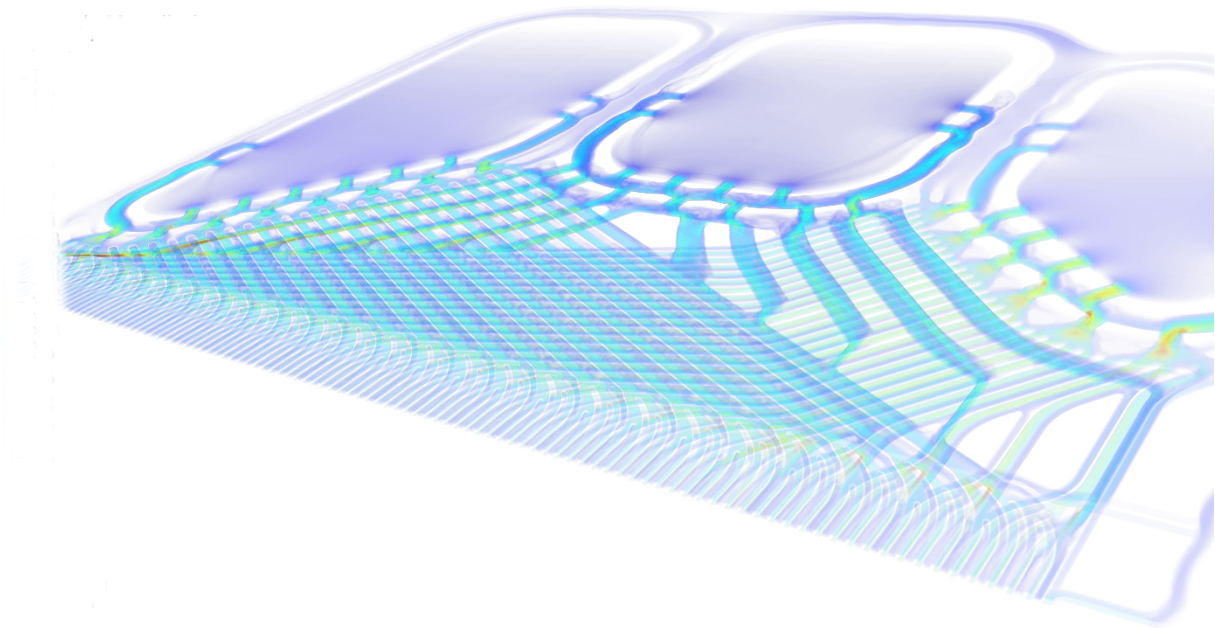




OpenFoamZSWPemfcToolbox

Example



July 2023

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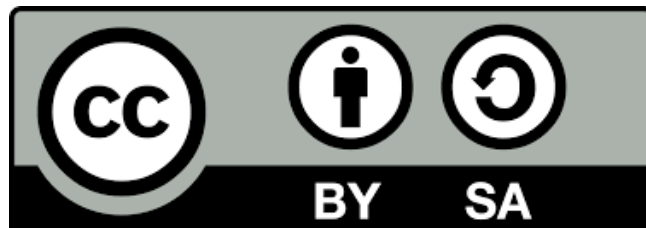
Compatibility

OpenFOAM v7

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

As a showcase example for the OpenFoamZSWPemfcToolbox a single channel simulation model is prepared. The file and folder structure of this example is illustrated in Figure 1. The simulation process can be performed by executing the *Allrun* file. The single steps of *Allrun* and the geometry of the example are described below.

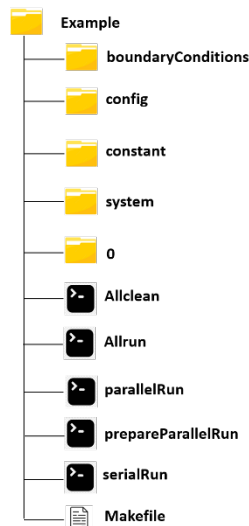


Figure 1: File and folder structure of example

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 (1/50 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 this table.

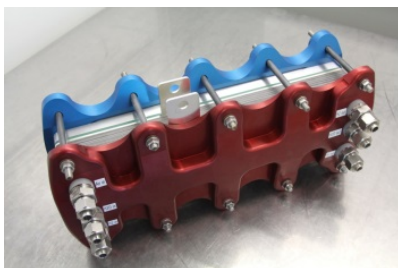


Figure 2: 5-cell short stack of ZSW 300 cm² automotive cell design

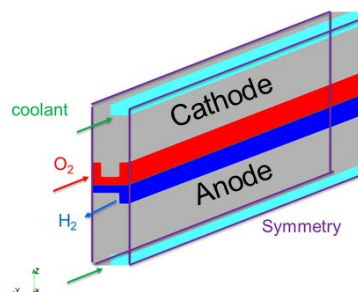


Figure 3: Single channel simulation model of repeating unit of ZSW 300 cm² automotive design active area channels (1/50)

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 (°)	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* file 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 comparable to 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*.

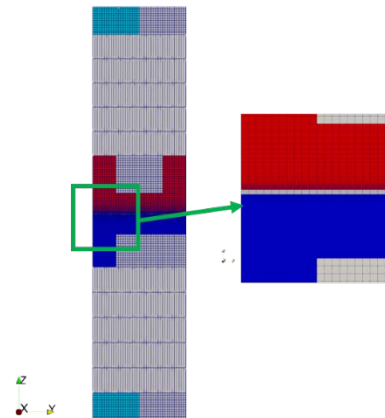
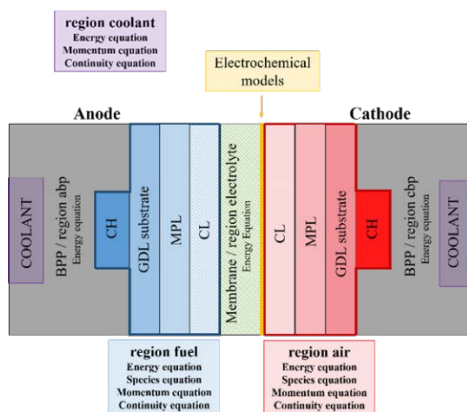


Figure 4: Schematic description of simulation model

Figure 5: blockMesh of single channel model

Simulation

The simulation is started by the *Makefile* file during performing *Allrun*. The simulation can be performed in serial mode by running *serialRun* script or in parallel mode by running *prepareParallelRun* and *parallelRun* scripts. The mode can be changed by adding *runSerial* or *runParallel* in line *All* within *Makefile*. In case of parallel mode, the solution is reconstructed after simulation is converged.

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