Three-dimensional modeling of argon flow in floating zone crystal growth process

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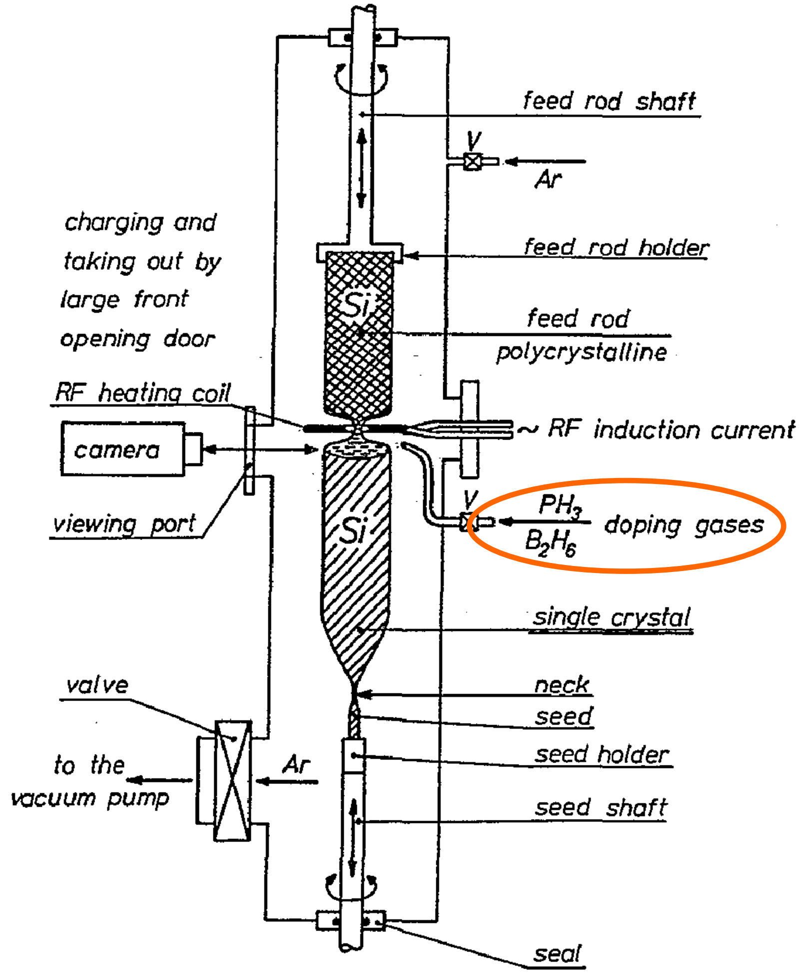
EIROPAS REĢIONĀLĀS ATTĪSTĪBAS FONDS
EIROPAS SAVIENĪBA
IEGULDĪJUMS TAVĀ NĀKOTNĒ

Introduction

Si single crystal growth with FZ technique

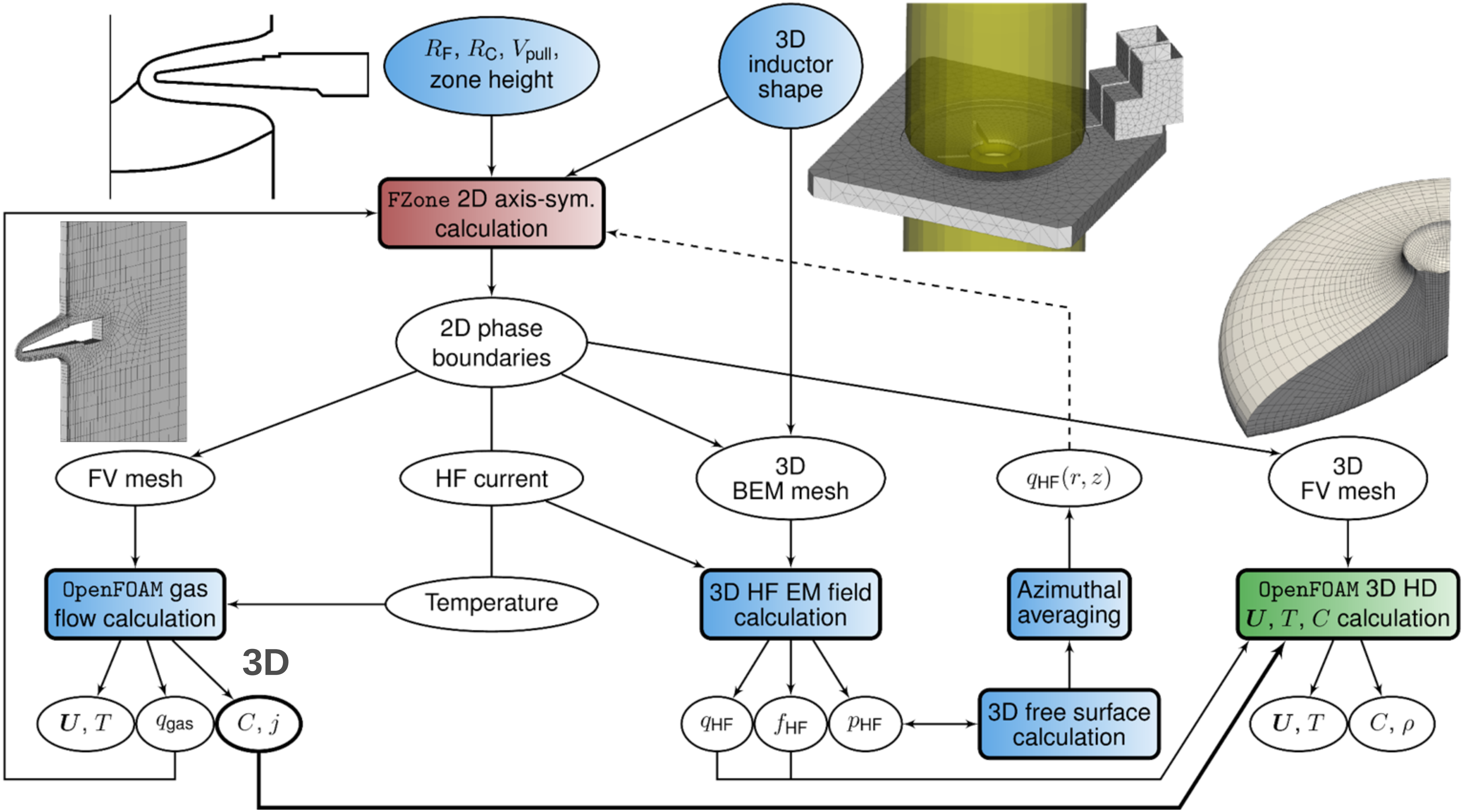
Courtesy of Dr. H. Riemann (ICG, Berlin)



W. Zulehner. Mater. Sci. Eng. B, 73(1):7-15, 2000

Introduction

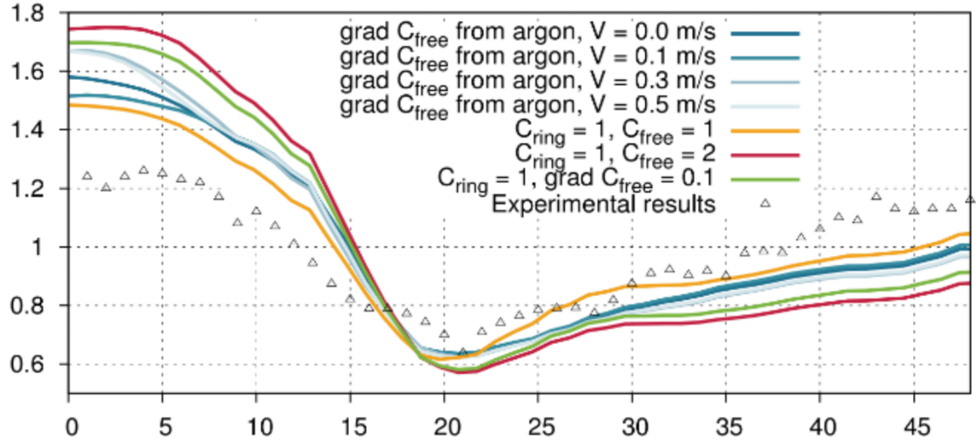
Actual mathematical model

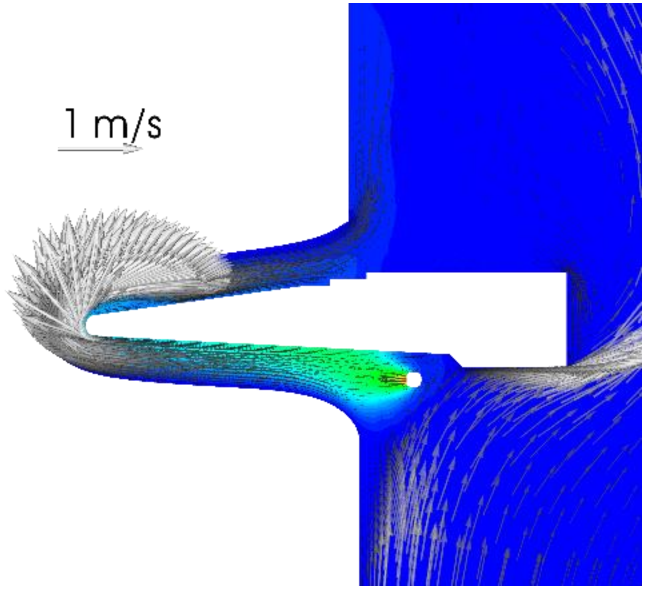


Introduction

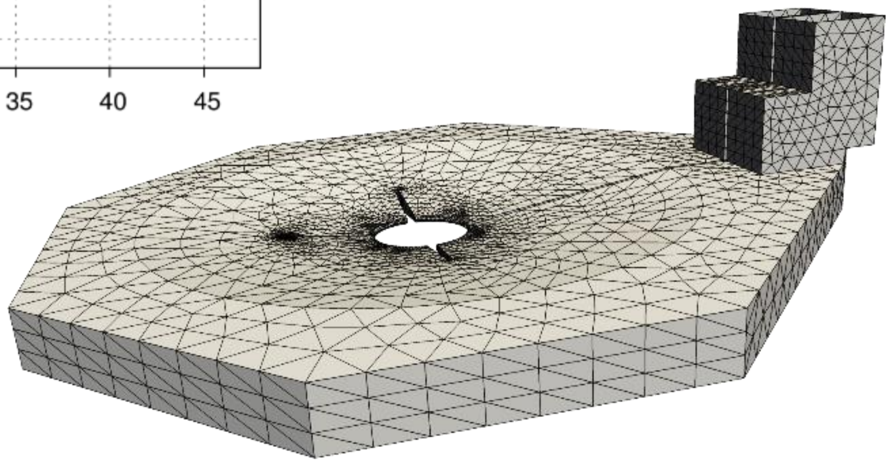
Motivation for 3D gas flow calculations

- Previous axisymmetric calculations: insufficient agreement of radial resistivity variations with experiment





- 3D inductor shape and non-symmetric dopant inlet



Mathematical models

3D gas flow and dopant transport

Continuity and momentum equations

$$\nabla(\rho \boldsymbol{U}) = 0$$

$$\nabla\left(\rho \boldsymbol{U} \otimes \boldsymbol{U} + \frac{2}{3}\mu_{\text{eff}}\nabla \boldsymbol{U} - 2\mu_{\text{eff}} e\right) = -\nabla\, p_{\text{rgh}} - \boldsymbol{g}\boldsymbol{x}\nabla\rho,\ \ p_{\text{rgh}} = p - \rho\boldsymbol{g}\boldsymbol{x}$$

Turbulence:
k-omega SST

Energy equation

$$\rho \boldsymbol{U}\nabla\left(\tilde{h} + \frac{U^2}{2}\right) = \nabla(\alpha_{\text{eff}}\nabla h)$$

Specific enthalpy $\tilde{h} = c_p T$

Viscosity: Sutherland's law

$$\mu(T) = \frac{A_S\sqrt{T}}{1 + T_S/T}$$

Ideal gas law

$$\rho = p\frac{M_g}{RT}$$

Dopant transport equation

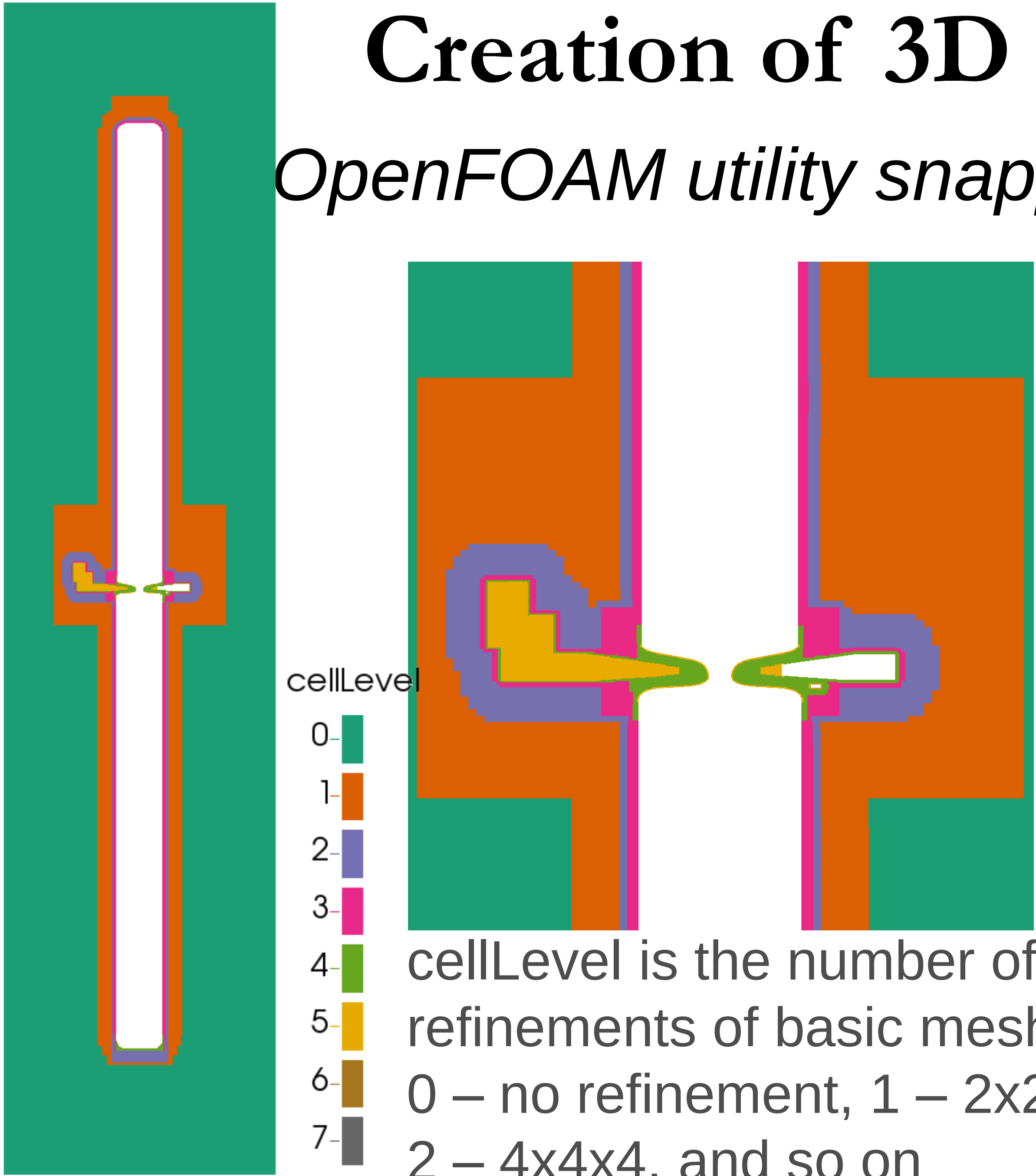
$$(\rho \boldsymbol{U}\nabla)C = \nabla(\rho D_{\text{eff}}\nabla C),\ \rho D_{\text{eff}} = \frac{\mu}{\text{Sc}} + \frac{\mu}{\text{Sc}_t}$$

Dopant mass flux

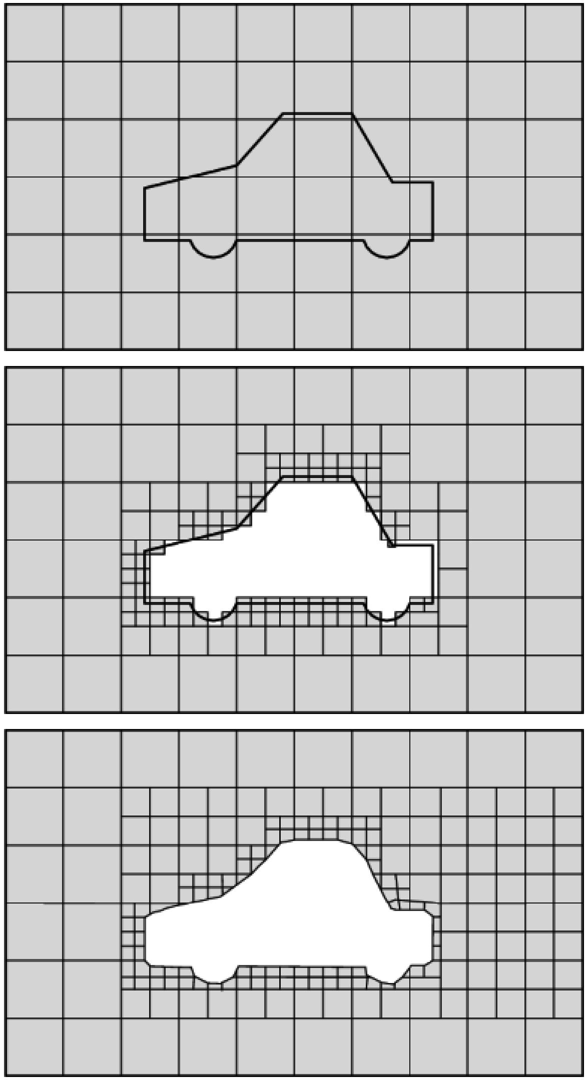
$$j = -\rho D_{\text{eff}}\frac{\partial C}{\partial n}$$

Creation of 3D mesh

OpenFOAM utility snappyHexMesh



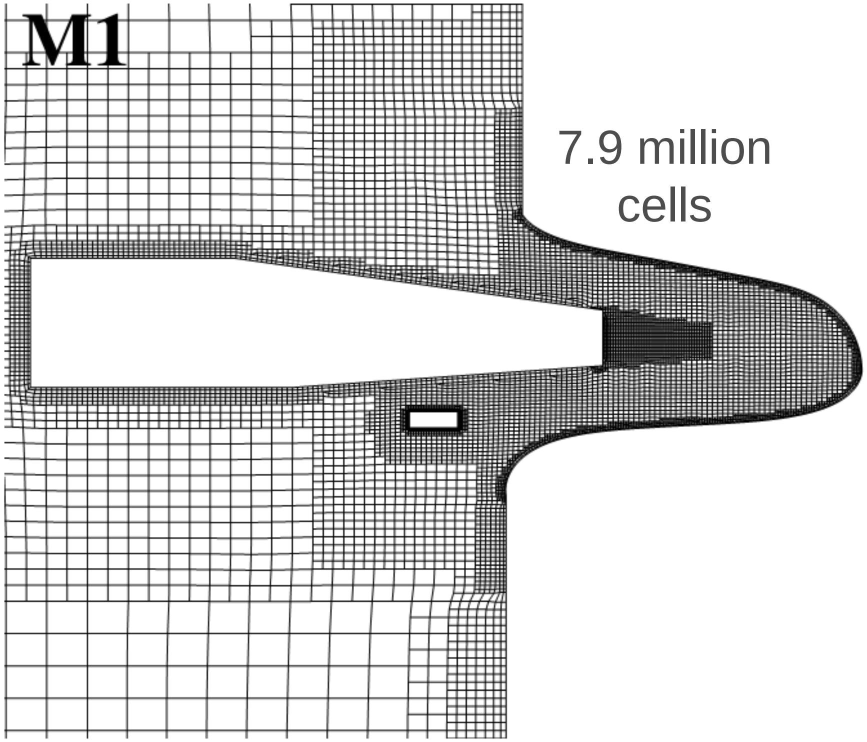
cellLevel is the number of refinements of basic mesh: 0 – no refinement, 1 – 2x2x2, 2 – 4x4x4, and so on



http://www.openfoam.org/docs/user/snappyHexMesh.php

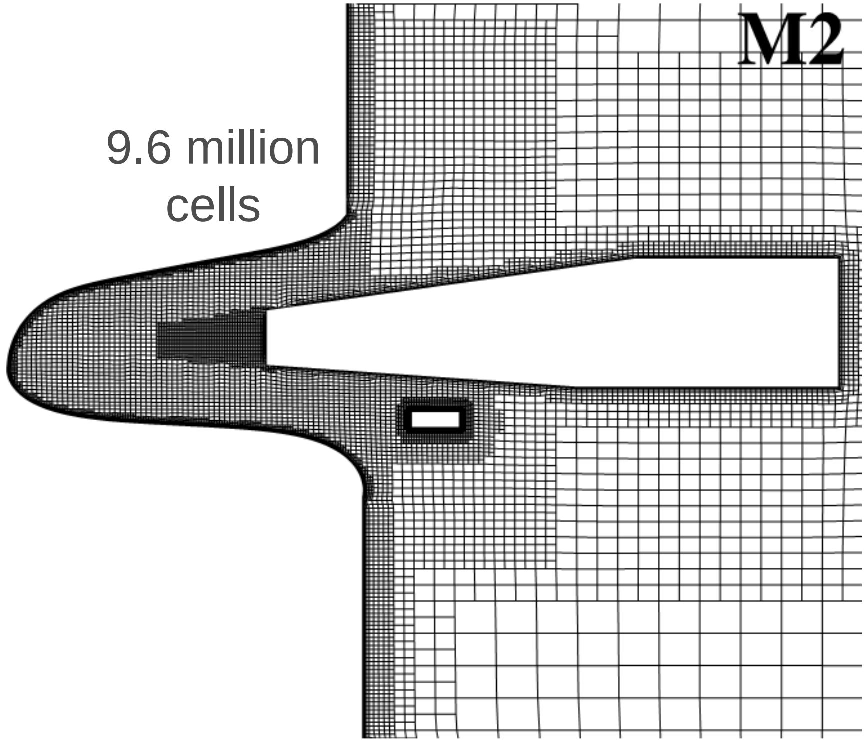
Creation of 3D mesh

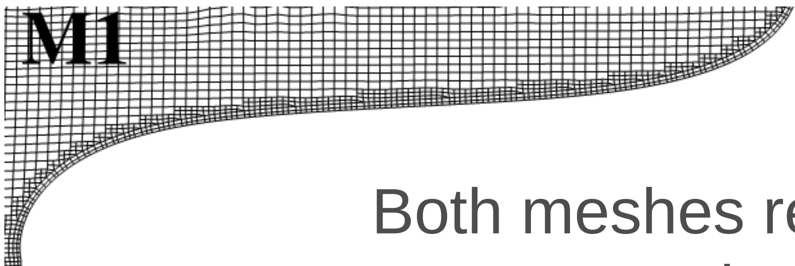
Mesh influence study



7.9 million cells

9.6 million cells

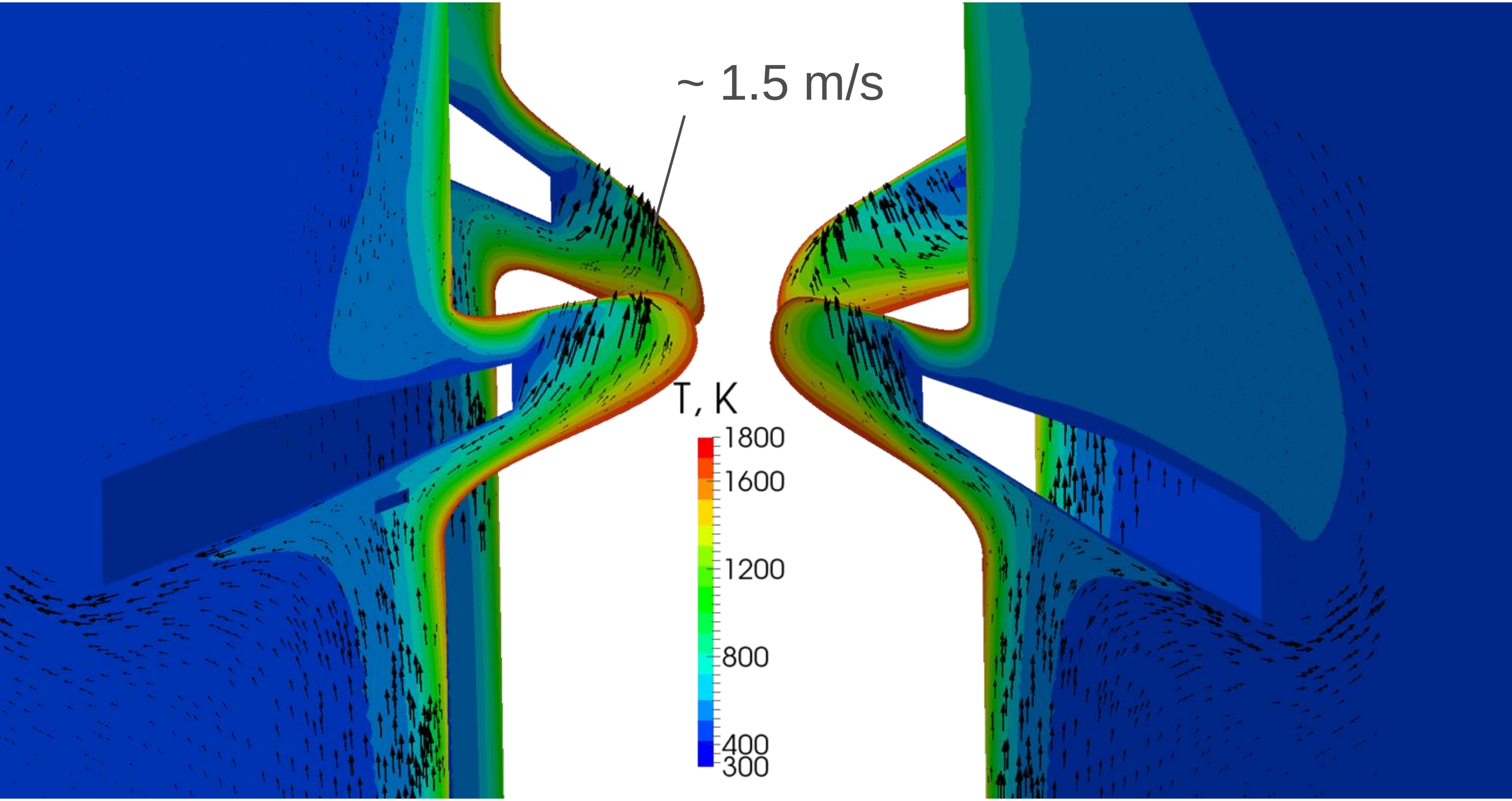




Both meshes resolve temperature and concentration boundary layers well

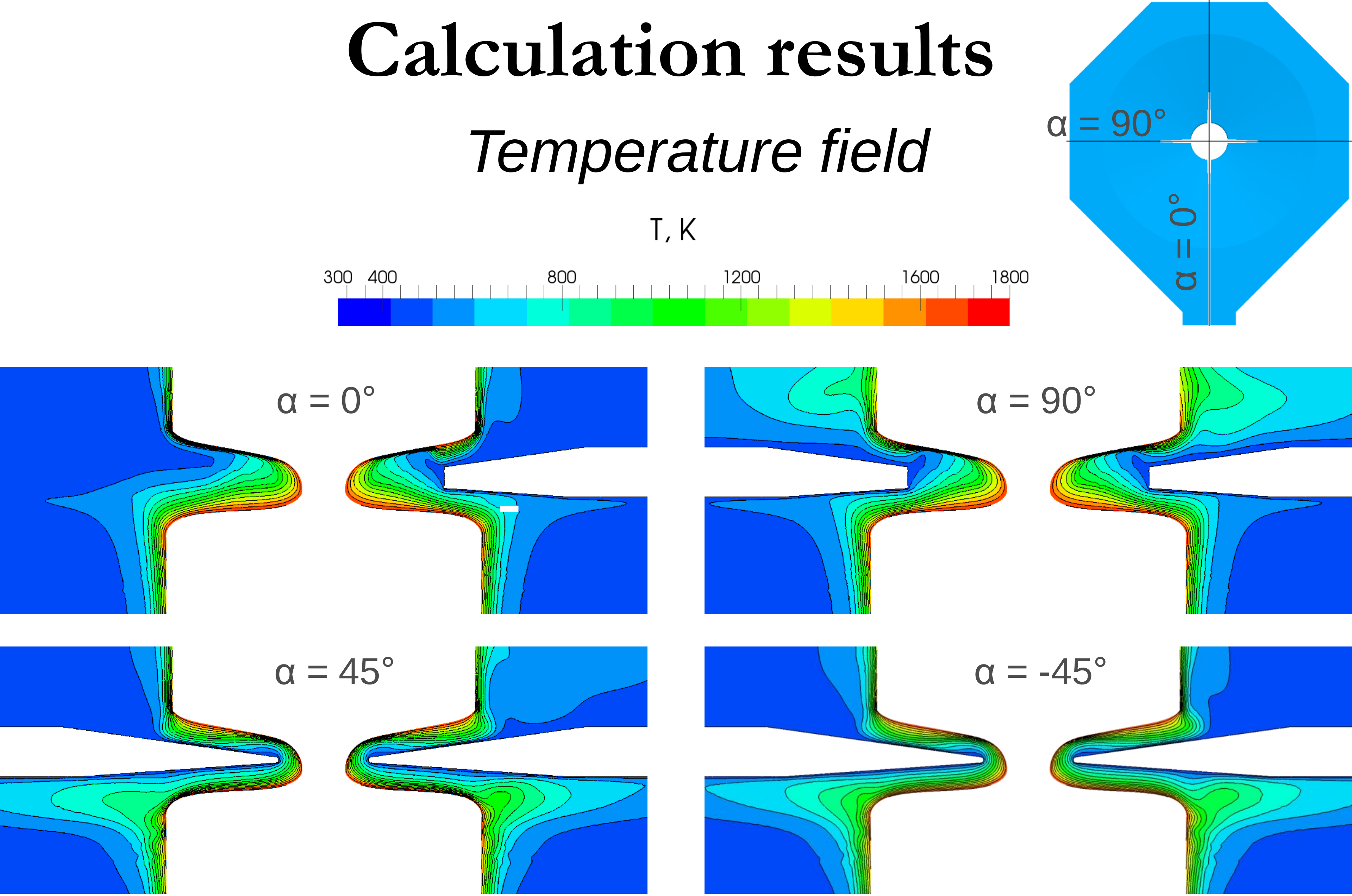
Calculation results

Temperature field



Calculation results

Temperature field



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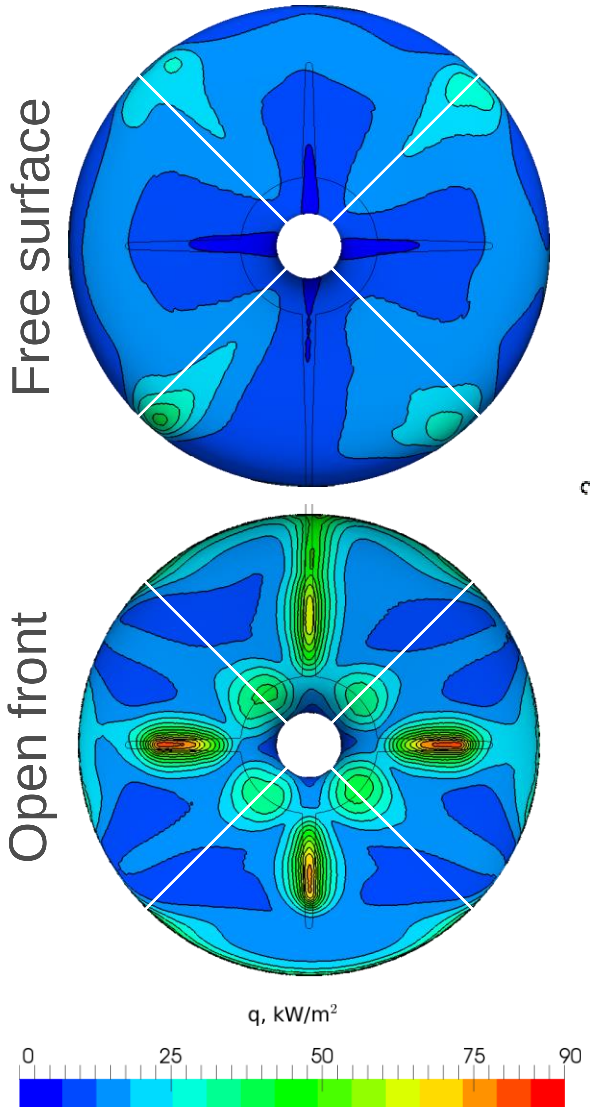
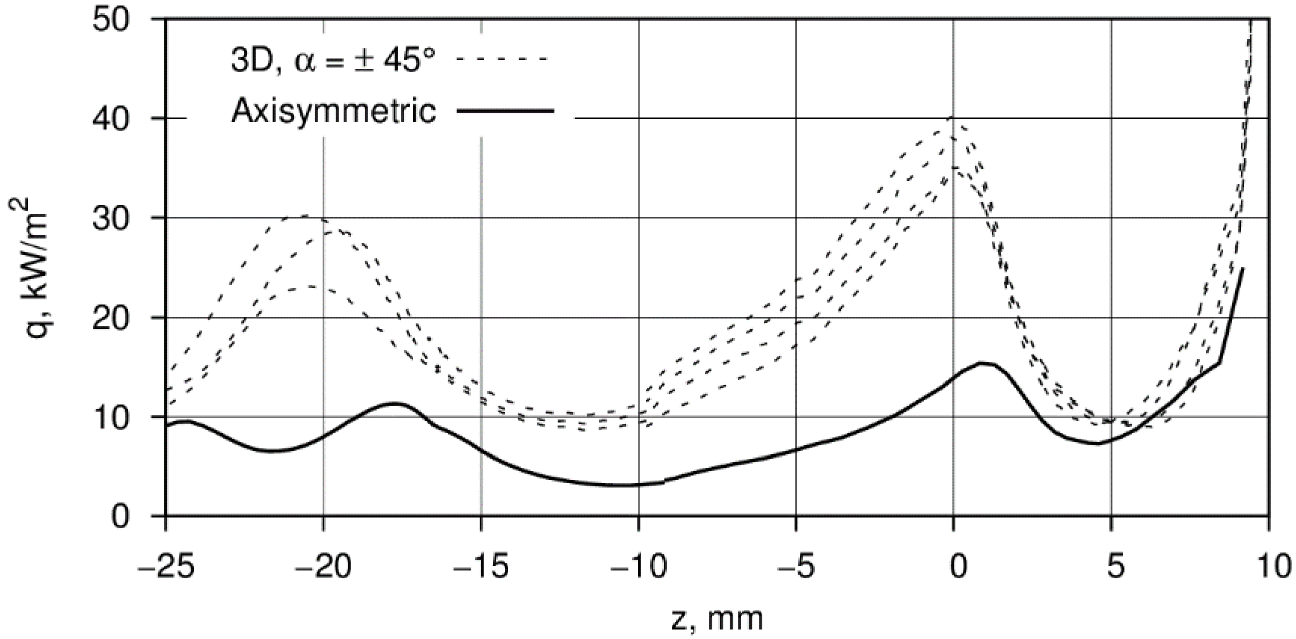
Calculation results

Gas cooling heat flux density



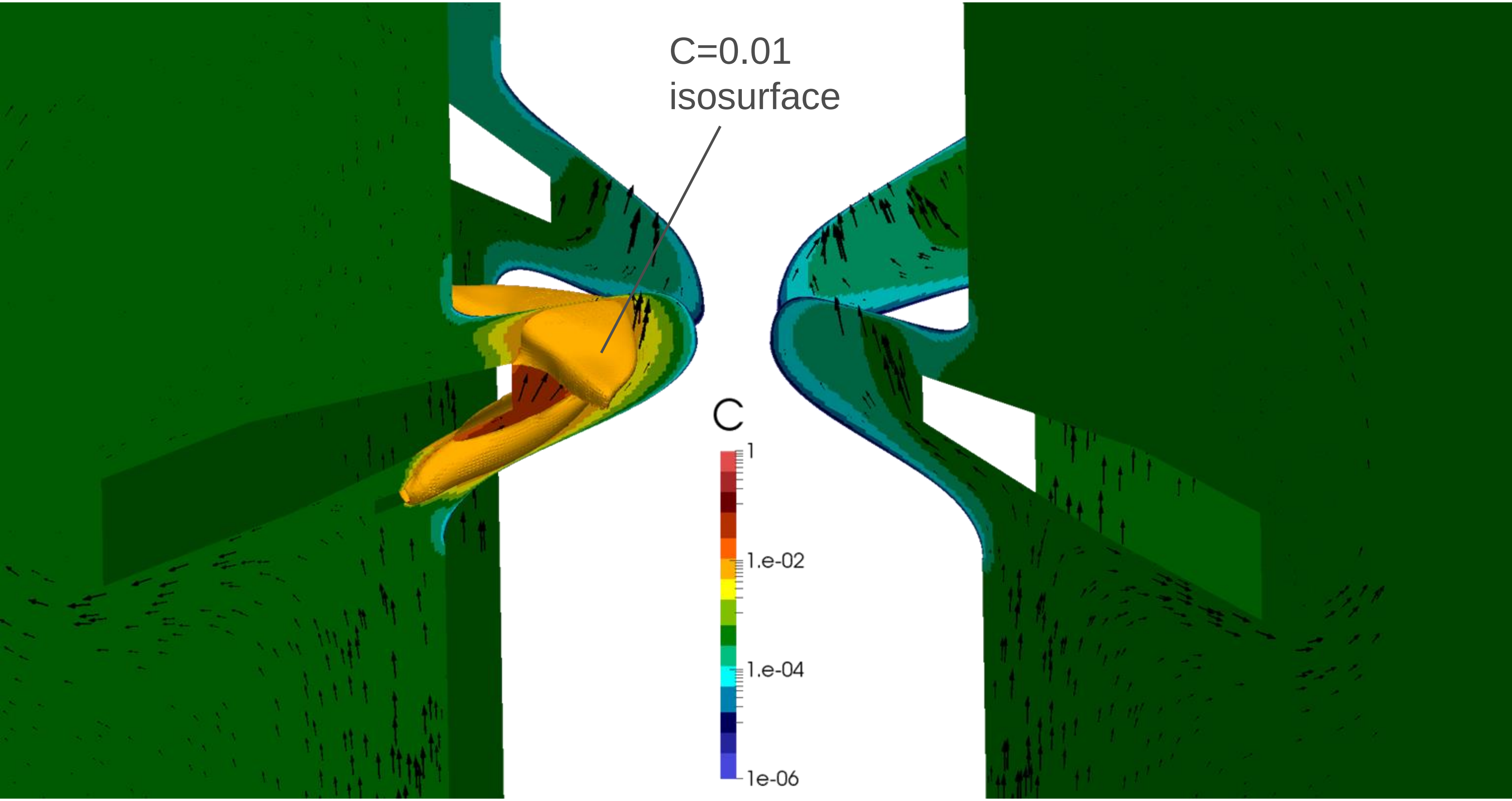
Comparison with previous axisymmetric calculations



Free surface ← → Open front

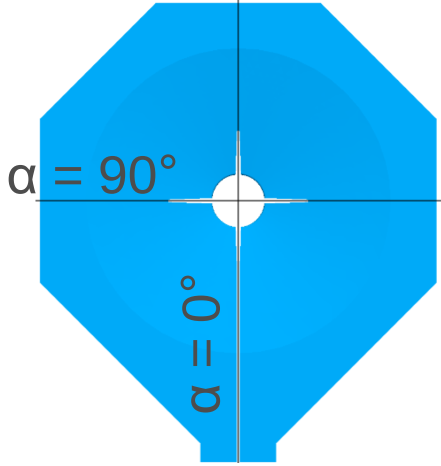
Calculation results

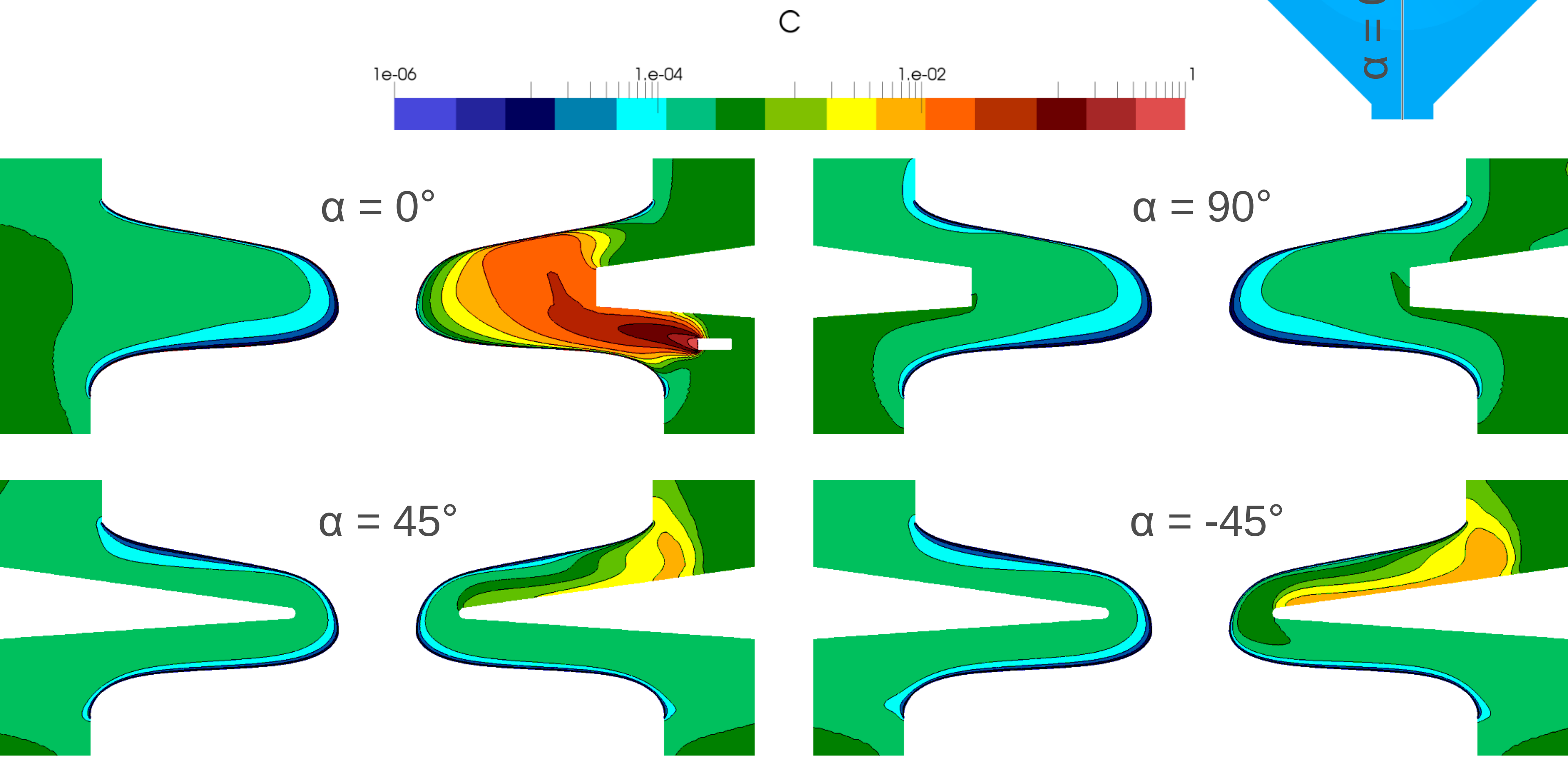
Dopant concentration



Calculation results

Dopant concentration





Conclusions and outlook

1. 3D gas flow calculations in FZ puller have been carried out for the first time
2. snappyHexMesh is hard to master, but it is suitable for mesh generation in a complex geometry
3. Calculated fields are strongly three-dimensional; symmetry is obtained with respect to the plane of main inductor slit
4. 3D calculations predict stronger gas cooling than previous axisymmetric simulations
5. The obtained concentration field and dopant mass fluxes at Si surfaces are used to create non-symmetric boundary conditions for 3D HD simulation of liquid Si flow (these results are not included in the present talk)