Fig. 17.

Subsequently, the cumulative deposition efficiencies were evaluated for each temperature scenario. The results are presented in Figs. 18 and 19, corresponding to the SiO<sub>2</sub> and GeO<sub>2</sub> deposition, respectively. A clear trend is observed: higher torch temperatures lead to enhanced deposition efficiency across the axial coordinate  $\xi$ . This behavior may be attributed to two combined effects: the increased oxidation reaction rates at elevated temperatures and the enhancement of thermophoretic forces due to steeper temperature gradients, which drive more precursor particles toward the inner wall.

#### 4.5. Effect of mass flow rate on deposition efficiency

To further investigate the parameters influencing deposition efficiency, a parametric analysis was conducted by varying the inlet mass flow rate while maintaining constant the relative proportions

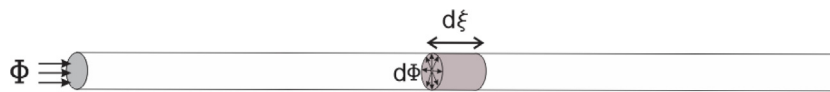


**Fig. 14.** Schematic representation of the inlet halide mass flux  $\Phi$  and the local deposited mass flux  $d\Phi$  on an infinitesimal wall element  $d\xi$ .

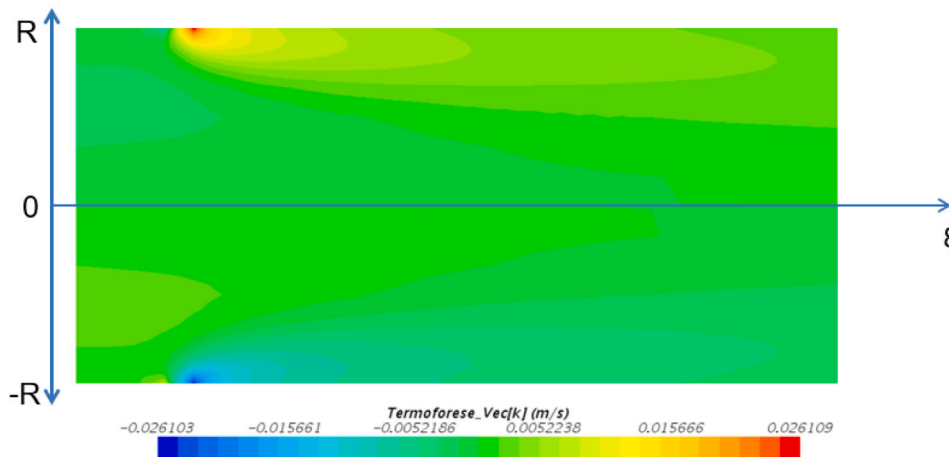


**Fig. 15.** Radial thermophoretic velocity field obtained via CFD (in m s<sup>-1</sup>).

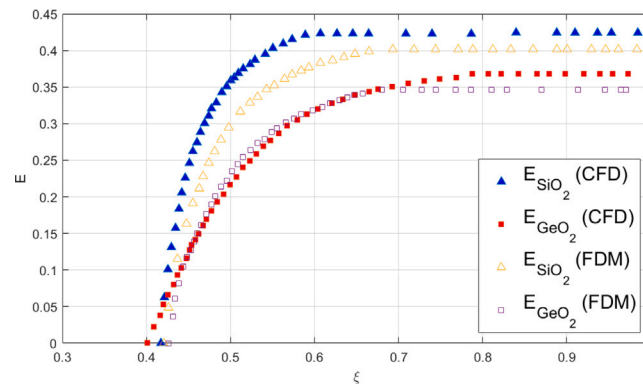


Fig. 16. Cumulative deposition efficiencies of  $\text{SiO}_2$  and  $\text{GeO}_2$  computed using CFD and FDM along the dimensionless axial coordinate  $\xi$ .

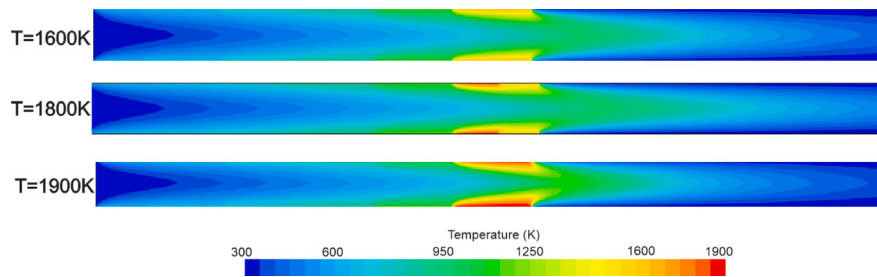


Fig. 17. Temperature fields computed via CFD for each maximum torch temperature.

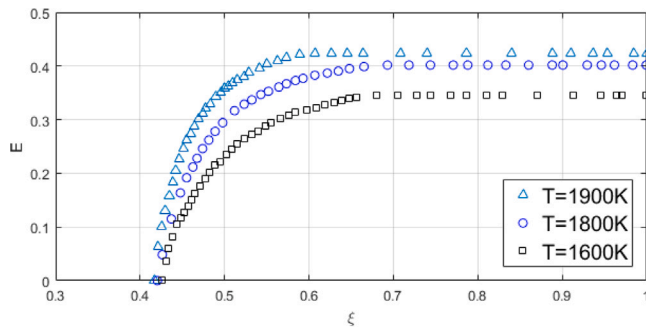


Fig. 18. Effect of peak torch temperature on the cumulative deposition efficiency of  $\text{SiO}_2$  along the dimensionless axial position  $\xi$ .

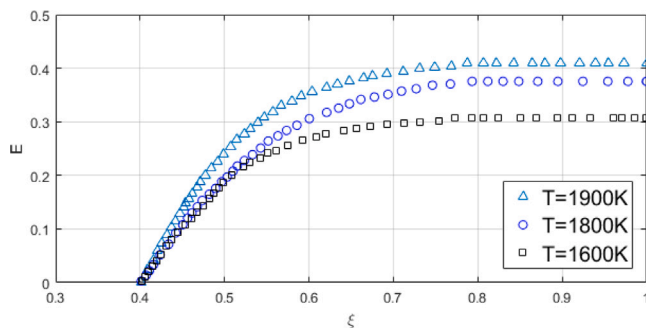


Fig. 19. Effect of peak torch temperature on the cumulative deposition efficiency of  $\text{GeO}_2$  along the dimensionless axial position  $\xi$ .

of chemical precursors and a fixed maximum torch temperature of 1800 K. Two volumetric flow rates were evaluated:  $\Phi_1 = 2 \text{ L}\cdot\text{min}^{-1}$  and  $\Phi_2 = 3 \text{ L}\cdot\text{min}^{-1}$ . The resulting deposition efficiency profiles for  $\text{SiO}_2$  and  $\text{GeO}_2$  are depicted in Figs. 20 and 21, respectively. The analysis reveals an inverse relationship between mass flow rate and deposition

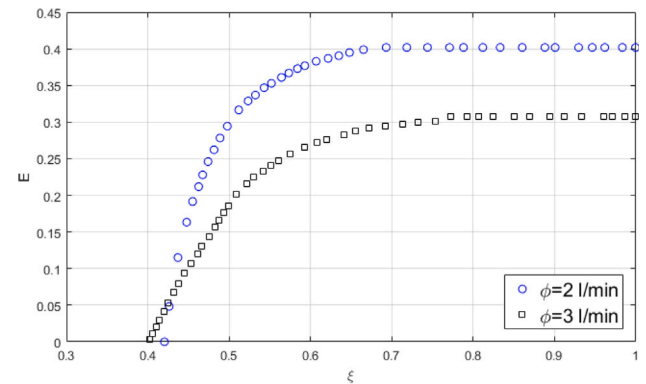


Fig. 20. Effect of inlet mass flow rate on the cumulative deposition efficiency of  $\text{SiO}_2$  along the dimensionless axial coordinate  $\xi$ .

efficiency. This phenomenon, also reported by [15], can be explained by the competing effects of thermophoresis and residence time. While higher flow rates intensify radial temperature gradients—potentially enhancing thermophoretic velocities, they also accelerate the gas-phase transport, reducing the residence time available for particle deposition and thereby increasing particle losses through the outlet.

#### 4.6. Particle trajectory prediction

Particle transport and deposition during the MCVD process were predicted using a Lagrangian tracking approach. Particle motion was computed by integrating the total velocity field, defined as the superposition of the carrier gas velocity and the thermophoretic drift induced by local temperature gradients. Deposition was assumed to occur when particle trajectories intersect the inner tube wall, a criterion commonly adopted in engineering-scale aerosol transport models and physically justified under MCVD conditions, where strong thermophoretic forces dominate and particle rebound is negligible.

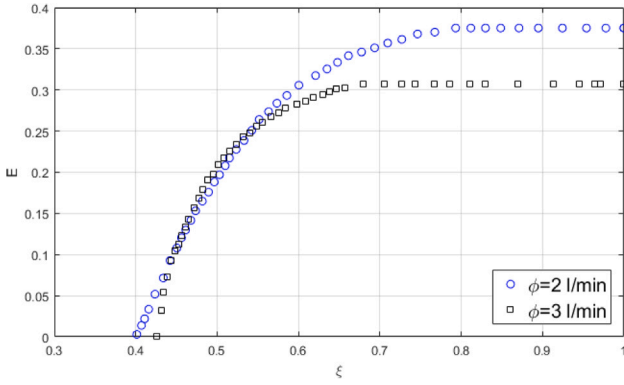


**Fig. 21.** Effect of inlet mass flow rate on the cumulative deposition efficiency of  $\text{GeO}_2$  along the dimensionless axial coordinate  $\xi$ .

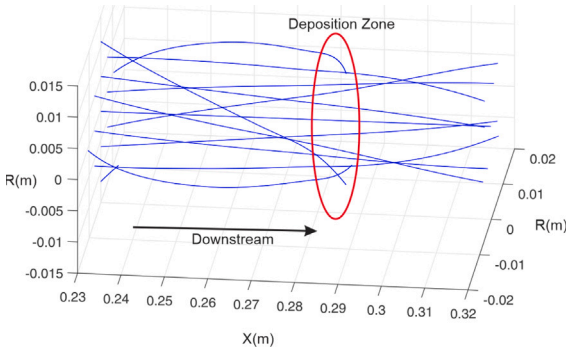


**Fig. 22.** Particle trajectories computed using the FDM approach. The red ellipse highlights the deposition region where particles reach the inner wall.

Oxide particles were modeled as spherical with a constant diameter of  $d_p = 1 \mu\text{m}$  throughout the analysis. This size is representative of oxide particles typically formed in MCVD oxidation zones [3,12]. Under these conditions, the Knudsen number spans the continuum-to-transition regime and is treated consistently in both Eulerian and Lagrangian formulations, as discussed in Section 2.

Particle trajectories  $\vec{r}_i$  were computed using a second-order Runge-Kutta integration scheme:

$$\vec{r}_{i+1} = \vec{r}_i + \frac{1}{6} \Delta t \vec{v}_i + \frac{1}{3} \Delta t \vec{v}_{i+1}, \quad (30)$$

where  $\vec{v}_{i+1} = \vec{v}_i + \frac{1}{2} \Delta t \nabla \vec{v}_i$ , and  $\Delta t$  is a pseudo-time step used exclusively for trajectory integration.

Trajectories were computed using velocity fields obtained from both FDM and FVM simulations. Particles were released at the onset of the oxidation zone identified in Fig. 10, enabling the identification of deposition regions along the inner tube wall.

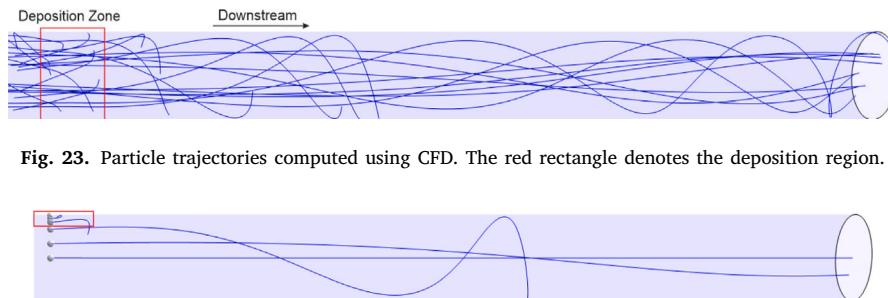


**Fig. 23.** Particle trajectories computed using CFD. The red rectangle denotes the deposition region.

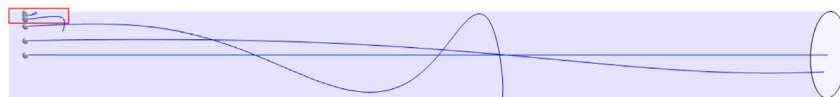


**Fig. 24.** Effect of initial radial position on CFD particle trajectories. The red rectangle highlights the region between 90% and 100% of the inner tube radius where deposition occurs.

Fig. 22 shows particle trajectories computed using the FDM approach, with deposition initiating near  $x = 0.28 \text{ m}$ . Considering a total tube length of  $0.5 \text{ m}$  and a torch centered at  $x = 0.25 \text{ m}$ , deposition begins shortly downstream of the heated region.

CFD-based trajectories, shown in Fig. 23, indicate deposition onset near  $x = 0.27 \text{ m}$ , in close agreement with the FDM results. Non-depositing particles follow helical paths due to the imposed rotational motion of the tube.

The influence of the initial radial position was further investigated by releasing particles at the same axial location and varying radial distances (Fig. 24). Particles injected beyond 90% of the tube radius were efficiently deposited, whereas particles originating closer to the center were transported downstream with minimal influence from rotational motion.

Particle growth, coagulation, and size polydispersity were not considered in the present formulation. While these effects may influence deposition under specific conditions, the constant-diameter assumption allows isolation of the dominant transport mechanisms — namely thermophoresis and convection — without introducing additional modeling uncertainty. Incorporation of particle size distributions is left for future work.

## Conclusion

This work presented a numerical investigation of the MCVD process using a Finite Volume Method implemented in a commercial CFD solver and an in-house Finite Difference Method. The comparison between both approaches aimed at assessing the consistency of global transport features and dominant physical mechanisms governing heat transfer, species transport, and particle deposition, rather than local pointwise agreement.

Despite local differences in the predicted velocity and temperature fields, both numerical formulations reproduced the same qualitative structure of the flow and thermal fields and yielded comparable orders of magnitude for the relevant transport quantities. The conclusions of this study rely on integral and mechanism-based metrics, which were found to be robust with respect to the adopted numerical approach.

The results emphasized the importance of thermophysical properties and kinetic parameters, particularly for the oxidation of  $\text{GeCl}_4$ , which remains a major source of uncertainty in MCVD modeling. Even under these limitations, the predicted deposition efficiencies lie within the range reported in the literature, and the trends with respect to flame temperature and precursor mass flow rate are consistent with previous experimental and numerical studies.

By combining convective transport with thermophoretic drift induced by strong radial temperature gradients, the particle-tracking framework enabled the identification of preferential deposition regions and confirmed the dominant role of thermophoresis in driving oxide particles toward the heated substrate under typical MCVD operating conditions.

The simplifying assumptions adopted in the model, including monodisperse particles with fixed diameter and an adiabatic tube wall, affect the quantitative interpretation of the results but do not alter the main physical conclusions. The predicted deposition efficiency should therefore be interpreted as representative of an effective particle size, while the dominant thermal gradients imposed by the external burner are expected to remain the primary driver of deposition behavior.

Future developments will focus on incorporating wall heat conduction, particle size distributions, and more realistic geometrical features, as well as on further assessing the sensitivity of local fields to numerical discretization while preserving the robustness of the predicted deposition trends.

#### CRedit authorship contribution statement

**Rubens Cavalcante da Silva:** Writing – review & editing, Writing – original draft. **Davi Pontes Nacaratti:** Writing – review & editing. **Elbis Santos Cardoso:** Writing – review & editing. **Paulo Jorge Duda de Morais:** Writing – review & editing, Software. **Wagner de Rossi:** Writing – review & editing, Supervision.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

#### Data availability

Data will be made available on request.

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