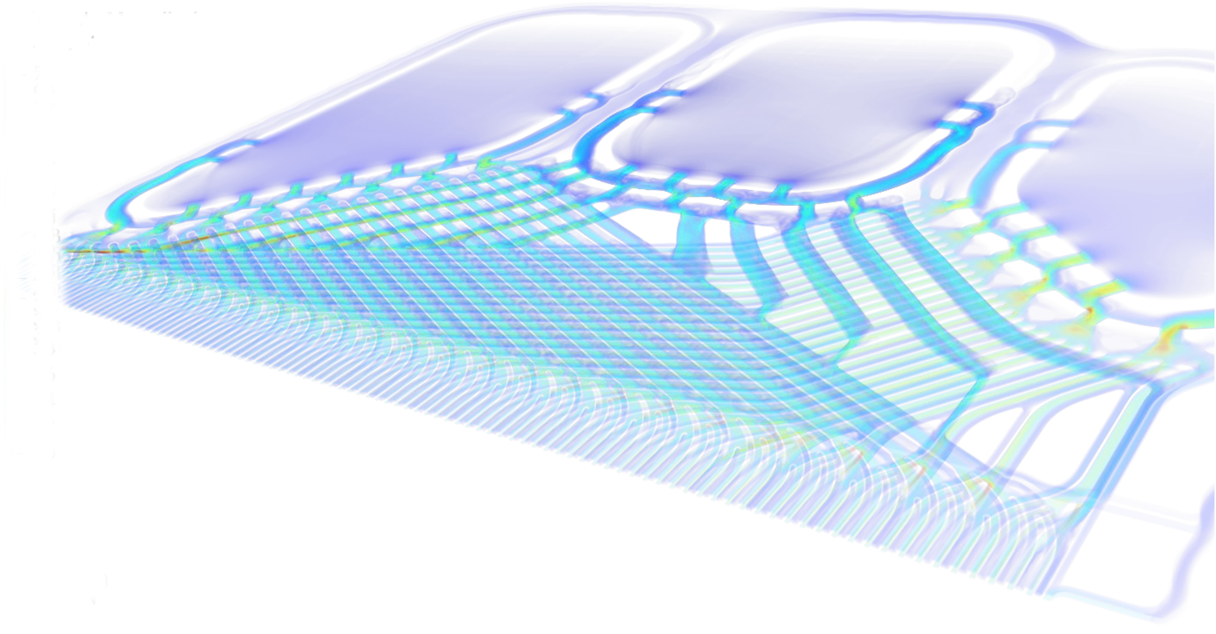
OpenFoamZSWPemfcToolbox

Example



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Compatibility

OpenFOAM v7

Getting started

- Installation of OpenFOAM v7 https://openfoam.org/version/7/
- Compiling pemfcFoam solver

Cover picture:

Generic fuel cell stack: open development platform for industry

https://www.zsw-bw.de/en/projects/brennstoffzellen/generic-fuel-cell-stack-open-development-platform-for-industry.html

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Single channel model of ZSW 300 cm² automotive cell design

To demonstrate the Toolbox, an example of a single channel simulation model is prepared. The file and folder structure of this example is shown in Figure 1. The simulation process can be performed by executing *Allrun* files. The single steps of *Allrun* and the geometry of the example are described below.

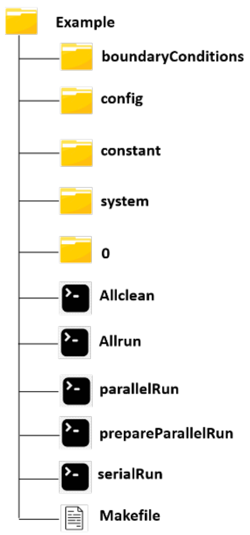

Figure 1: File and folder structure of example

Cell design and operating condition

For the single channel simulation model the ZSW automotive cell design (300 cm² active area, see Figure 2) is used. This graphite bipolarplate cell design consists of 100 straight rectangular cathode and 50 straight rectangular anode channels. For the simulation one-half of the repeating unit (1/100 of active area width) is modelled (cf. Figure 3). At the domain borders, symmetry boundary conditions are defined. As operating conditions automotive conditions are used (cf. Table 1). The mass flow rates and mass fractions, which are needed for boundary condition definition, are calculated based on Table 1.

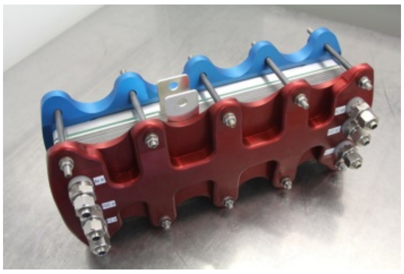

Figure 2: 5-cell short stack of ZSW 300 cm² automotive cell design

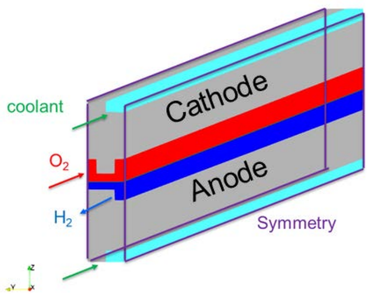

Figure 3: Single channel simulation model of repeating unit of ZSW 300 cm² automotive design active area channels (1/100)

Table 1: Operating Conditions

	Cathode	Anode
Pressure Stack Outlet (bar_a)	2.0	2.2
Temperature Stack Inlet (°C)	73.0	73.0
Stoichiometry	1.6	1.6
Dew point temperature (°C)	48.5	53.0
Gas composition	100% Air	30% N_2 / 70% H_2
Coolant Temperature Stack Inlet (°C)		68

Mesh generation

The mesh generation is done by *mesh* section (*bmesh, regionMesh, defineZones*) within *Makefile* files called by *Allrun*. The hexahedral mesh itself is generated with *blockMesh*. The mesh is refined both, inside the gas and coolant channels, and even more in the GDL and catalyst layer (cf. Figure 5). Grading from channels to membrane is used. Six mesh regions are defined cf. Figure 4:

- **air**: cathode gas channel, GDL (substrate + MPL) and catalyst layer (CL)
- **fuel**: anode gas channel, GDL (substrate + MPL) and catalyst layer (CL)
- **coolant**: coolant channel
- **cbp**: cathode bipolar plate (BPP)
- **abp**: anode bipolar plate
- **electrolyte**: membrane

The naming of this regions is mandatory. Identical *cellZones* has to be defined. Additional *cellZones* for gas channel, GDL substrate, MPL and catalyst layer in region air and fuel are defined with *topoSet*.

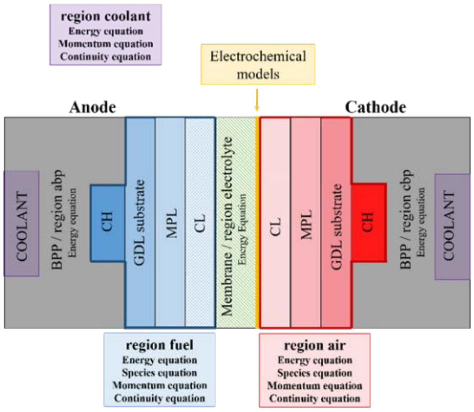

Figure 4: Schematic description of simulation model

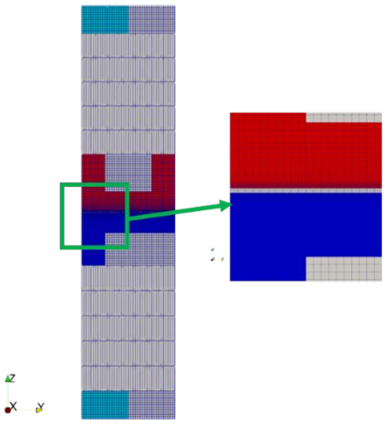

Figure 5: blockMesh of single channel model

Two different *blockMesh* files considering two different mesh resolutions (coarse and fine) are prepared. The coarse mesh resolution can be used for testing solver compilation in serial mode. The fine mesh resolution should be used in parallel mode because of high calculation time. It provides a more accurate results than the coarse mesh resolution.

Simulation

The simulation is started by the *Makefile.Serial* or *Makefile.Parallel* file during performing *Allrun.Serial* or *Allrun.Parallel.* In serial case the coarse mesh resolution is used. Performing *Allrun.Serial* takes 1.04 hours on an Intel® Xeon® Gold 6154 machine. Performing *Allrun.Parallel* takes 10.2 hours on 20 cores on an Intel® Xeon® Gold 6154 machine.

For defining boundary conditions and material properties *codeStream* is used. The values can be described within the files located in the *boundaryCondtions* folder:

- **Air**: boundary conditions for region air (U, p, T, YO2air, YH2Oair, rho, diffO2air)
- **Coolant**: boundary conditions for region coolant (U, T, p, rho)
- **Material**: material properties of GDL (substrate + MPL), CL, BPP and membrane
- **Fuel**: boundary conditions for region fuel (U, p, T, YH2fuel, YH2Ofuel, rho, diffH2fuel)
- **Electrochemistry:** parameters of the electrochemical models