

## **Response to the comments of the reviewers**

I thank the referee for their insightful comments. I have greatly benefited from the comments, and the response to all comments is provided here. All the comments of the reviewer are retyped below in bold while the responses are given in normal font, and the changes in the thesis are highlighted in yellow.

### **Examiner 1**

#### Major Issues:

**Q.1. In section 4.5, validation of the simulation is conducted by comparing its predictions with the results of an experiment. The full geometry of the reactor with dimensions and a list of relevant properties of the reactor material and gaseous medium inside the reactor should be revealed somewhere, perhaps in an appendix. (For example, the coefficient of thermal conductivity. Also tell how the coefficient of convective heat transfer,  $h$ , was determined. Also, give details of the flow type boundary conditions implemented at the inlets and outlets of the gases. Where and how were the boundary conditions associated with the heating of the reactor implemented? All this information is necessary in case some reader wants to redo the simulation and experiments. If the reactor was supplied by a company and there is a product number associated with it, then that also should be revealed. Also, section 4.5 should be presented before starting the discussion on results since one wants to see the accuracy of the simulation before launching the discussion of numerical results.**

The full geometry of the reactor with dimensions and a list of relevant properties of the reactor material and gaseous medium inside the reactor, coefficient of convective heat transfer, and boundary condition are mentioned in Appendix A (page no. 83-87). Section 4.5 is now presented before starting the discussion on results in the revised section 4.1 (Page no. 62).

**Q.2. Give details of how all the equations listed in Table 3.1 were solved in ANSYS Fluent. If user-defined functions were used, give their details.**

The built-in chemical kinetics models in ANSYS Fluent were used to solve the gas-phase reactions. All species involved in the reactions were added to Fluent's species transport model, and each reaction from Table 3.1 was added to Fluent's Reaction Editor, specifying the reactants, products, and kinetic parameters.

**Q.3. It is not clear how the ML-based optimization was implemented in practical terms. Was it done within the commercial software Fluent, or externally using some other code?**

**These details are missing and should be provided. The practical aspects of the implementation of the algorithm are shown in Fig. 3.3.**

The ML-based optimization for the study was implemented externally using custom code rather than directly within the commercial software ANSYS Fluent. This model was integrated with a parameterization study and optimization algorithm (Nelder-Mead) to refine the input parameters and achieve optimal conditions. The details of the code written in R are given in Appendix B (page no. 88).

**Q.4. Some terms are intriguing and confusing. For example, what is the deposition rate? What is the uniformity index? A glossary defining such terms along with the SI units involved should be furnished. In the same vein, a list of all mathematical symbols used along with their units should be presented right in the beginning.**

The average rate of deposition (RD) and uniformity index (UI) was calculated as:

$$\overline{RD} = \frac{\int RD dA}{A}$$

$$UI = \frac{\int |RD - \overline{RD}| dA}{A}$$

where A is the total area of the substrate (page no. 48). A list of special or unusual words and their meanings are given in nomenclature at the beginning of the thesis (page no. xi) and glossary defining such terms is added (page no. 98).

**Q.5. Wherever possible, the printouts of the codes used in the simulation should be attached as appendices. This will not only bring authenticity to the work but will also be helpful to anyone planning to replicate the results.**

The code details regarding the support vector machine and Nelder-Mead algorithm, written in R, are provided in Appendix B (page no. 88).

**Q.6. In the mesh refinement study, some more details are needed. For example, convergence of which variables were monitored?**

The grid independence study was also performed by varying the number of elements from 2,012,374 to 2,952,435 in various steps. In this study, several key variables including velocity, temperature, C<sub>2</sub>H<sub>2</sub> concentration and deposition rate were monitored for convergence to

determine the adequacy of the mesh. To this end, the convergence of the above-mentioned variables at various critical points in the domain was closely monitored. This included points near the inlet, outlet, and regions with high gradients to ensure an accurate representation of the flow field. It was found that the relative increase in the cell values abovementioned was <1% after 2,360,910 elements (pages 52, 53).

### **Q.7. How was it ensured that the computations converged? What criteria were used?**

The following points summarize the approach and criteria used to ensure computational convergence in the present study:

- i) *Residual Monitoring*: The residuals of the governing equations (continuity, momentum, energy, and species transport) were closely monitored. Convergence was deemed achieved when all residuals fell below  $10^{-3}$ .
- ii) *Key Variable Monitoring*: Specific variables such as velocity, temperature,  $C_2H_2$  concentration, and deposition rate were tracked to ensure they reached steady-state values.
- iii) *Mass and Energy Conservation*: The overall mass and energy entering and leaving the system were checked to ensure they balanced within an acceptable tolerance, preventing unphysical accumulation or depletion. By adhering to these criteria, I ensured the accuracy and reliability of the computational results. (page 58)

### **Minor Issues:**

#### **1) What is the full form of slm, the units used for flow rate? Use SI units.**

SLM, Standard litre per minute is a unit of volumetric flow rate, specifically, it is commonly used to express the flow rate of gases under standard conditions of temperature and pressure.  $1\text{slm} = 1.67 \times 10^{-5} \text{ m}^3/\text{s}$ . (page 69).

#### **2) Explain how distance was normalized in Fig. 4.2.**

The vertical distance mentioned in Fig. 4.2 is normalised by the total distance of the substrate containing four plates (page 63).

#### **3) Explain how Grashoff and Reynolds numbers are estimated in Fig. 4.6. (For example, which temperature differences and velocities were used in the estimation? How and at what temperatures were the properties of gases estimated?)**

The Reynolds number was calculated based on the reactor diameter, while the Grashof number was calculated using the vertical distance from the first plate. A cross-sectional average of

velocity and concentration was used to estimate the various dimensionless numbers. The difference between the inlet temperature and the averaged temperature at a given cross-sectional position was used to calculate the Grashof number (page 66).