A numerically highly efficient dynamic quasi-2D PEMFC model including non-isothermal and phase change processes

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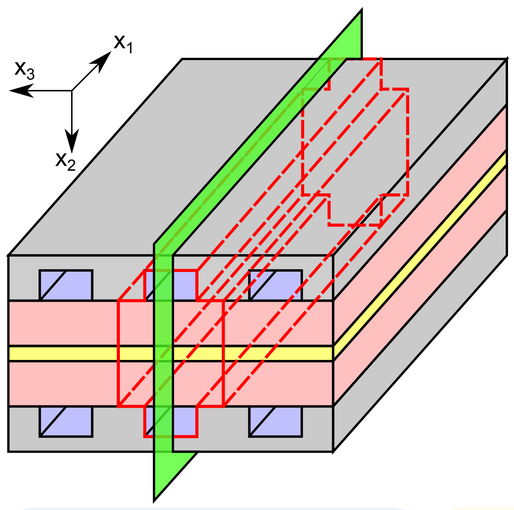
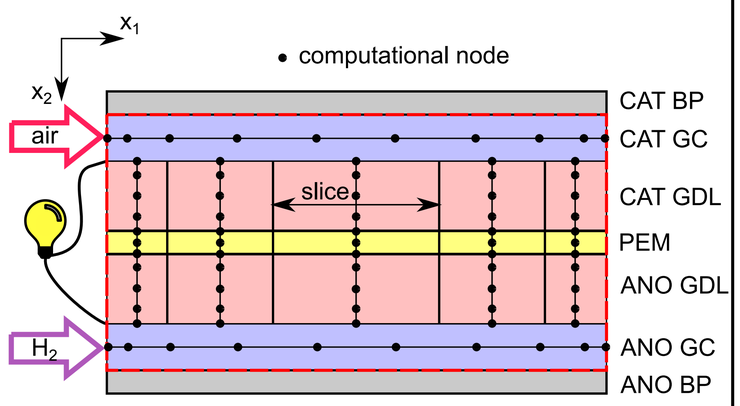
Model based fuel cell control

- Identification of degradation relevant operating conditions
- Development of test cycles for performance and degradation analysis
- Development of control strategies for transient operation
- Increase the lifetime and efficiency of fuel cells

transient simulation — **spatial resolution depth**

Quasi-2D[1] multiphase mixture[2] approach





$N_{GC} = 12$, $N_{GDL} = 5$, $N_{PEM} = 3$, $N_{SL} = 5$

GCs & GDLs
- ✓ Convection
- ✓ Multicomponent diffusion
- ✓ Capillary fluxes
- ✓ Phase change

PEM
- ✓ Electro-osmotic drag
- ✓ Diffusion
- ✓ Joule heating
- ✓ Thermal conduction

Catalyst layers
- ✓ Chemical reactions
- ✓ Polarisation losses
- ✓ Finite rate PEM sorption
- ✓ N_2 crossover

3D integral conservation laws — **non-dimensionalization**

System of non-linear PDEs (GC)

Mixture mass
$$\partial_t \rho_m + \partial_{x_1}(\rho_m u_{m,1}) = -K_T\, \varepsilon \rho_m u_{m,2}\,|_{GDL}$$

Liquid mass
$$\partial_t s_l + \partial_{x_1}(s_l u_{m,1}) = K_\rho\, \dot{m}_l - [K_{L1}\, \varepsilon \rho_m u_{m,2} + K_{L2}\, \psi_l]\,|_{GDL}$$

Reactant mass
$$(1-s)\rho_g\left[\partial_t \xi_g^\alpha + u_{m,1}\partial_{x_1}\xi_g^\alpha\right] + K_{S1}\,\partial_{x_1} j_{g,1}^\alpha = \dot{m}_l \xi_g^\alpha - K_{S2}\, j_{g,2}^\alpha\,|_{GDL}$$

H_2O mass
$$(1-s)\rho_g\left[\partial_t \xi_g^{H_2O} + u_{m,1}\partial_{x_1}\xi_g^{H_2O}\right] + K_{S1}\,\partial_{x_1} j_{g,1}^{H_2O} = \dot{m}_l(\xi_g^{H_2O} - 1) - K_{S2}\, j_{g,2}^{H_2O}\,|_{GDL}$$

Energy
$$\rho_m c_m[\partial_t T + u_{m,1}\partial_{x_1} T] + K_{E1}\,(1-s)\rho_g \xi_g^{H_2O}[\partial_t T_{sat} + u_{m,1}\partial_{x_1} T_{sat}] + K_{E2}\, j_{g,1}^\alpha \partial_{x_1} T + j_{g,1}^{H_2O}[K_{E3}\,\partial_{x_2} T + K_{E4}\,\partial_{x_1} T_{sat}] = -(K_{E5} + K_{E6})(T - T_{BP}) - K_{E7}(T - T_{GDL})$$

Momentum
$$\partial_t(\rho_m u_{m,1}) + \partial_{x_1}(\rho_m u_{m,1}^2) + K_{M1}\,\partial_{x_1} p = K_{M2}\,\partial_{x_1}(\mu_g \partial_{x_1} u_{m,1})$$

Closure
$$K_{EOS}\,\rho_g \sum_\gamma \frac{\xi_g^\gamma}{\mathcal{M}_\gamma} = p \qquad \xi_g^\alpha + \xi_g^{N_2} + \xi_g^{H_2O} = 1 \qquad K_\rho[\rho_m - (1-s_l)\rho_g] = s_l$$

Equation of state — Mass fractions — Mixture density

1D description of domain/slice — **assessment of relevant effects**

Numerical treatment

Variable time-stepping [3]
$$\left(\frac{\partial r}{\partial t}\right)^{(n+1)} = \frac{(1+2\alpha)r^{(n+1)} - (1-\alpha)^2 r^{(n)} + \alpha^2 r^{(n-1)}}{(1+\alpha)\Delta t^{(n+1)}} + \mathcal{O}(\Delta t^2)$$

Chebyshev collocation [4]
$$r_i' = \sum_j D_{ij}^{(1)} r_j\,.$$

Linearisation in time **(LIT)** [5]
$$(rs)^{(n+1)} = r^{(n+1)}s^{(n)} + r^{(n)}s^{(n+1)} + r^{(n)}s^{(n)} + \mathcal{O}(\Delta t^2)$$

System of linear equations
$$\sum_j A_{ij}\, x_j = b_i$$

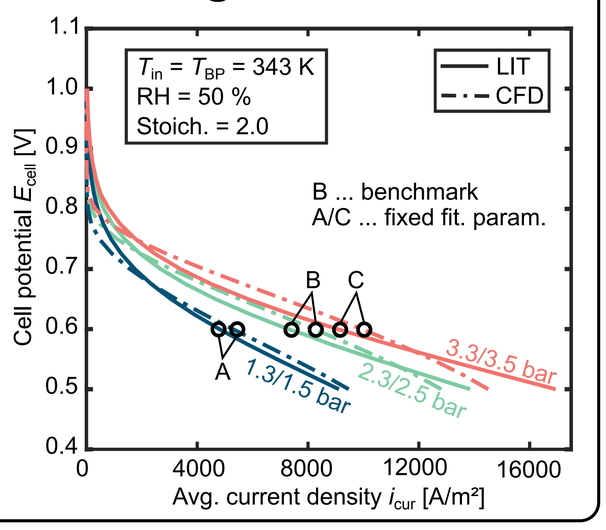
supplement experimental setups — **extract critical parameters**

Polarisation curve fitting

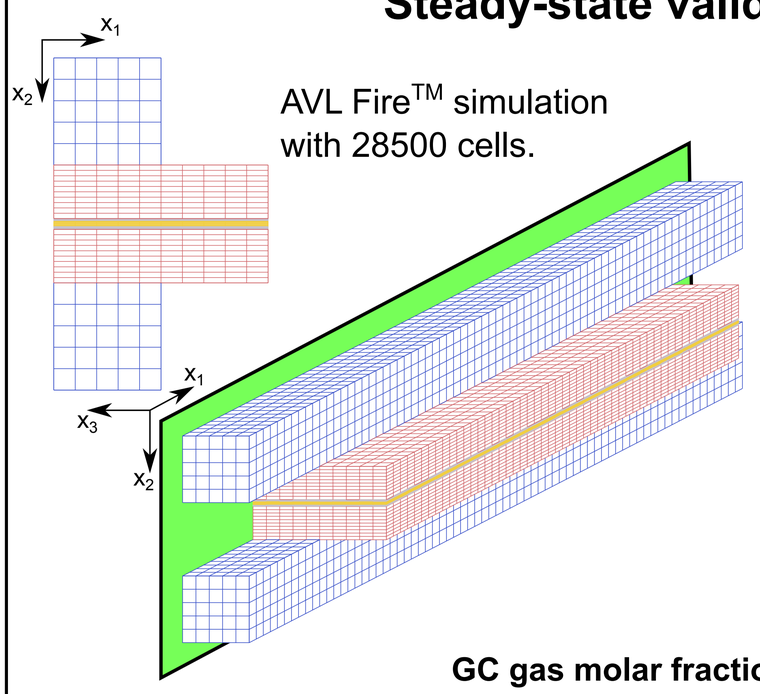
Multithreading particle swarm optimization adjusts the LIT model's electrochemical fitting paramters to match a reference polarisation curve, running several simulations in parallel.

$$\tilde{E}_{cell} = \tilde{E}_{OC} - \frac{\tilde{\mathcal{R}}\tilde{T}}{\alpha_C \tilde{F}}\ln\left(\frac{\tilde{i}}{\tilde{i}_0}\right) - \tilde{i}\int_0^{\tilde{H}_{PEM}} \frac{d\tilde{x}_2}{\tilde{\sigma}(\lambda)}$$

$$\tilde{i}_0 = \tilde{i}_{0,r}\tilde{a}_C\tilde{L}_C\left(\frac{\tilde{p}^{O_2}}{\tilde{p}_r^{O_2}}\right)^{\gamma_C}\exp\left[-\frac{\tilde{E}_{act}}{\tilde{\mathcal{R}}\tilde{T}}\left(1 - \frac{\tilde{T}}{\tilde{T}_{0,r}}\right)\right]$$



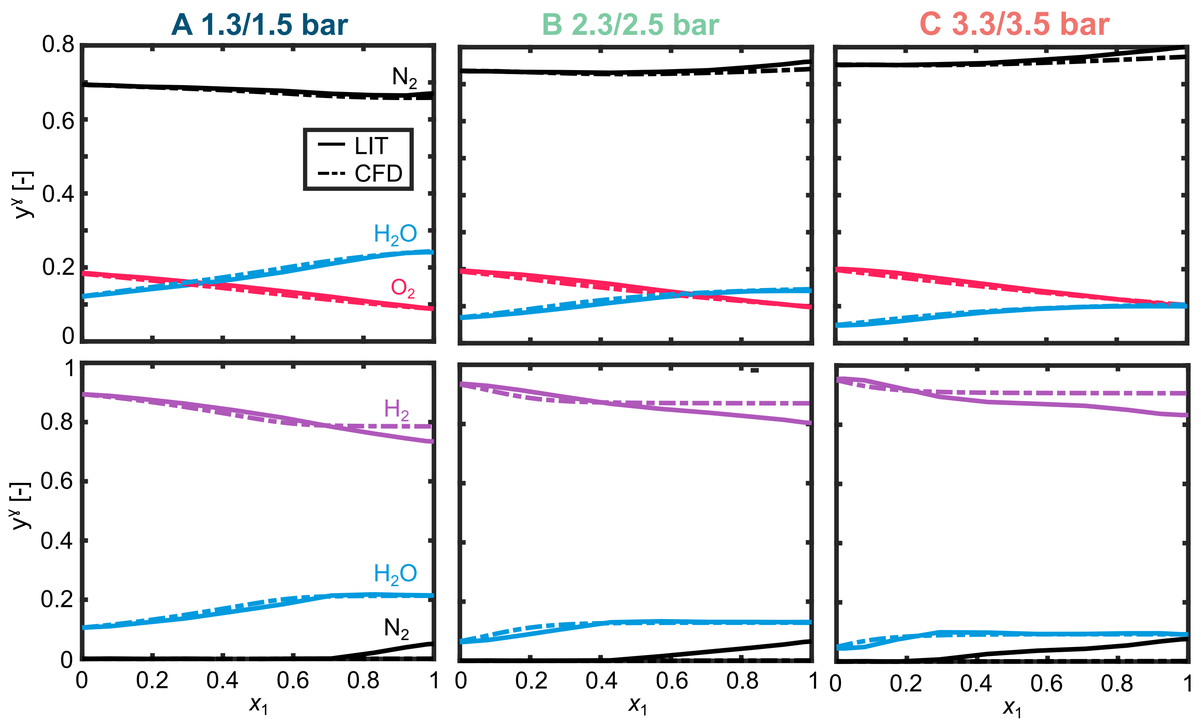
Steady-state validation



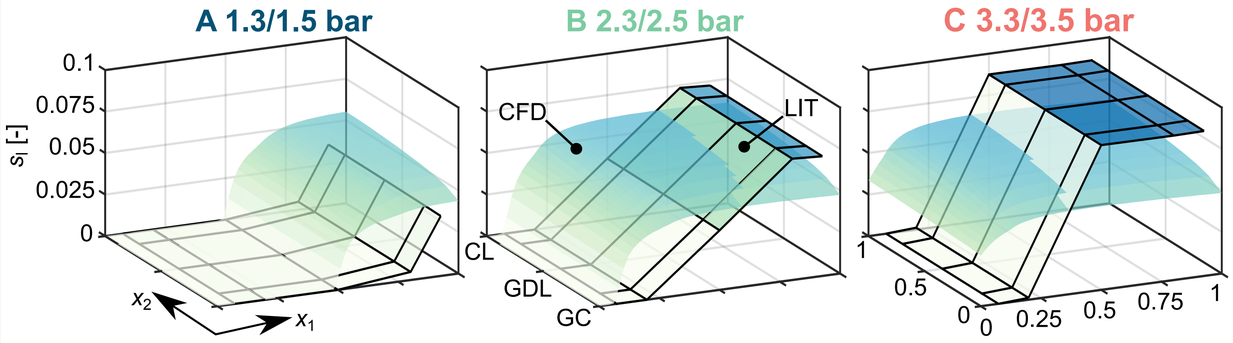
AVL Fire™ simulation with 28500 cells.

Predictive capabilities of the LIT model with fixed fitting parameters:
- ✓ Gas species distribution
- ✓ PEM hydration characteristics
- ✓ Flooding prediction
- ✓ Sufficient accuracy for control tasks
- ✓ LIT computation time < 1% of CFD simulation

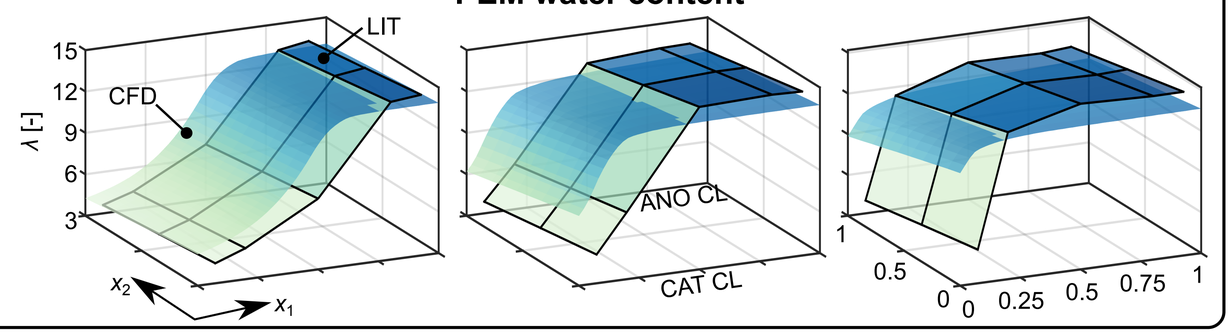
GC gas molar fractions



CAT GDL liquid water saturation

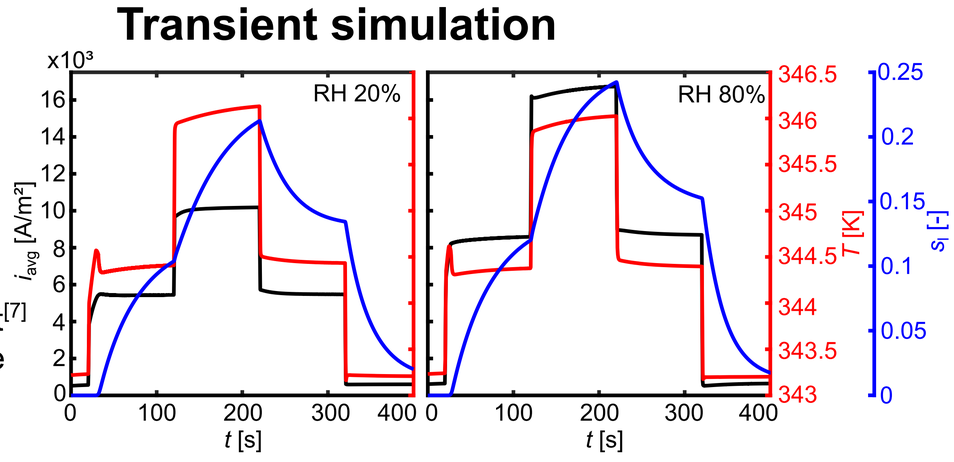


PEM water content



Transient simulation

Prescribed cell potential steps: 0.8 - 0.6 - 0.5 - 0.6 - 0.8 V:
- ✓ temperature overshoot[6]
- ✓ current density over-/undershoot[7]
- ✓ computation time ≈ 1200 s



Characteristic transport timescales obtained directly from dimensionless groups of the governing equations:

$$\tilde{\tau}_{heat} = \frac{\tilde{H}_{GDL}\tilde{\rho}_{GDL}\tilde{c}_{GDL}}{\tilde{\alpha}} \approx 0.8\,s$$

$$\tilde{\tau}_{liquid} = \frac{\tilde{H}_{GDL}\,E\tilde{W}\,\tilde{\rho}_l}{\tilde{M}_{H_2O}\,\tilde{\rho}_{PEM}\,\tilde{k}_{sorp}} \approx 122\,s$$

Outlook

- ↦ Parallelization of solution procedure to achieve real-time capability
- ↦ Coupling of several single cells to obtain efficient full stack model
- ↦ Add humidifier and recirculation model

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