Simulation of CVD Process in a Reactor

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INTRODUCTION:

Steel tools which are used in industrial high-throughout processes like injection molding, are susceptible for wear and corrosion due to rapid cyclic temperature and pressure fluctuation as well as the use of abrasive polymers. Chemical vapor deposition (CVD) offers the opportunity of depositing thin layers intending to protect, ennoble or functionalize given surfaces. Compared with other coating techniques CVD enables homogeneous layer thickness distribution even on highly complex surface geometries [1].
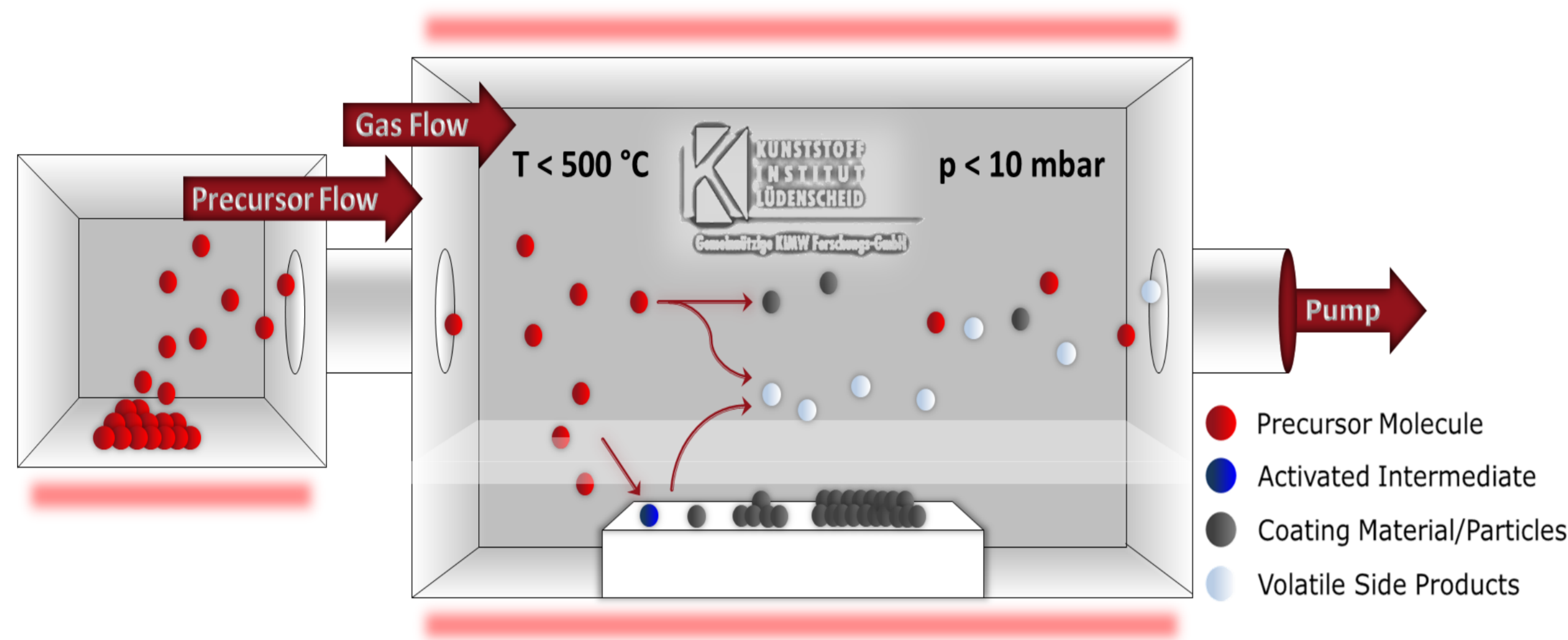

Figure 1. Schematic representation of CVD process (KIMW-F)

High quality tool surfaces can be achieved with CVD techniques. Such coating layers are able to thermally insulate the tool surface providing a more precise temperature regulation with intent to avoid the formation of surface flaws, e.g. weld lines in plastic fabricated parts. At the same time it enables shortening of cycle times as well as decrease of energy demands during molding processes [2]. The main aim of this work is to figure out how the test specimens and the tool inserts to be coated have to be arranged in the reactor so that the coating is homogeneously distributed on the functional surface. The influence of gas flow, temperature, and pressure on the flow behavior within the reactor and around and through the specimen can be simulated with COMSOL Multiphysics®.

COMPUTATIONAL METHODS:

The process parameters used for the real coating experiments are in the range of Re<2000 (Reynolds Number) hence the laminar flow was considered for the computation. The laminar flow is based on the Navier Stokes equation:

$$\rho\left(\frac{\partial u}{\partial t} + (u \cdot \nabla)u\right) = -\nabla p + \nabla \cdot \left[\mu\left(\nabla u + (\nabla u)^{\mathrm{T}} - \frac{2}{3}(\nabla \cdot u)\mathbf{I}\right)\right] + F$$

$$\frac{\partial p}{\partial t} + \nabla \cdot (\rho u) = 0$$
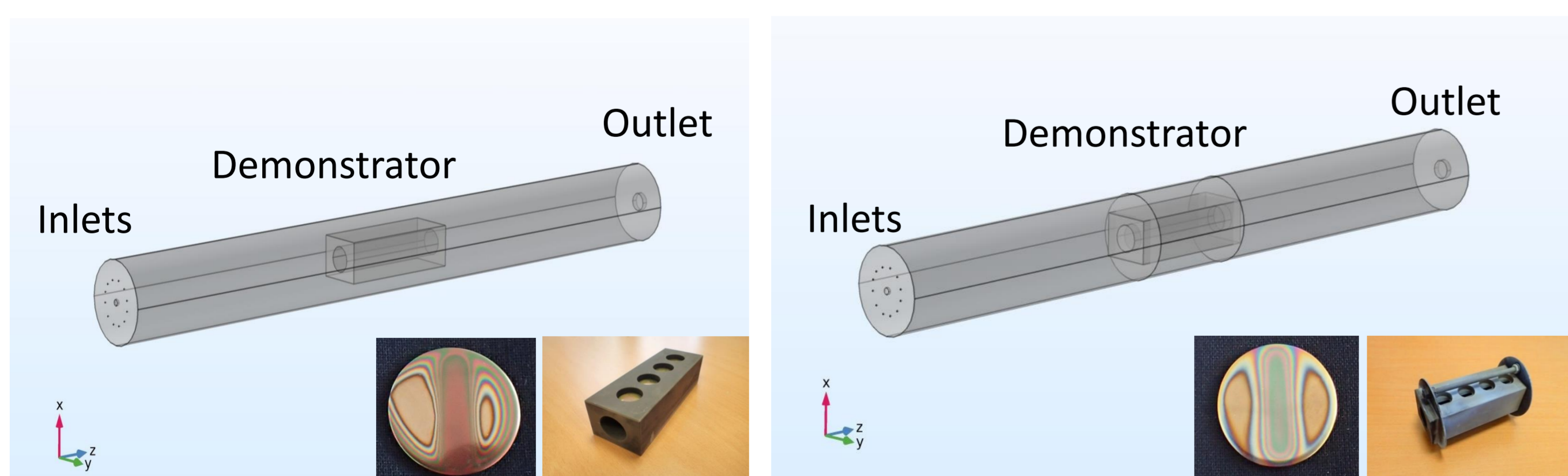
$$\rho = \rho(p, T)$$

Figure 2. Simulation geometry, specimens and real CVD reactor

RESULTS:

To develop an optimized arrangement of the specimens in the gas flow as well as to enhance the coating efficiency and layer thickness distribution, a demonstrator was developed with which the thickness of coating at the inner surface of the tool could be determined. Therefore small metal plates can be placed into the demonstrator, so that they are part of the inner surface and are coated as well. The plates can then be used to determine coating layer thickness distribution at the inner surface of the demonstrator (figure 2). Different geometries were evolved and used for simulation as well as for the experiments. In so doing, a comparison between the gas flow within the reactor and the resulting coating thickness on the specimens after the process was feasible. Figure 2 represents the reactor geometry considering the demonstrator without plate (left) and with plate (right). Due to the gas flow from the inlets a high amount of swirls (figure 3) are developed in the front area of the reactor. To optimize the coating on the inside of the cylindrical cavity a plate was installed around the demonstrator forcing the whole gas to stream through the cavity. Thus the gas velocity inside the demonstrator increases dramatically (figure 5) and the activated molecules have less time to react with the surface and to reach small slits, which becomes obvious regarding the flow pattern on the specimens (figure 2) and the gas velocities (figures 4 and 5).
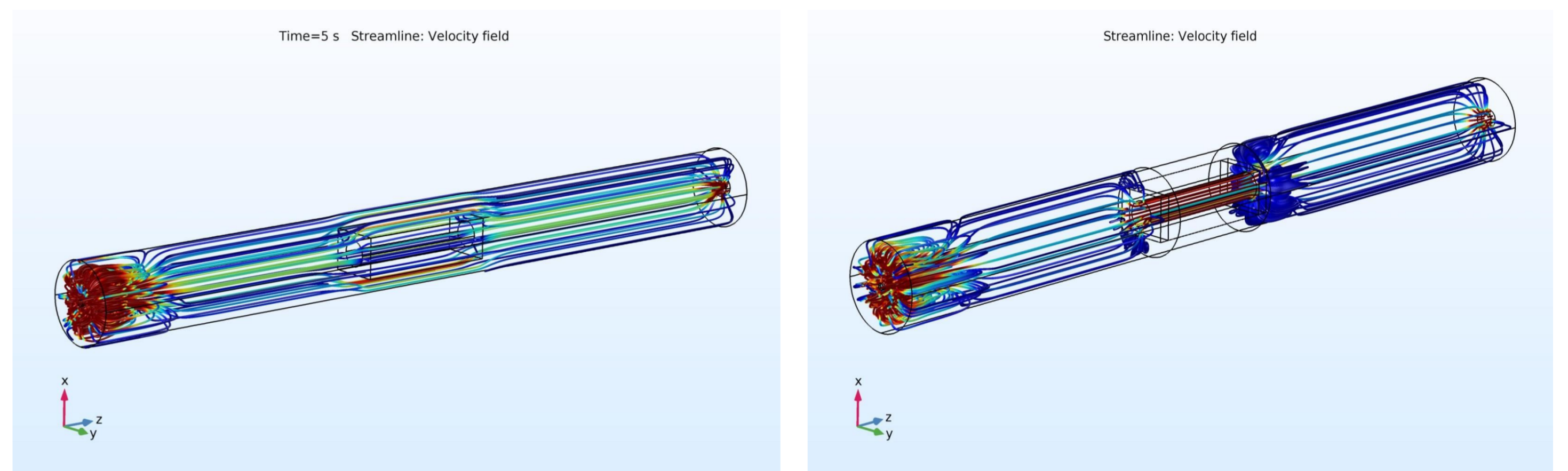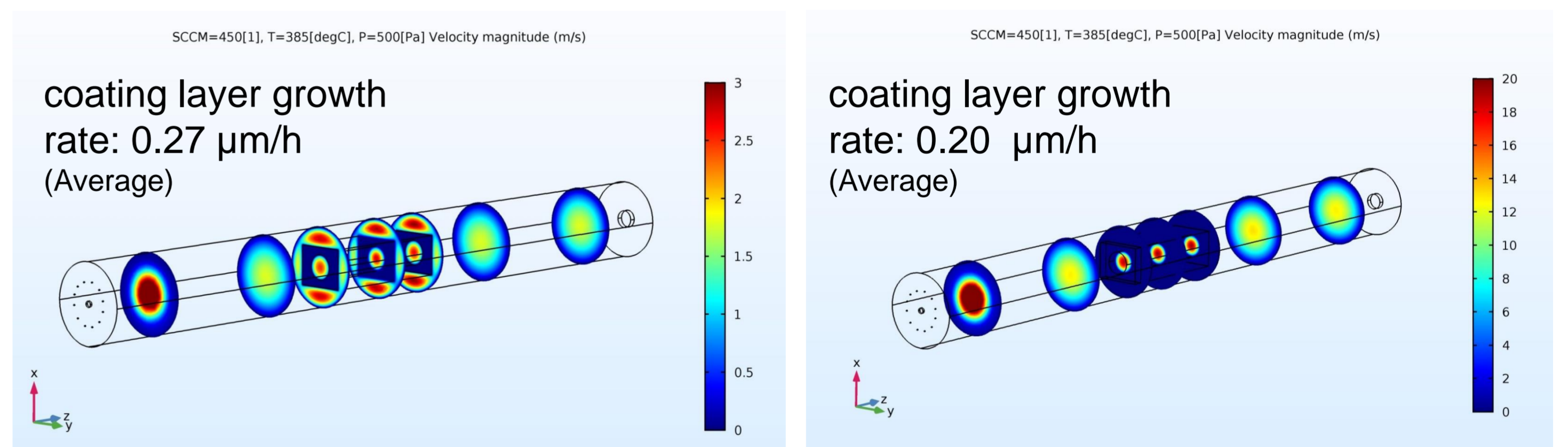

Figure 3. Velocity streamlines (refer scale figure 4)
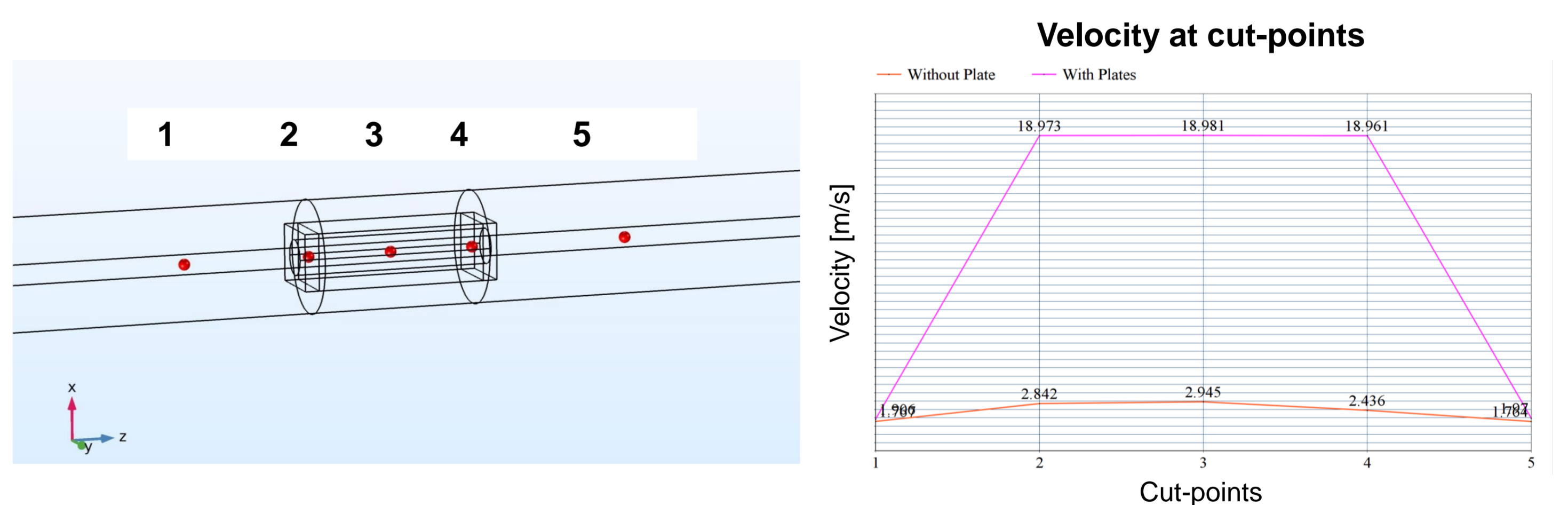

Figure 4. Velocity cut-sections

Figure 5. Velocity values with plate at cut-points (1-5)

CONCLUSIONS:

Simulation results show the differences in velocity range due to volume reduction. Since the molecules have shorter time to react, the growth rate of the coating is reduced (figure 4). By implication, the amount of gas used can be reduced, reaching decreased gas velocities and therefore a more efficient, homogeneous coating.

REFERENCES:

1. G. Fornalczyk, et. al.: Yttria-Stabilized Zirconia Thin Films via MOCVD for Thermal Barrier and Protective Applications in Injection Molding, Key Engineering Materials 742, 427-433, (2017)
2. B. Atakan, V. Khlopyanova, S. Mausberg, F. Mumme, A. Kandzia, C. Pflitsch: Physica Status Solidi C12 878, (2015)