

## Annex 37: Modelling for Fuel Cells Systems

Annex 37 focuses on the design, development, and application of suites of *open source computational fluid dynamics* (CFD) software for application to fuel cells, as well as electrolysers and other electrochemical applications. Computational models provide unique insight into the science and engineering of fuel cells systems and system components. Multi-scale models ranging from nano-scale to systems-level balance-of-plant, complement and enhance the physical gathering of experimental data in the laboratory. In some situations a model can even provide a more realistic picture of reality than an artificial physical experiment.

In the last century, fuel cell scientists often wrote their own source codes, from scratch, in FORTRAN or C. Subsequently a number of commercial houses developed proprietary CFD codes which were adapted/modified to simulate fuel cells. More recently, the development of well-written and optimised open-source CFD software has stimulated activities in fuel cell application and development by member groups. The IEA Modelling Annex coordinates the activities and developments of the group, fostering communication, and co-locating activities in an aligned manner. The groups' activities range from fundamental pre-competitive science and research to practical industry-oriented technology. At present, the activities of the Annex are focused on continuum-level models and codes. All code must be in the source, openly-shared, and cost-free (not for sale). The IEA Annex 37 provides a suitable platform for the joint development of such a global, freely available toolkit, with the aim to enable more effective progress modelling science. By sharing the interface, duplication of resources is avoided, while at the same time, privacy of sensitive data, particular to any design, is maintained.

An important related activity is code validation and verification by comparison with other CFD codes, physical experiments, development of benchmarks and standardised 'round-robin' tests. The main focus, at this time, is on solid oxide fuel cells (SOFCs) and polymer electrolyte fuel cells (PEFCs). Other fuel cells and electrochemical devices may be included within the scope of the Annex, in due course.

There are presently three subtasks:

Subtask 1: Code development. This is focused on the development of suites of open source software for application to fuel cells.

Subtask 2: Experimental validation. The subtask will gather experimental data for model validation for both SOFCs and PEMFCs. This includes the adoption of common experimental protocols

Subtask 3. Model equations: best practices. Output will be a report outlining recommended state-of-the-art physics/mathematics. Subtask 3 is deferred until subtasks 1 and 2 are substantially complete.

Currently active members are (in alphabetical order): Croatia, Denmark, France, Germany, Italy, Netherlands, Sweden, USA.

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