

Pseudo-3D Multiphysics Simulation of a Hydride Vapor Phase Epitaxy Reactor

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Hydride Vapor Phase Epitaxy of GaN

- Gallium nitride is the main material for the production of LED's and LD's e.g. for data storage by the blue laser diode
- Boule growing of GaN is a complicated technology
- HVPE is the most promising technology for GaN production

Model of Hydride Vapor Phase Epitaxy

- Coupled Simulation of Non-Isothermal Flow (nif) and Transport of Diluted Species (chds)
- Velocity field of N_2 shows the the highest flow rates in the region of the gas inlet nozzles (**Fig. 1**)
- Temperature field shows the coupling between velocity field and heat flux (**Fig. 2**)
- Concentration field of NH_3 illustrates increasing dispensation with increasing z-coordinate (**Fig. 3**)
- The model can be applied for a variation of several physical parameters and reactor geometry
- Temperature was found to be independent from reactor length whereas concentration fields are strongly influenced

Main Definitions

- Exploration of the structure of the FEM model (**Fig. 4**)
- Axisymmetric pseudo-3D model
- Laminar gas flow at the inlets
- Variation of concentration and speed at the inlets
- Physical properties of the domain calculated by help of ideal gas law
- Compressible fluid flow is considered
- Gas inlets are defined as mass flow
- Gas outlets are defined as pressure-outlet
- Temperature at the substrate holder is 1320 K

Geometry and Mesh

- Geometry was derived from a commercial reactor (**Fig. 6**)
- Simulation area limited from nozzles to substrate holder
- Mesh consists of 31.369 mesh elements (**Fig. 5**)
- Surface layer mesh along the no-slip boundaries which consists of rectangle elements

Acknowledgements

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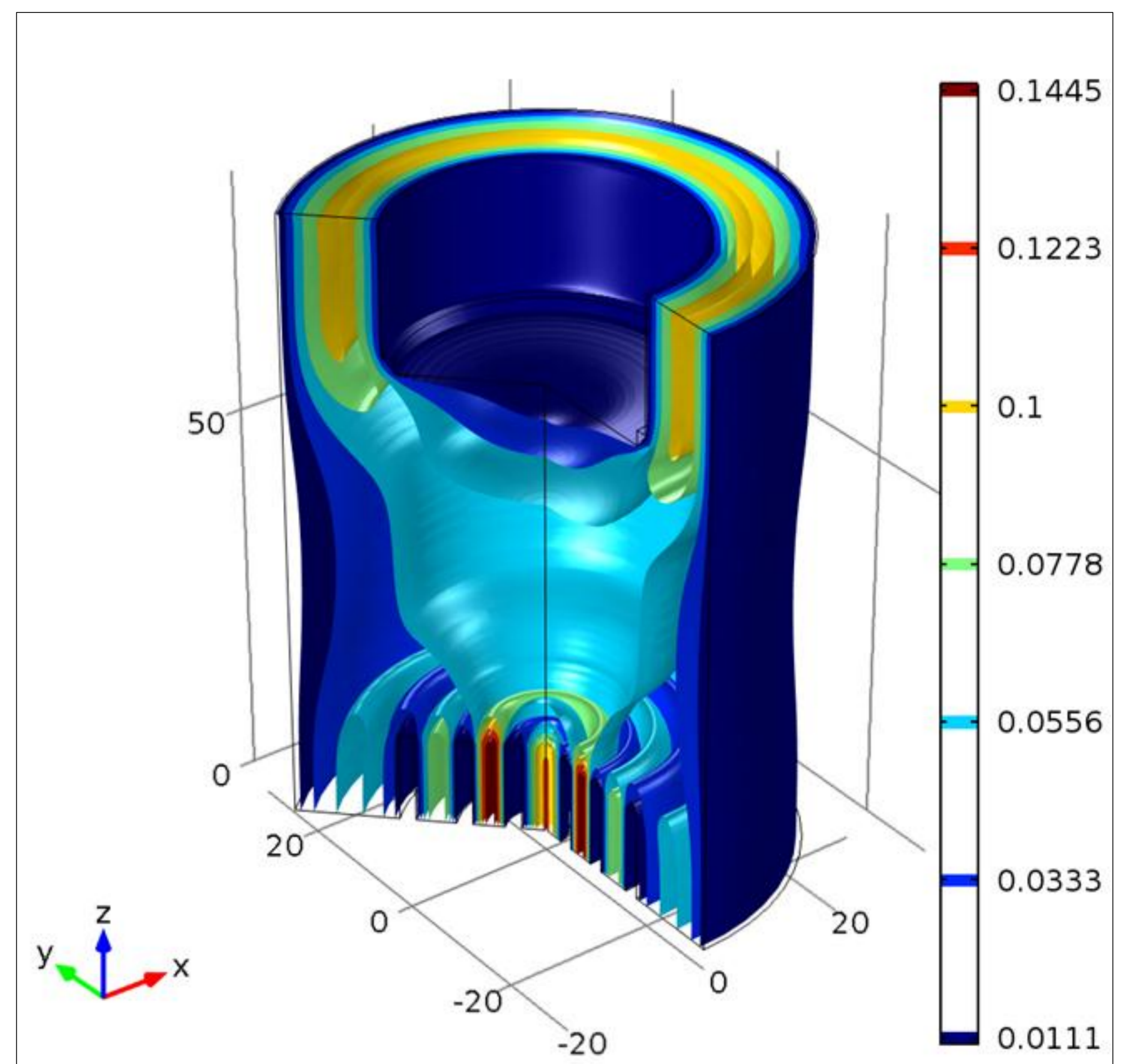


Fig. 1 Sectional view of the velocity field of N_2 based on iso-surfaces [m/s]:

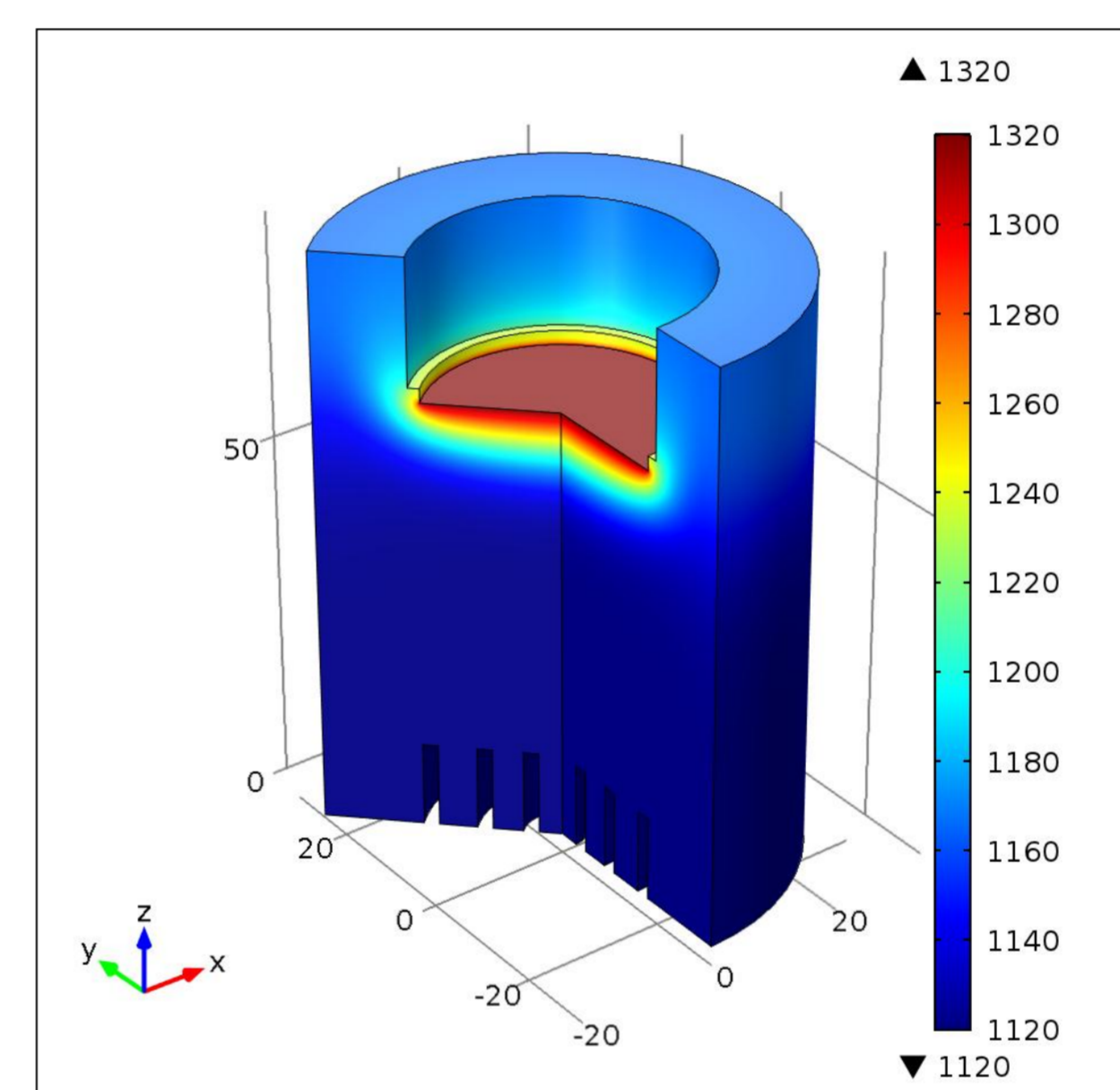


Fig. 2: 3D iso-plot, temperature field [K]

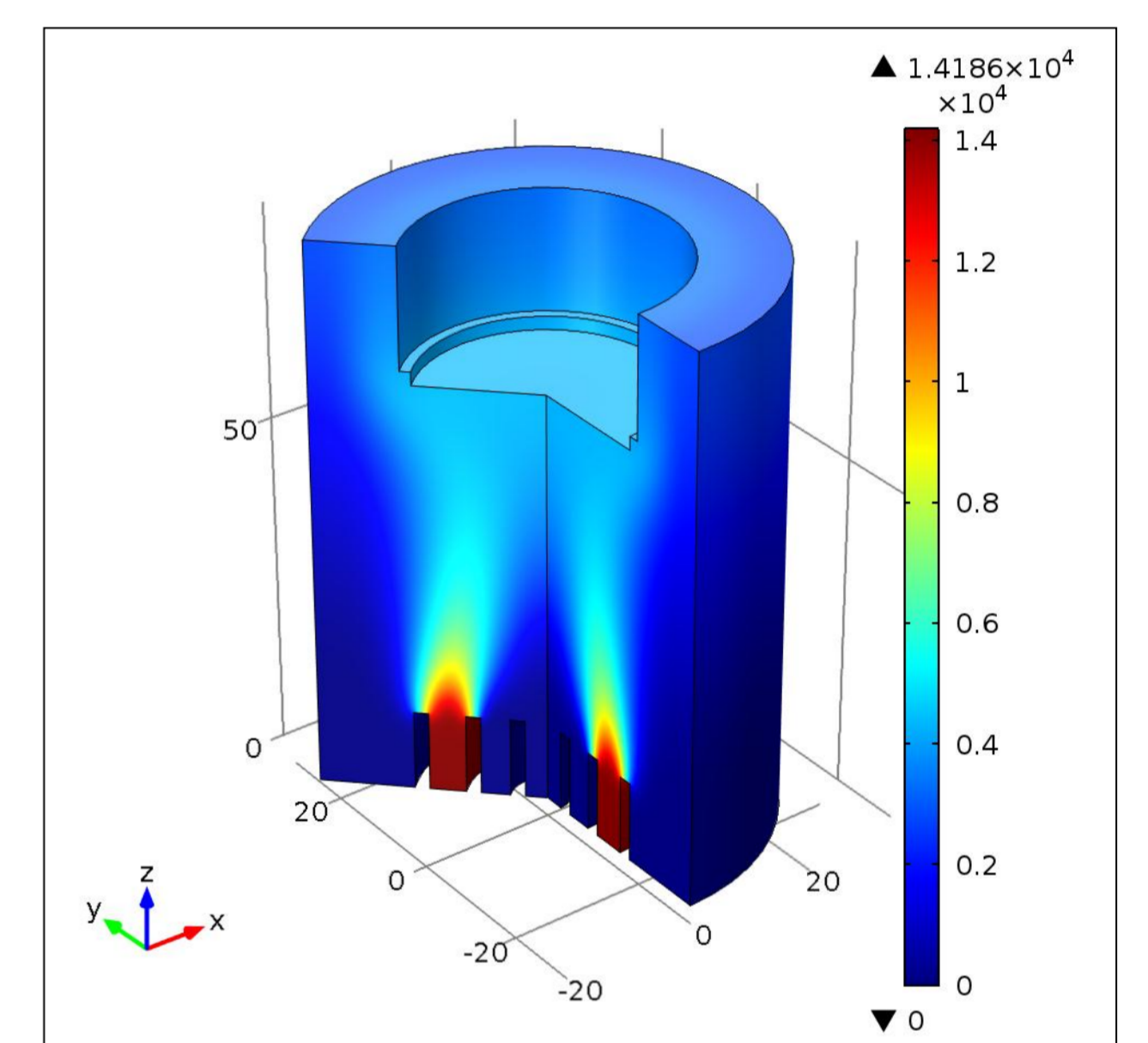


Fig. 3: 3D iso-plot, concentration of NH_3 [mol/m³]

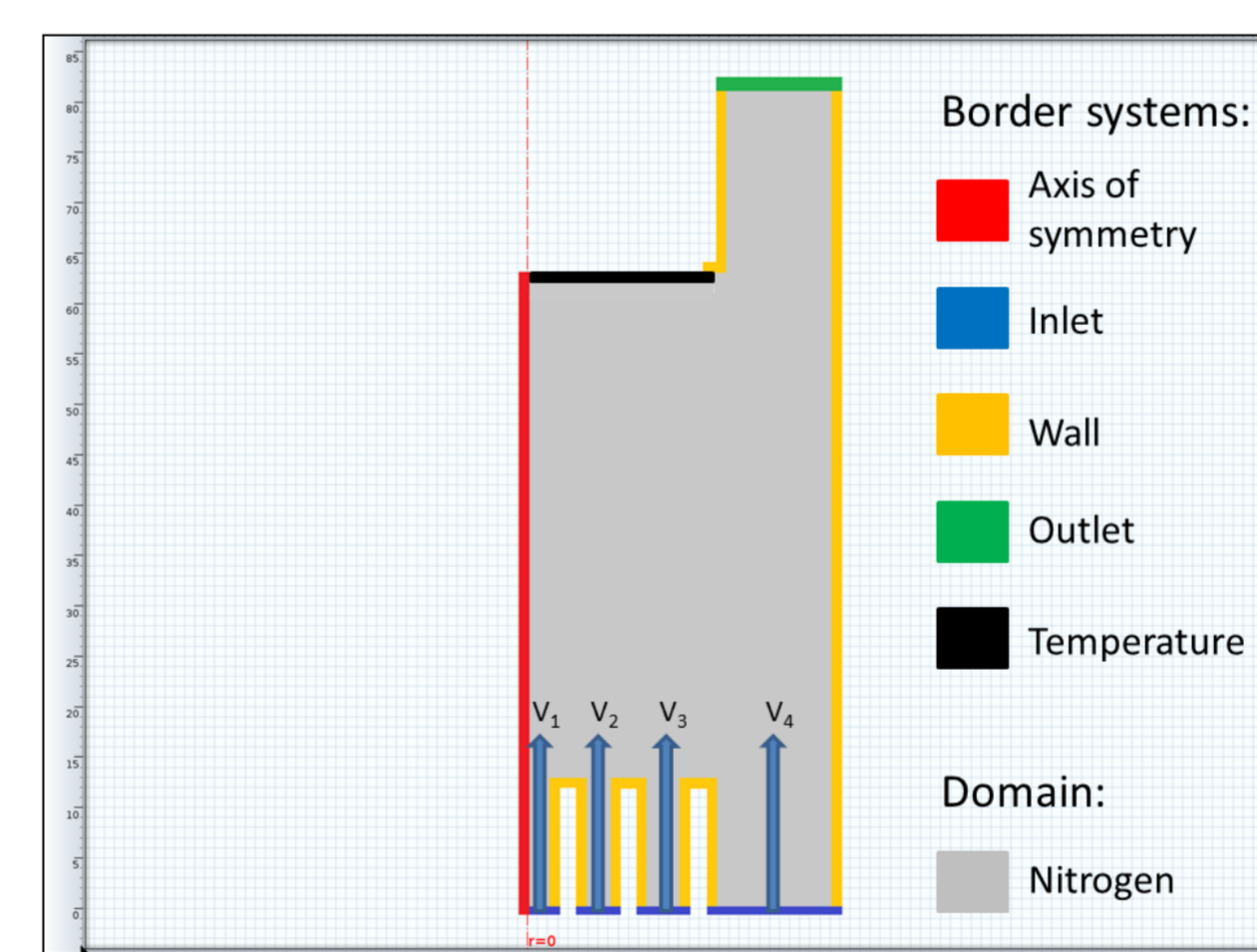


Fig. 4: Axis symmetric reactor model with color coded border systems and fluid

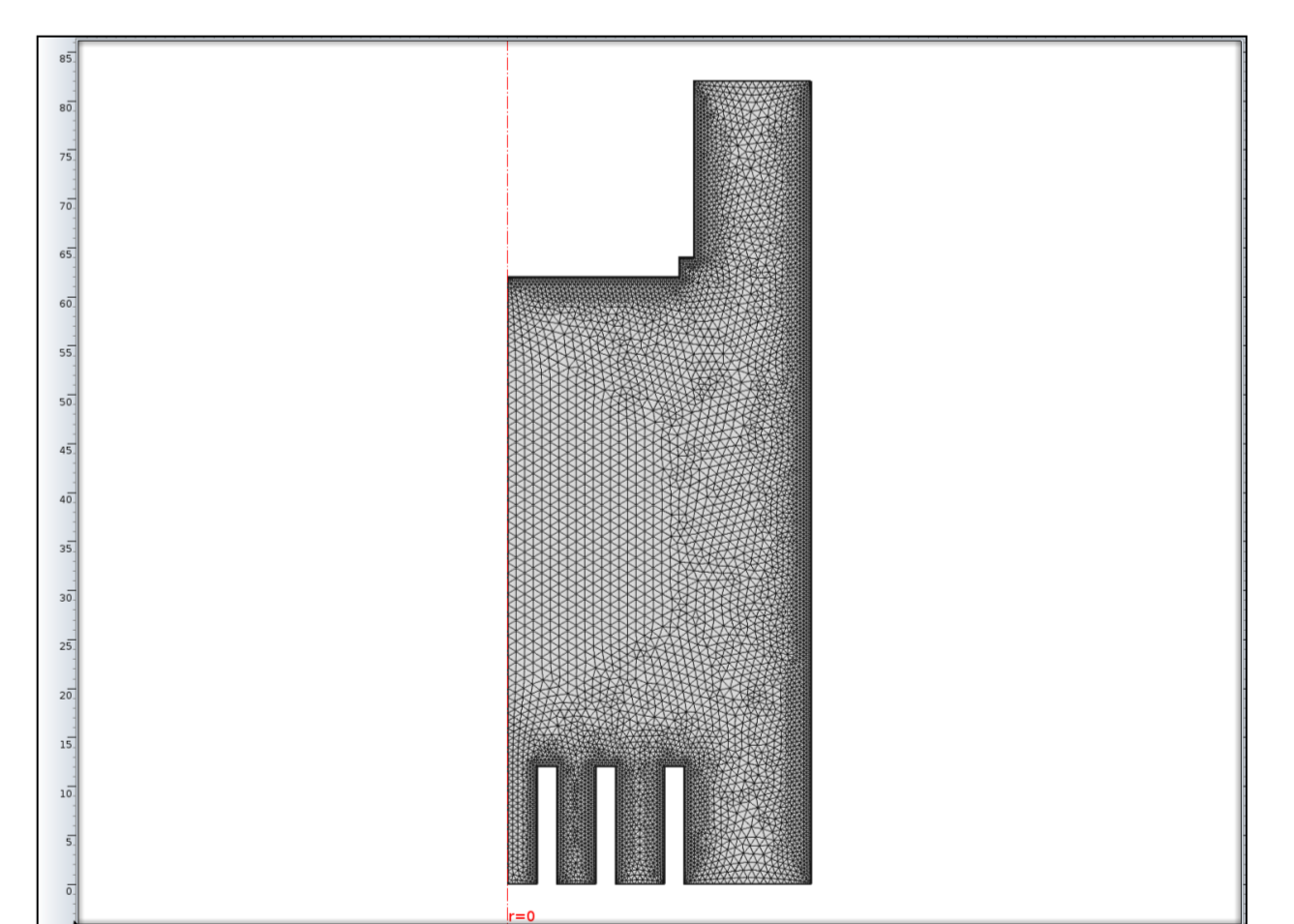


Fig. 5: Mesh of the model with 31.369 mesh elements

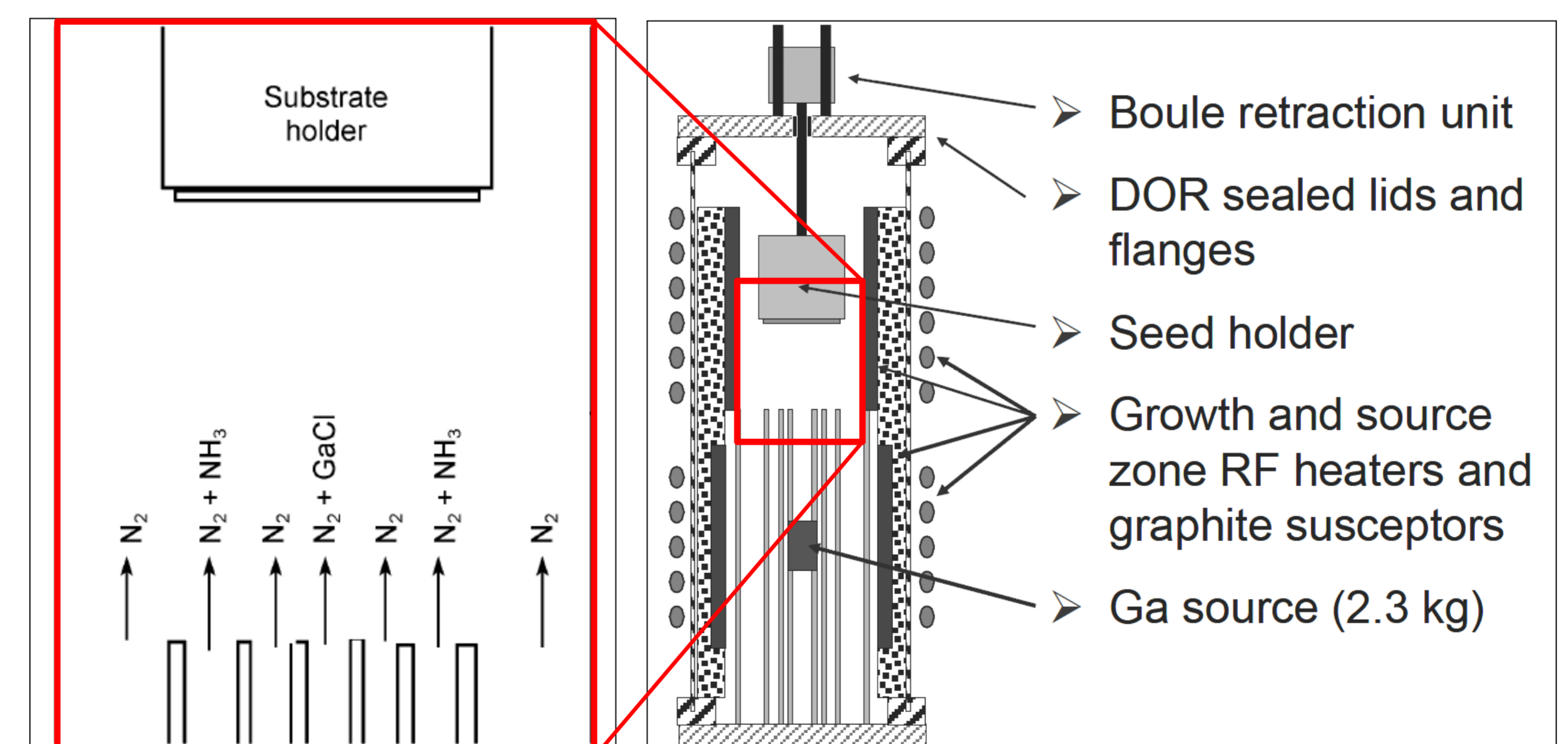


Fig. 6: Schematic cross section of the gas inlet nozzles with incoming species and the substrate holder of the observed vertical HVPE reactor from AIXTRON AG (Aachen, Germany)

