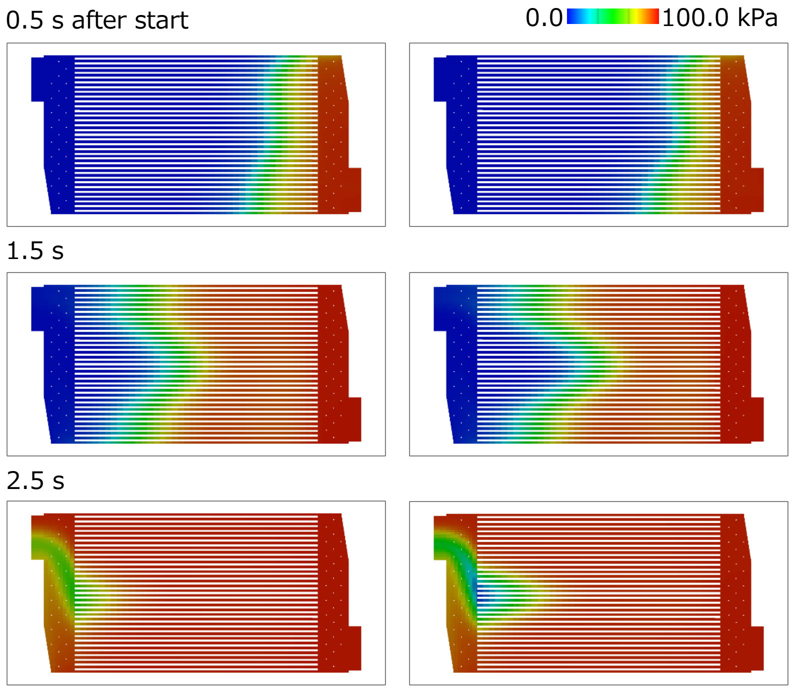
Example 3: Prediction of Durability Performance

Effect of Thinning on Carbon Corrosion

226th ECS meeting, Cancun (2014)

To enhance the durability of polymer electrolyte fuel cells, it is crucial to prevent carbon corrosion during activation. In this example, we analyze the effect of channel thickness on carbon corrosion in a cathode catalyst layer. The right figures compare changes of hydrogen partial pressure distribution for (a) the base cell and (b) the thinner cell whose channels are downsized by 20%. Hydrogen exchange in center channels occurs slowly because of channel thinning. Consequently, the amount of carbon corrosion in a cathode catalyst layer increases by 10%. This indicates that an even flow distribution is also important in terms of durability.



(a) Base cell (b) With thinned channel

Changes of hydrogen partial pressure during activation

Product Specification

Analysis Target	Polymer electrolyte fuel cell (PEFC) From single cell to entire stack (up to 400 cells)
Applications	For power generation performance: ■ Evaluation of flow channels by estimating the distribution of flow-rate balance between cells and uniformity of various internal states ■ Estimation of cell performance and internal states (e.g., water content and current density) under severe operating conditions (e.g., low stoichiometry and high temperature (over 100°C)) ■ Analysis of the effects of MEA characteristics’ change due to a reduction of the Pt content on power generation performance ■ Estimation of heat generation and transfer, i.e., whether warm-up time meets the criteria for activation from low temperature For durability performance: ■ Estimation of carbon corrosion in a cathode catalyst layer during activation/deactivation ■ Prediction of areas where the dry/wet cycle intensively occurs
Calculation Status	I–V characteristics and distributions of various internal states: current density, overpotential, water content, gas concentration, gas–liquid volume ratio, pressure, temperature, and so on
Numerical Models	Well-validated reliable models achieving fast simulation for full-scale cells and stacks: ■ Electromotive force models: open-circuit voltage with consideration of hydrogen cross leak, electrochemical reaction (Butler–Volmer equation), catalyst layer model (transport resistance owing to catalyst layer), and so on ■ Mass transport through MEA: water back diffusion, electro-osmotic drag, proton conduction, and gas transport ■ Two-phase flow model (channel/GDL/MPL), single-phase flow model, and heat transport (coolant) ■ Heat and mass transport model (channel/GDL/MPL) and Heat transfer model (solid part)
Computational Time	One day for a stack of 400 cells (fixed load) Note: One core is used per cell. The computational time depends on computer performance.
System Requirements	【GUI】OS: Windows 10, 11 (64 bit, Microsoft .NET Framework 4.7 or later) 【Solver】OS : Linux（Red Hat Enterprise Linux7, 8)

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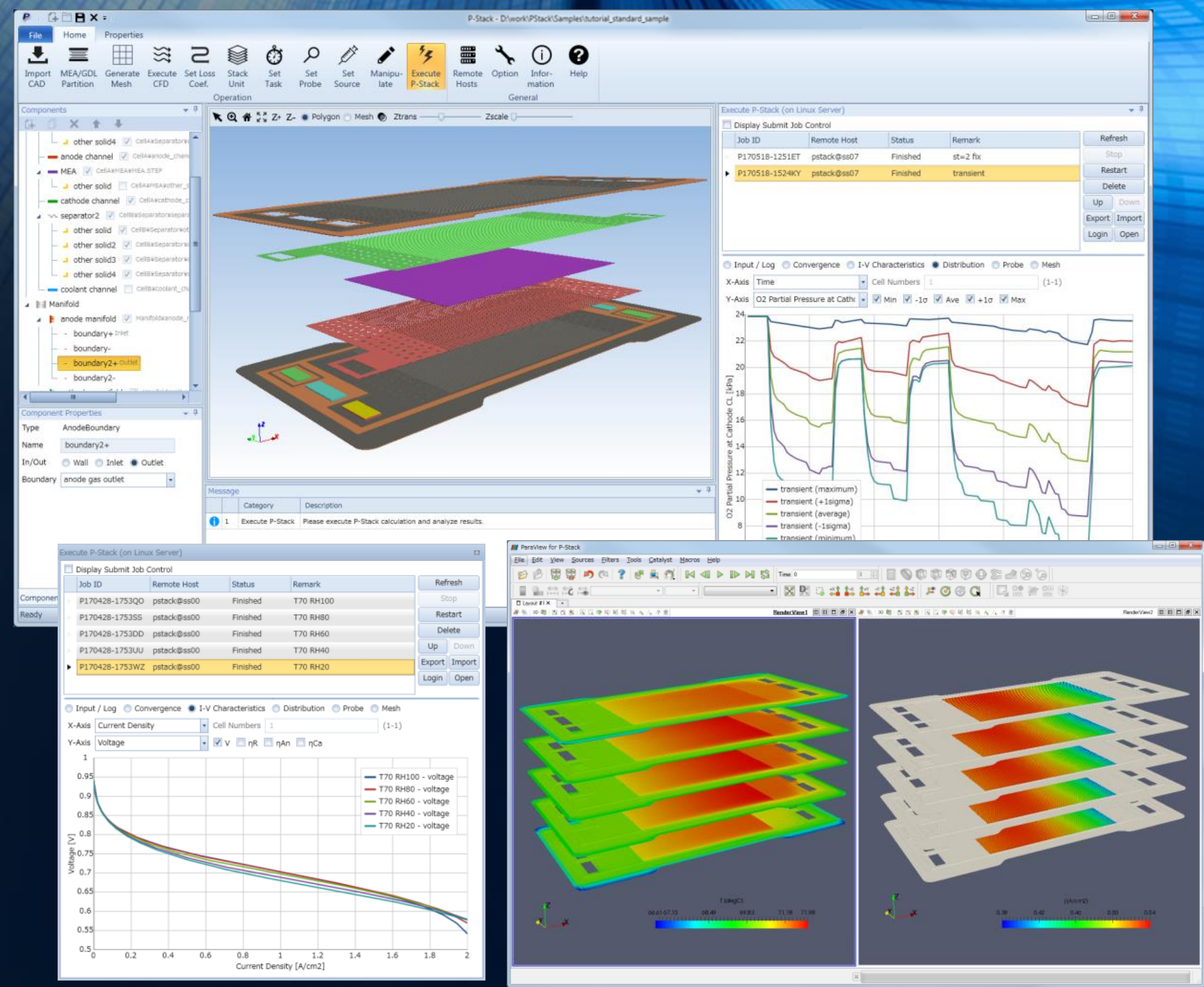
PEFC Simulation Software Package

P-Stack®

P-Stack accelerates the developments of cells and stacks for PEFC by

- ✓ ***revealing internal phenomena that cannot be observed by experiments***
- ✓ ***reducing the trial manufacturing cost through performance estimations of new cells and stacks***
- ✓ ***predicting material degradation under various conditions***



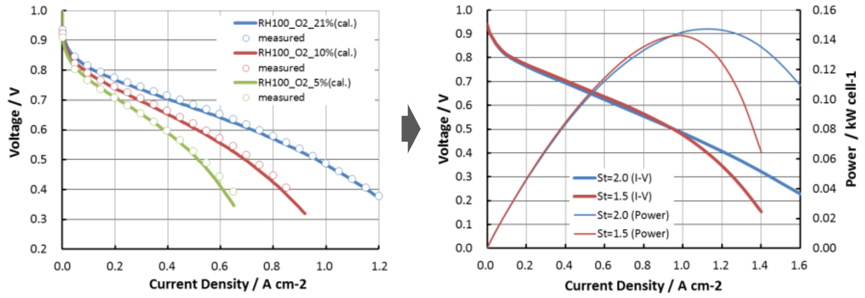
Features:

- ✓ **rapid estimation of power generation performance and analysis of internal states for full-scale cells and stacks**
- ✓ **analysis of various internal states, including current density, water content and temperature, under various operating and structural conditions**

P-Stack: Fast and Reliable Simulator for Full-Scale Cell and Stack

Strategy for Fast Computation

Because internal phenomena in fuel cells are related to multiple physics aspects, computational costs for their simulation tend to be high using general CAE software. P-Stack® rapidly simulates the performance and internal states of full-scale fuel cells and stacks. A drastic reduction of computational costs is achieved by well-validated numerical models such as the MEA model, which reproduce measured I–V characteristics.

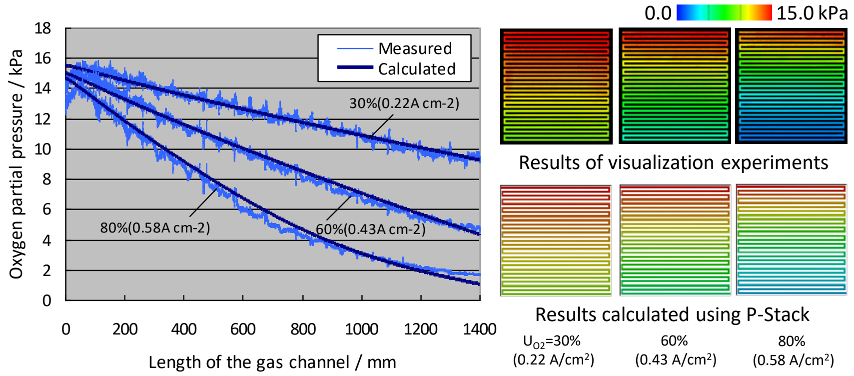


Numerical models are fitted to reproduce the measured I–V characteristics of mini-cells

Characteristics of actual-sized cells and stacks can be rapidly obtained

Well-Validated Reliable Numerical Models

Numerical models in P-Stack well reproduce not only the I–V curve but also various internal states. The figures on the right hand side present a comparison of the measured and calculated oxygen partial pressure distributions in a cathode channel under different utilization ratios U_{O2}. The calculated results are in good agreement with the measured data for all U_{O2} cases. Oxygen is consumed almost constantly in low-U_{O2} condition, while a relatively faster consumption of oxygen is observed in the upper-flow region for U_{O2} = 80%. These behaviors are also well reproduced by P-Stack. These results indicate that the MEA model in P-Stack can quantitatively estimate oxygen consumption owing to the ORR reaction.



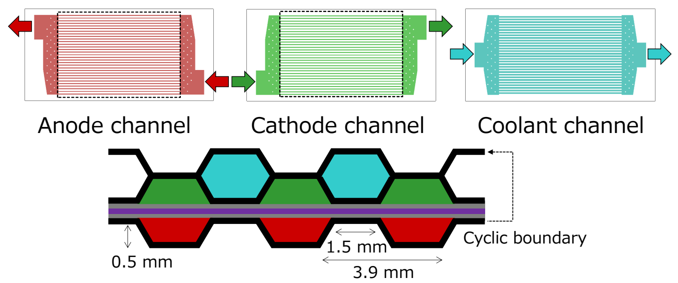
Comparisons of the measured and calculated oxygen partial pressure distributions in a cathode channel for different utilization ratios U_{O2}.
The experimental data are provided by the University of Yamanashi, Japan

M. Yoneda, et al., ECS Trans., 11, 1105 (2006). 11th ASME, Minneapolis, (2013)

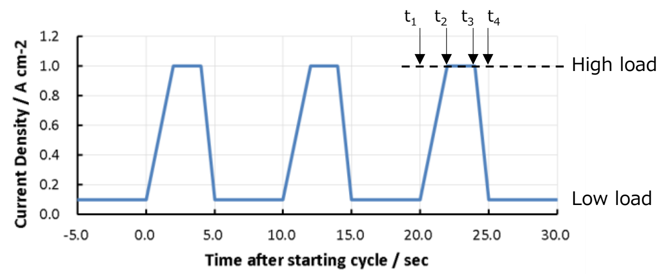
Example 1: Effect of Load Fluctuation on Full-Scale Cell

Dry and Wet Cycles of Membrane due to Load Fluctuation

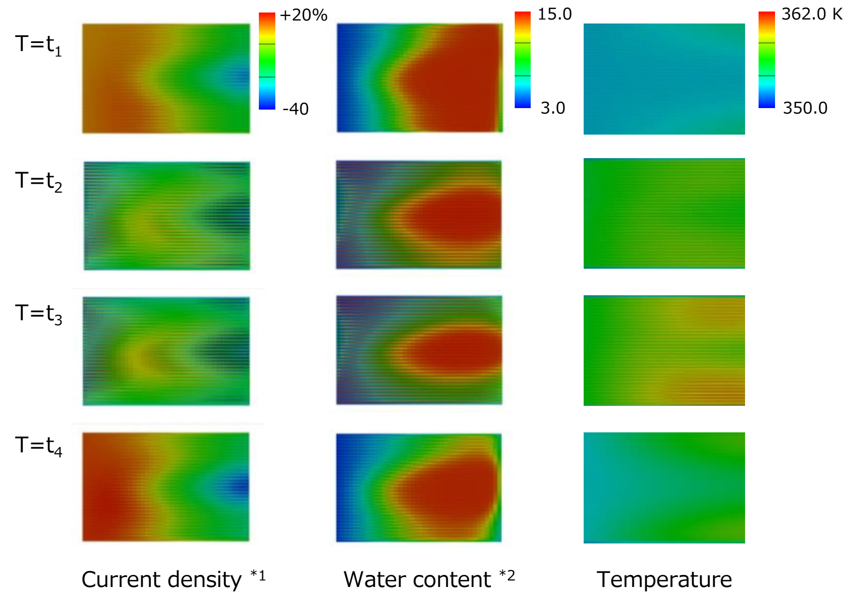
Dry/wet cycle causes mechanical deterioration of electrolyte membranes. The internal states of a full-scale cell were simulated under loading cycles, which imitate actual operating conditions. The distributions of current density, water content, and temperature in a membrane are shown in the right-hand-side figures. A large difference was observed in the water content between channels and ribs (see horizontal stripes in the distributions). High-temperature areas appear in both sides of the coolant outlet at T = t_3, and the water content decreases in these areas because of the temperature. As indicated in the example, P-Stack can estimate the area where the dry/wet cycle intensively occurs and predict the area where mechanical deterioration is likely to occur.



Cross-sectional diagram of the cell



Pattern of the loading cycle



Changes of the MEA internal states at each load fluctuation

*1 Relative deviation from average current density
*2 Number of water molecules per one sulfonic acid group

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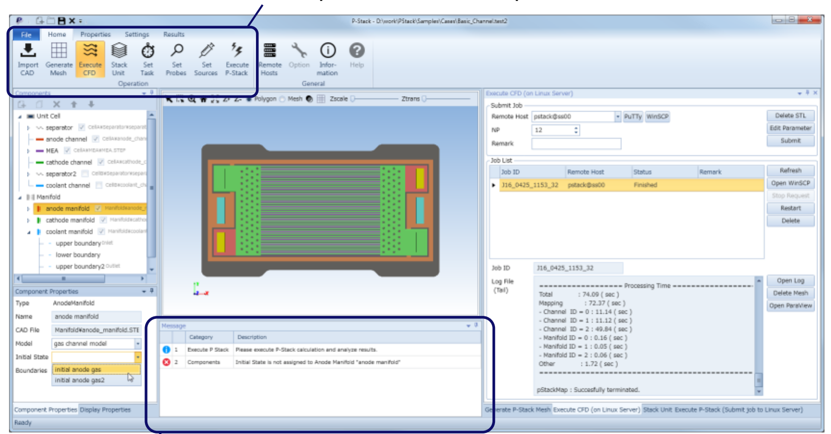
Semi-Automated Workflow and User-Friendly GUI for P-Stack

3D CAD
Automatic Mesh Generation
Mesh
CFD (for Single Cell + Manifold)
Fluid Parameters
Thermofluid Dynamics
Exp. Data
Pressure, Flow Rate
MEA Parameter Fitting
Parameters for MEA
Power Generation Simulation
Performance, Durability
Done

Output Useful for Designing Optimal Cell and Stack

- pressure drop and flow rate balance in a cell
- predicting area where liquid water stagnates
- pressure drop and flow rate balance in a stack
- pressure fluctuation and hydrogen exchange during activation/deactivation
- current density, water content, and temperature distributions depending on conditions
- effect of load fluctuation

These buttons correspond to each step of the workflow



Displays directions and warnings/errors with regard to settings

Semi-Automated Workflow

The typical simulation procedure using P-Stack is shown in the left-hand-side flowchart. 3D CAD data of an actual cell and MEA characteristics measured in a mini-cell are required as input data.

Mesh generation from 3D CAD data and the determination of fluid parameters using CFD are automatically performed. These features drastically reduce the required manpower to setup simulations. Combined with the low computational costs of P-Stack, the total work period can be much shorter than that of general CFD-based approach.

* The auto meshing was implemented based on the algorithm developed by Elysium Co. Ltd.

User-Friendly GUI

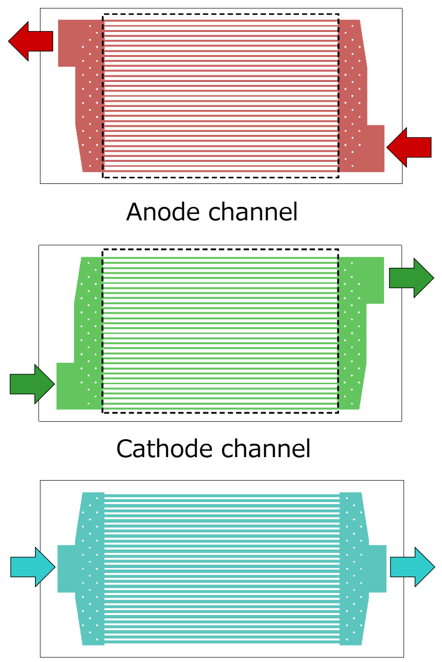
The GUI of P-Stack is designed such that it can be intuitively used without requiring operation manuals. By sequentially clicking buttons on the ribbon tab, a user can proceed with the workflow steps. The message panel displays directions and warning/error messages to guide users (left-hand-side figure).

Parallel computations on Linux® servers can be easily executed by clicking a few buttons without fiddly command-line operations. Copy and paste from Microsoft® Excel® to the GUI are supported. Table data such as time-series data measured by experiments can be easily provided as an input.

Example 2: Performance and Internal State of Full-Scale Stack

Effect of Operating and Structural Conditions on the Internal state and Cell Performance

In this example, we investigate the effects of the operating and structural conditions on a stack of 100 cells, whose reaction area is 260 cm². The figures below show the distributions of the temperature and current density under stationary operating conditions: load current density 0.2 A/cm², anode utilization 75%, and cathode utilization 50%. This study indicates that manifold downsizing produces an uneven flow rate across cells, while a higher loading current causes an increase of water in the end cell. Both effects result in the performance degradation of the stack system.



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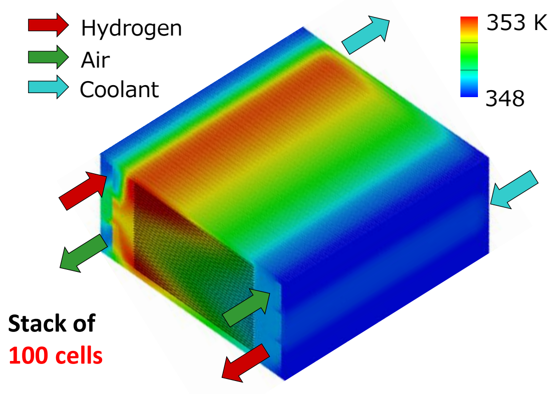
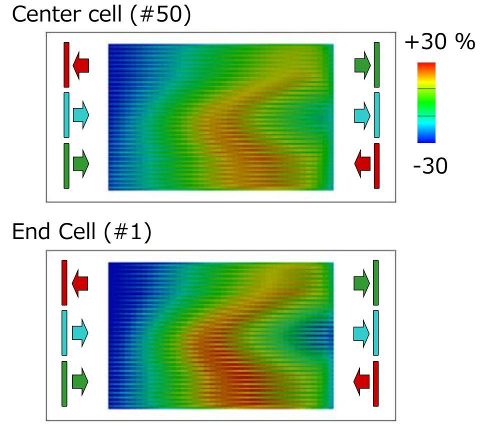
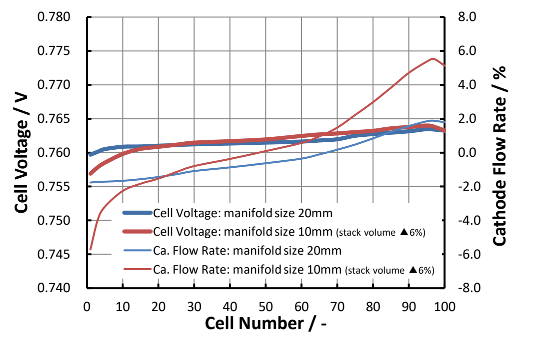


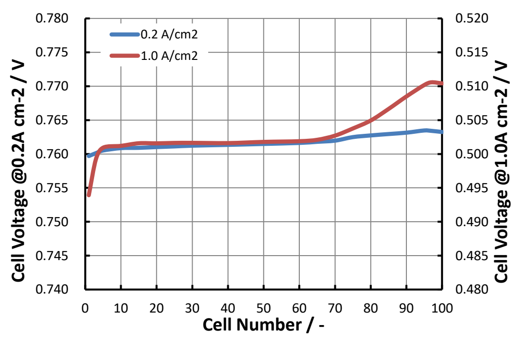
Temperature distribution in a stack of 100 cells



Local current density



Effect of manifold size on performance



Effect of loading current density on cell voltage