

Simulation of CVD process in a reactor

Presenting coating on a demonstrator within the reactor

Comsol conference 2018, Lausanne, Switzerland

CVD reactor at KIMW

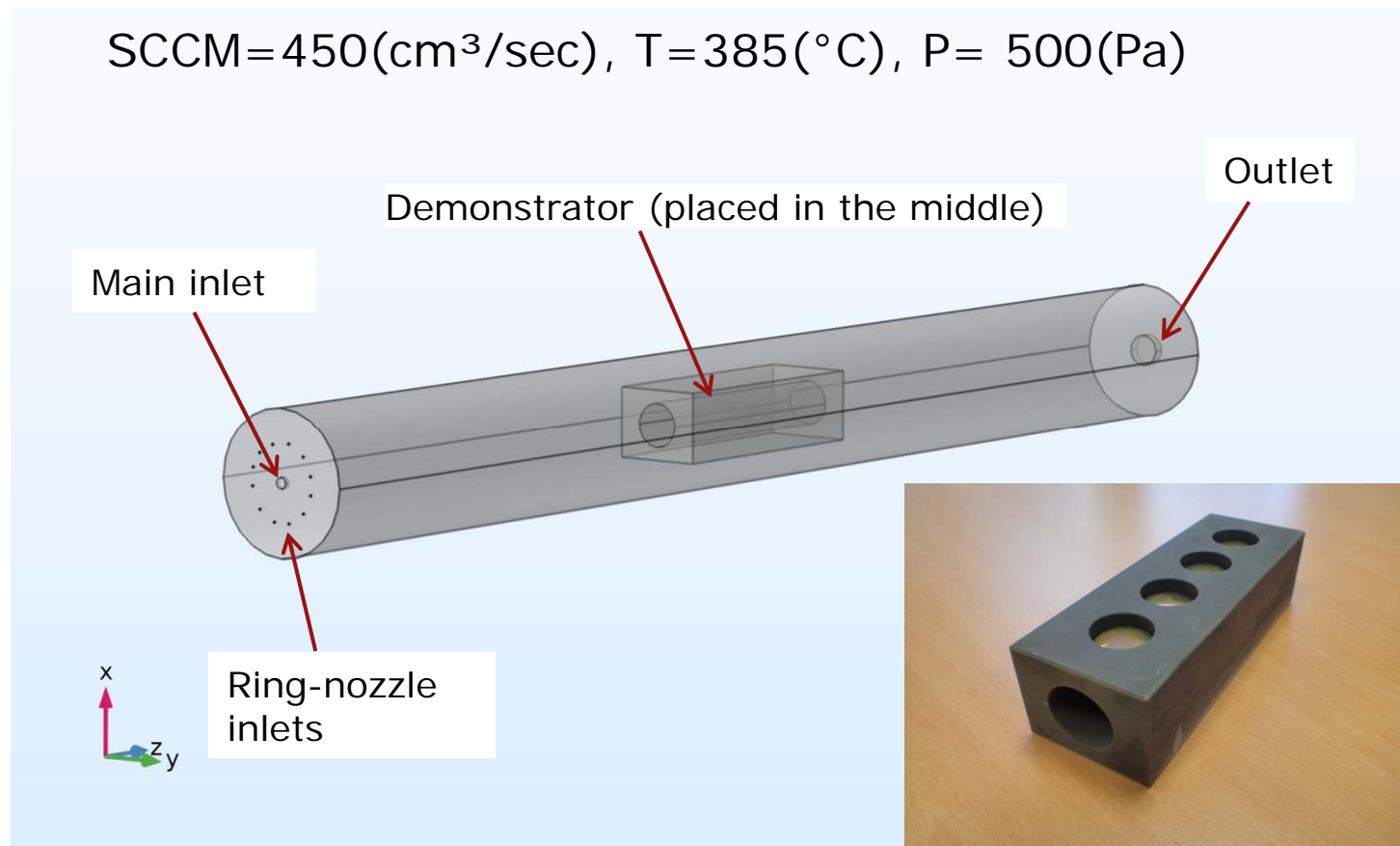
Main and
Ring-nozzle Inlets

Outlet



Hollow demonstrator calculation

► Comsol Geometry



Real Demonstrator

Equations considered for the computation

► Laminar Flow

- Solves Navier-Stokes and continuity equations
 - Only practical for low Re numbers, i.e. $Re < 2000$
 - Stationary or time dependent
 - Incompressible, weakly compressible, or compressible flow ($Ma < 0.3$)

Navier-Stokes, continuity and equation of state

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \nabla \cdot \left[\mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right) \right] + \mathbf{F}$$
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$
$$\rho = \rho(p, T)$$

Laminar Flow (spf)

- Fluid Properties 1
- Initial Values 1
- Wall 1

Equation form:
Study controlled

Show equation assuming:
Study 2 Both Inlets, Stationary

$$\rho(\mathbf{u} \cdot \nabla) \mathbf{u} =$$
$$\nabla \cdot \left[-\rho \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right] + \mathbf{F}$$
$$\nabla \cdot (\rho \mathbf{u}) = 0$$

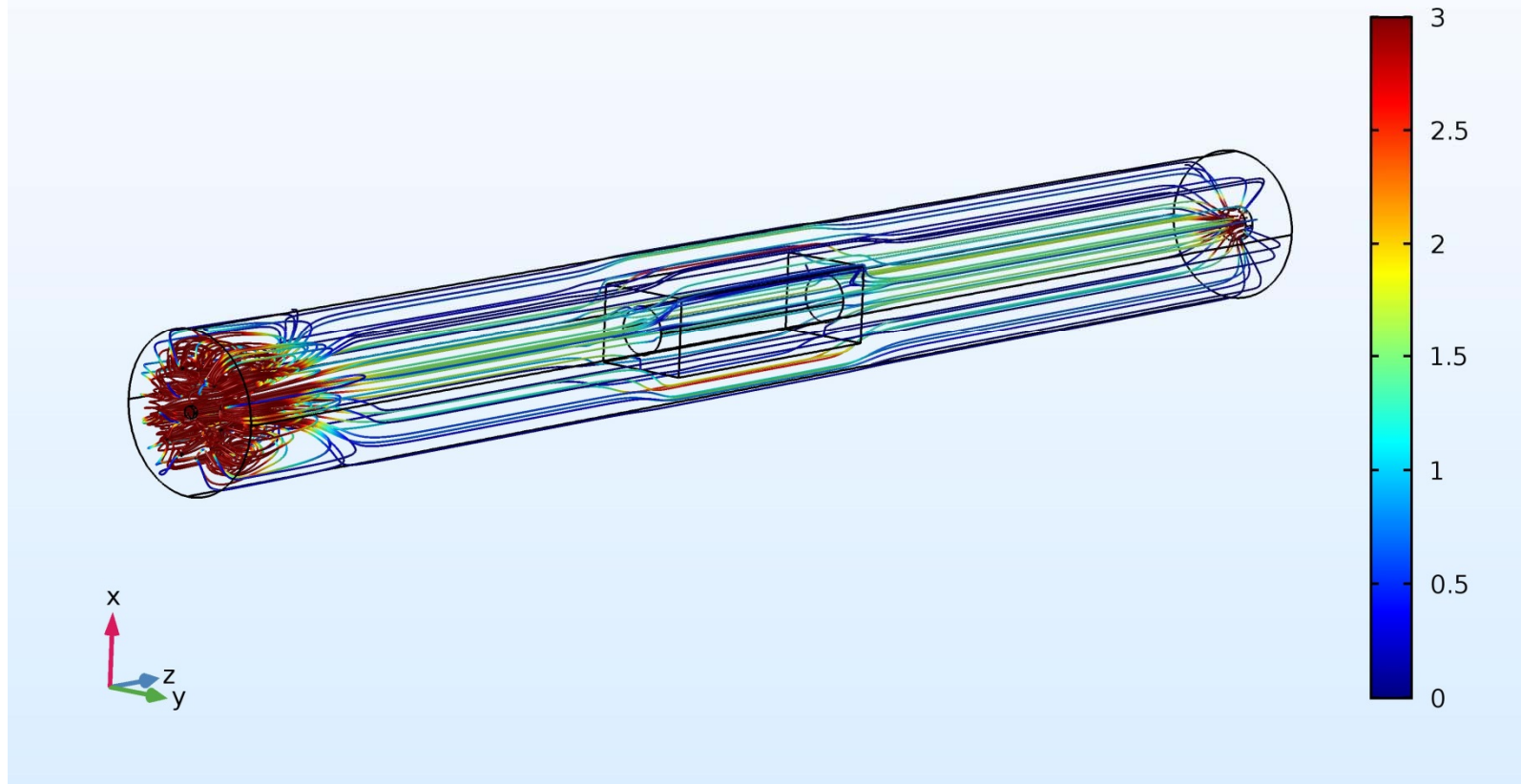
CASE 1: Without plates

FLOW THROUGH THE REACTOR

Hollow demonstrator calculation

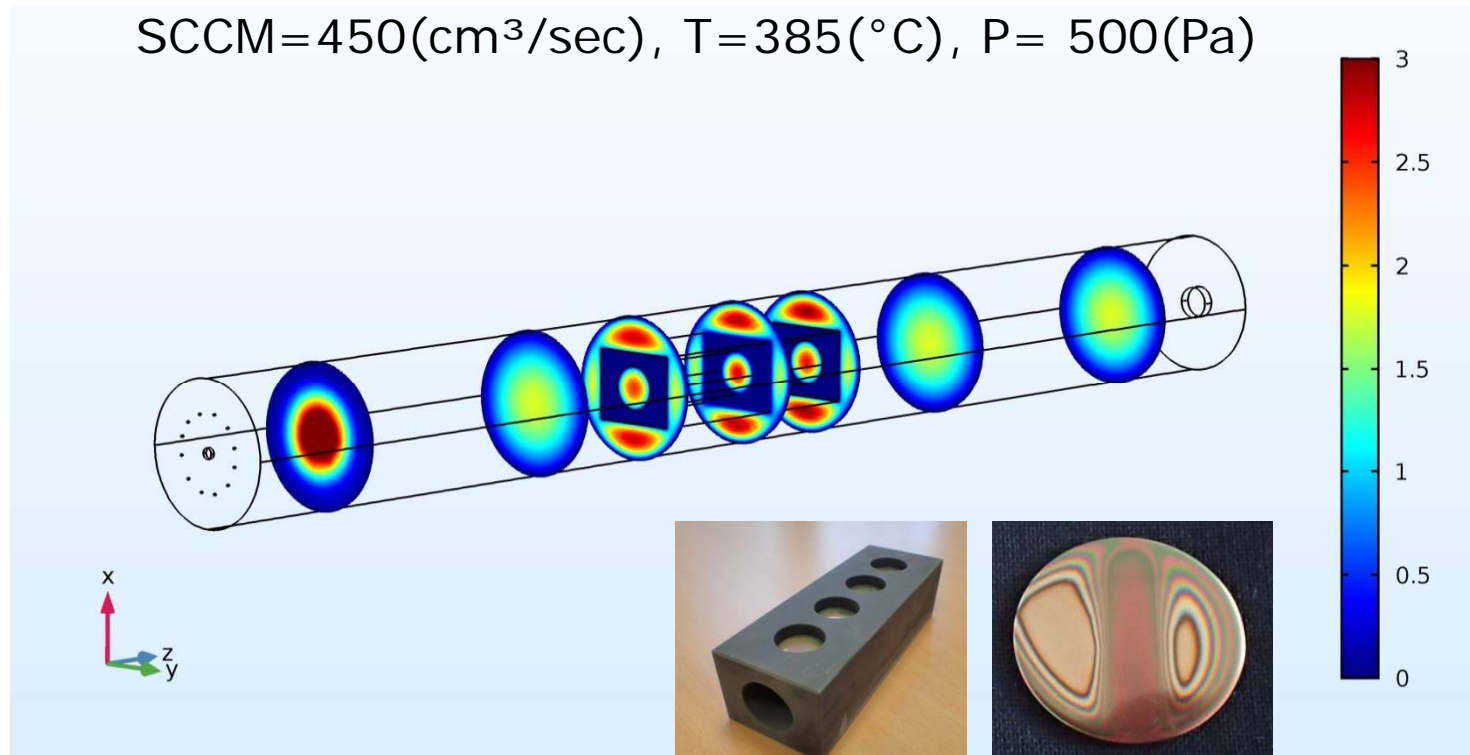
► Velocity Streamlines

Streamline: Velocity field
SCCM=450(cm³/sec), T=385(°C), P= 500(Pa)



Hollow demonstrator calculation

► Velocity Cut-section



- Higher velocity can be observed in the front section of the reactor because of the swirls.

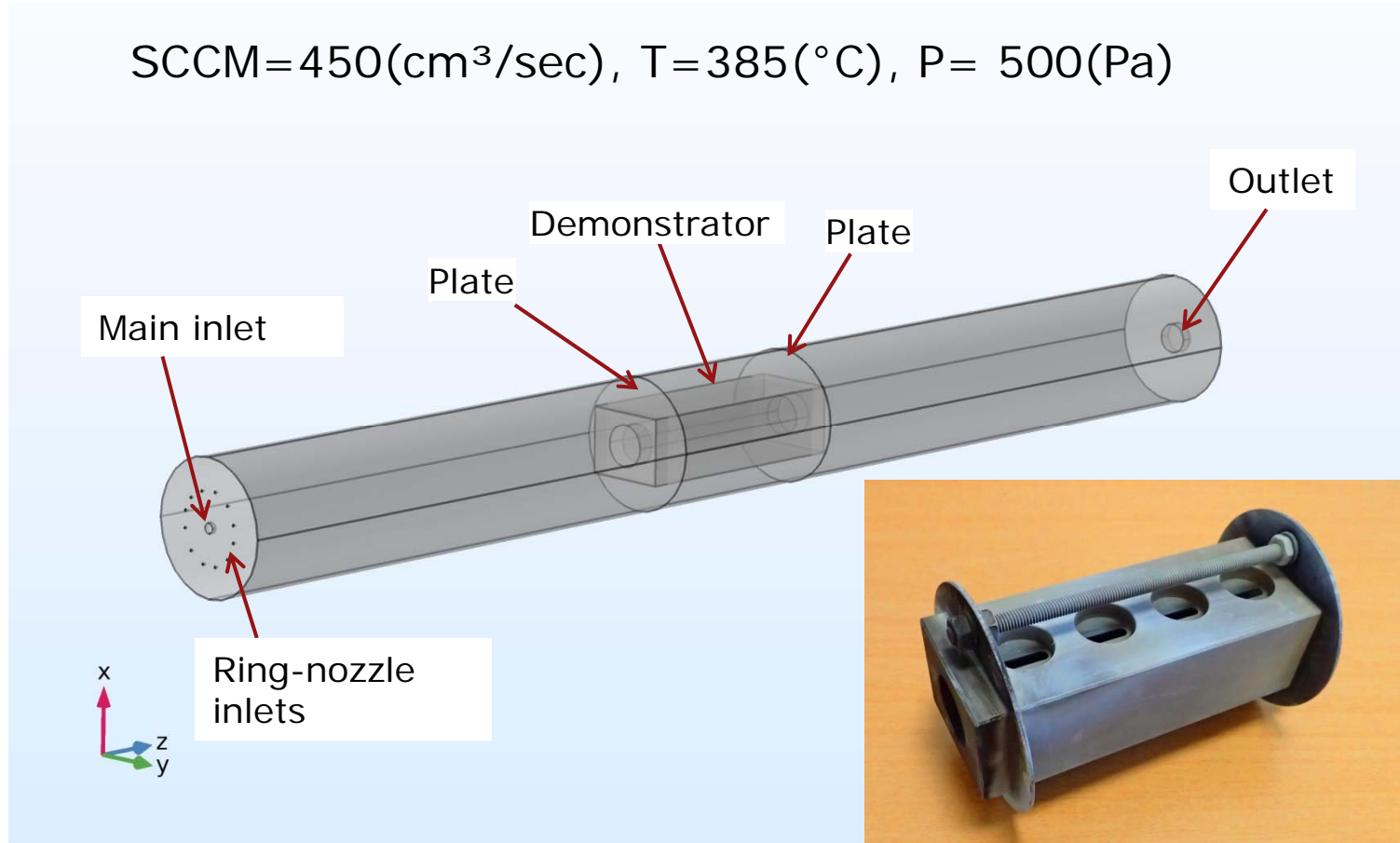
CASE 2: With plates

REDUCTION OF THE FLOW PATH

Hollow demonstrator calculation

► Comsol Geometry

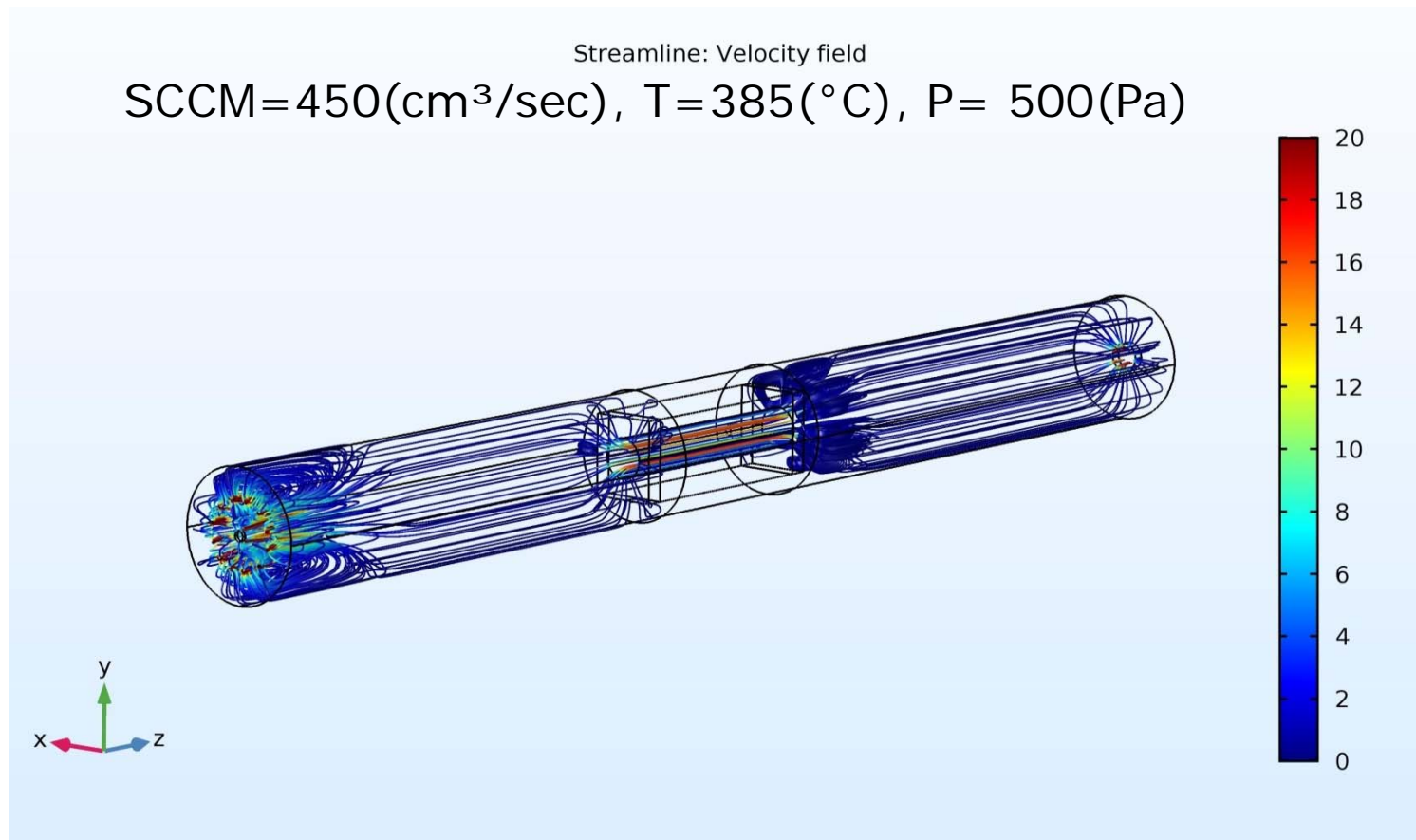
SCCM=450(cm³/sec), T=385(°C), P= 500(Pa)



Real Demonstrator

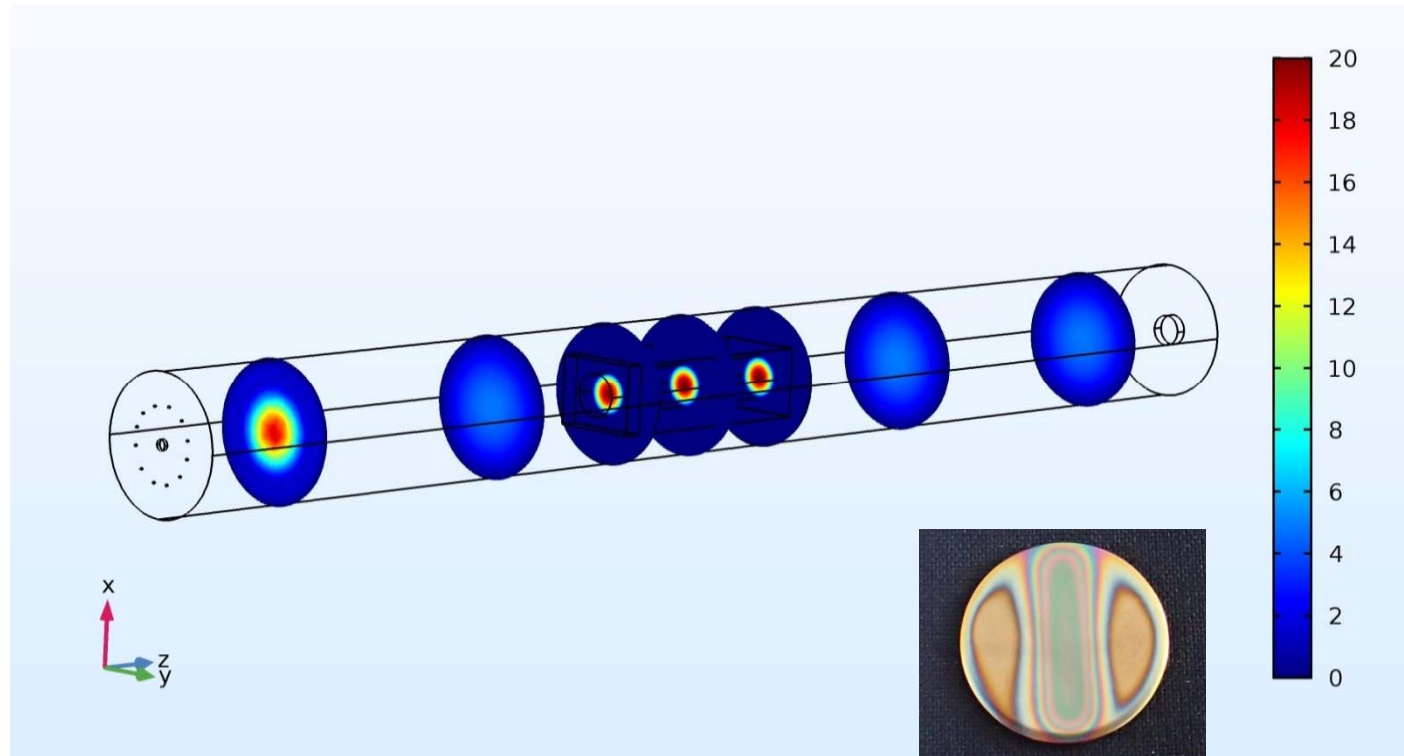
Hollow demonstrator calculation

► Velocity Streamlines



Hollow demonstrator calculation

▶ Velocity Cut-section



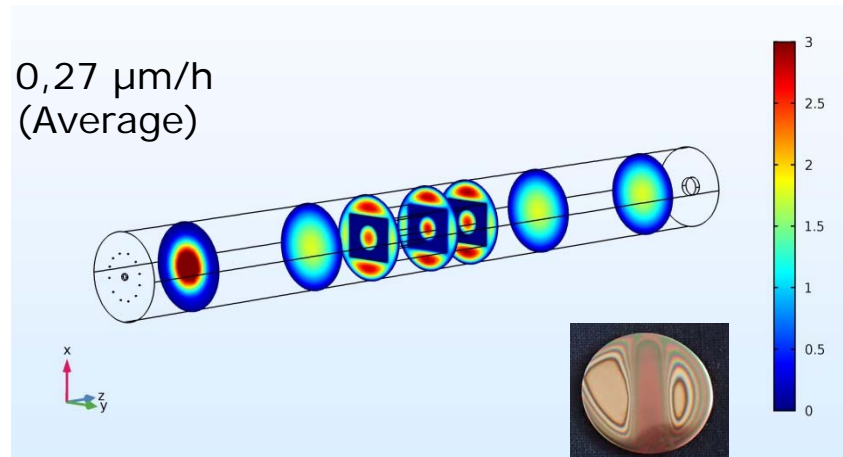
- ▶ Higher velocities can be observed in the front of reactor due to swirls caused by turbulence.
- ▶ Due to the volume reduction with the help of plates, one can also clearly observe higher gas velocities within the demonstrator.

Hollow demonstrator calculation

- ▶ Comparison of velocity cut-sections within reactor

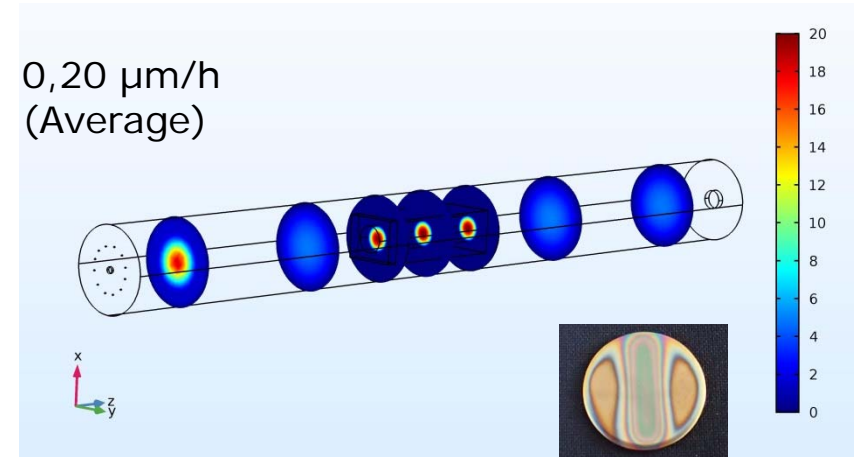
SCCM = 450, P= 500Pa, T=385°C

Without plates



SCCM = 450, P= 500Pa, T=385°C

With plates



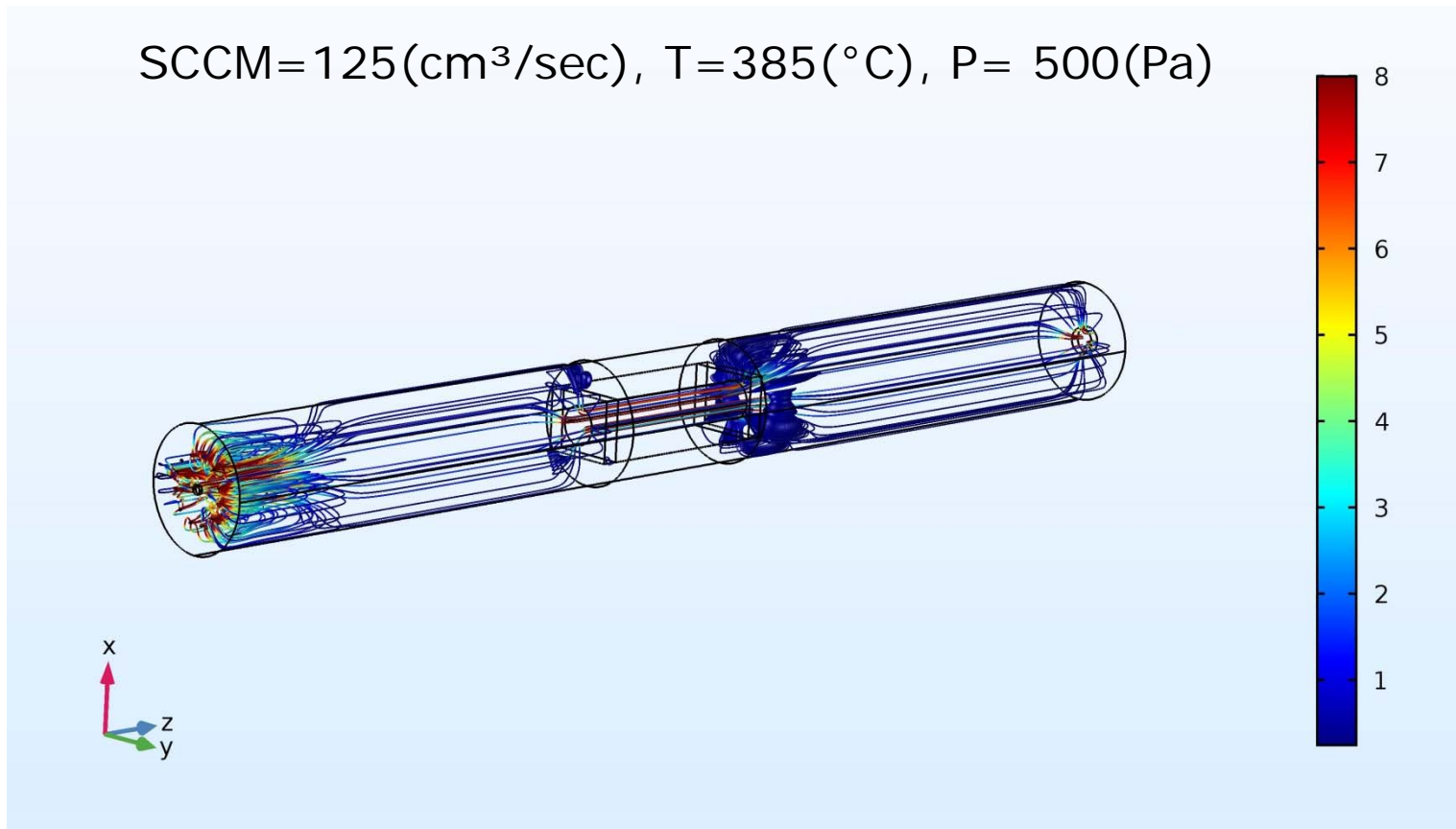
- ▶ The simulation shows higher velocity values due to the volume reduction, so that in this case, less gas flow can be used.
- ▶ Hence an efficient, homogeneous coating could be achieved.

REDUCED GAS FLOW THROUGH THE REACTOR

Hollow demonstrator calculation

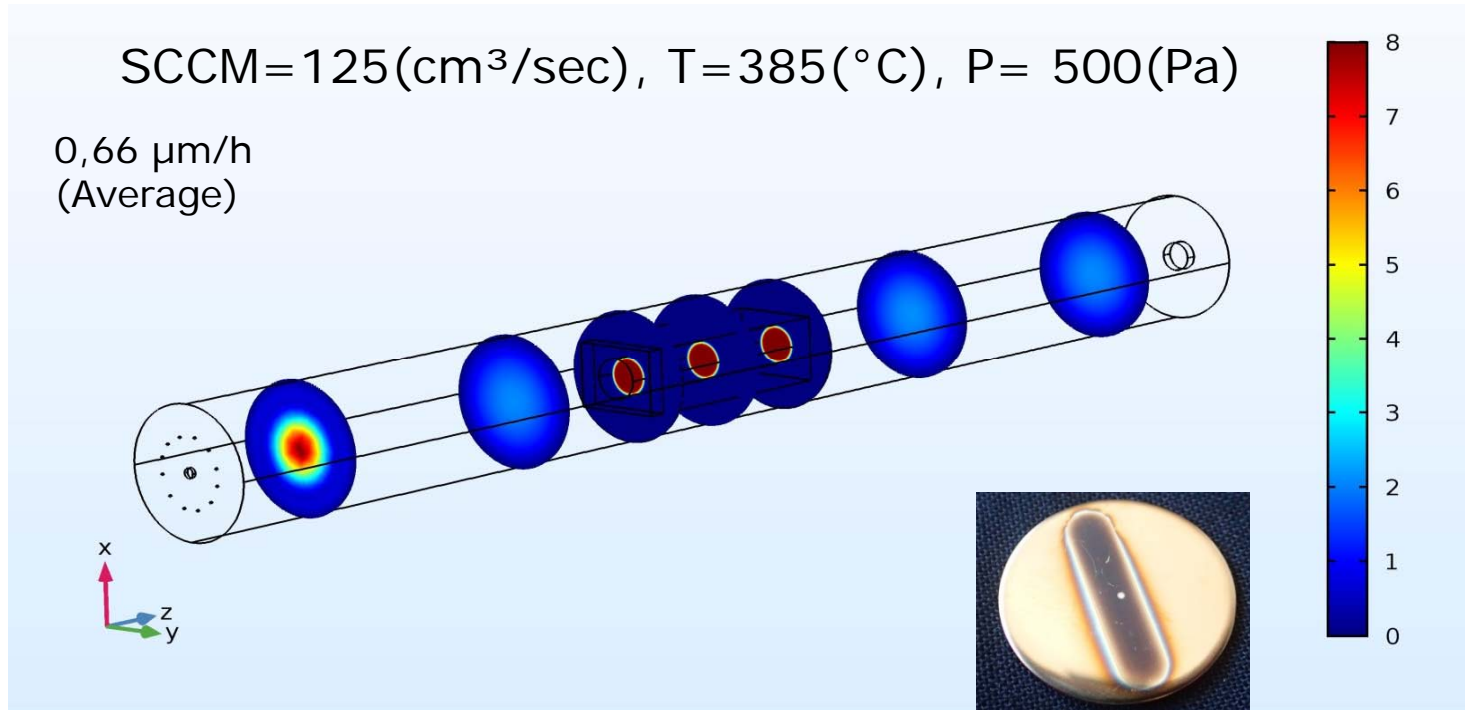
▶ Velocity Streamlines

SCCM= 125(cm^3/sec), $T=385(^{\circ}\text{C})$, $P= 500(\text{Pa})$



Hollow demonstrator calculation

▶ Velocity Cut-section

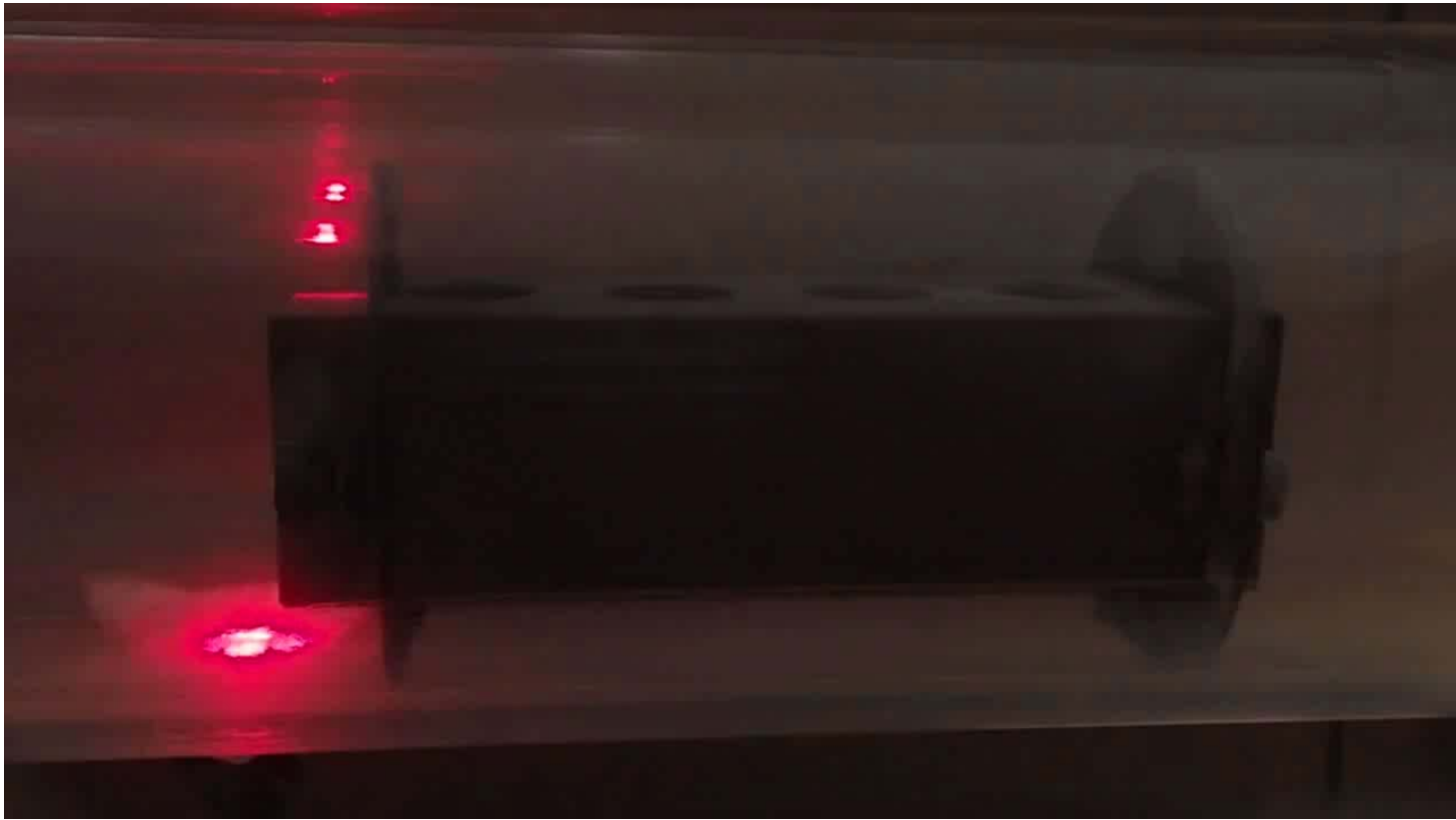


- ▶ Reduced velocities are obtained from simulations with reduced SCCM.
- ▶ As the gas flow is at a slower rate a much higher coating growth rate can be obtained on the specimens.

Hollow demonstrator calculation



Hollow demonstrator calculation





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