

Motivation

- Hydrogen will play a crucial role in energy transition and decarbonization.
- High-temperature reversible solid oxide cells (rSOCs) are a promising dual-mode technology to generate hydrogen and electricity.
- Intermittent renewable energy requires **flexible mode switching** of SOCs as the price of electricity fluctuates.
- Dynamic modeling, equipment health, and advanced process control** help to improve SOC **operational performance** and **thermal management** while **reducing cell degradation** during frequent mode-switching operations.

SOEC Dynamic Process Modeling

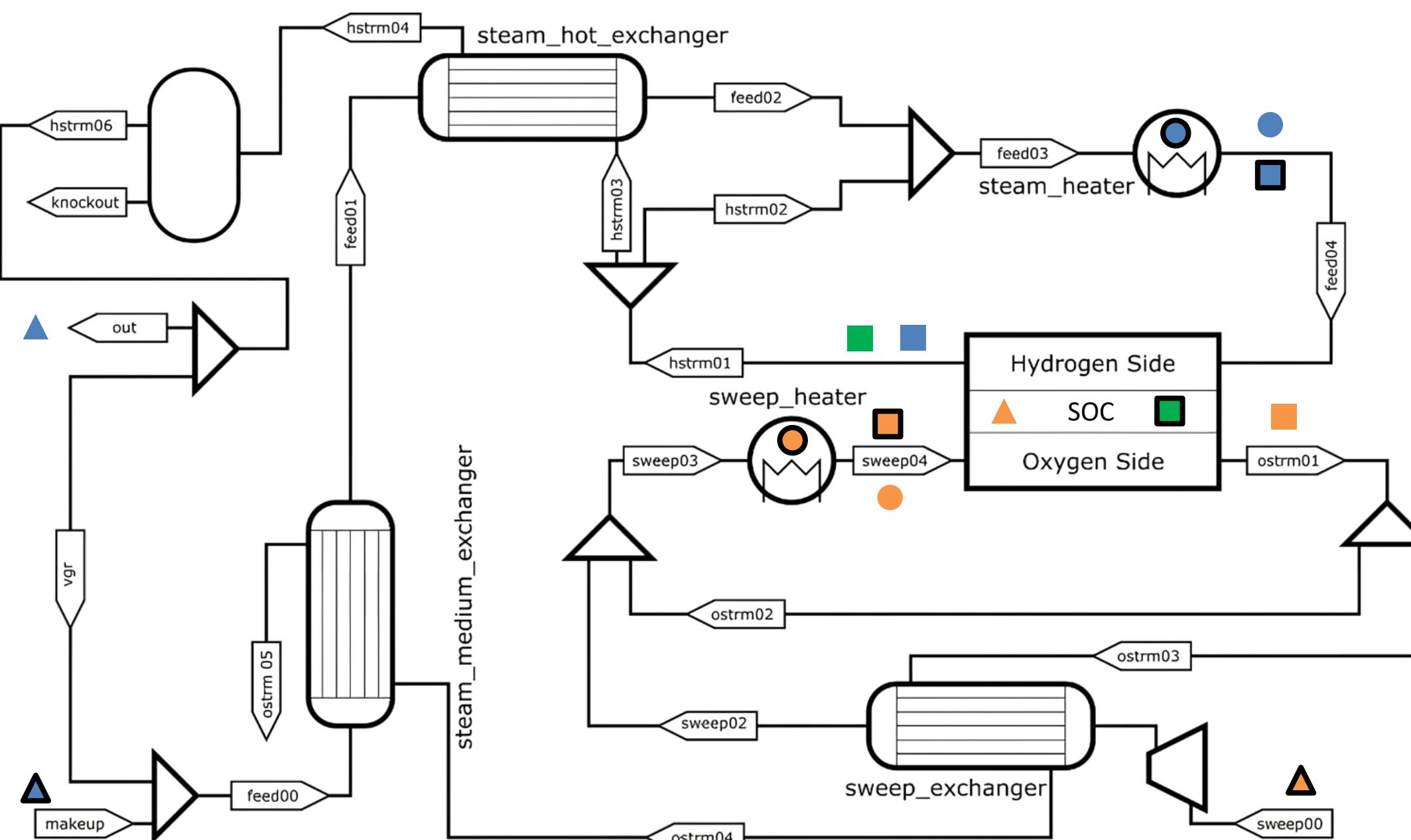


Figure 1. Process flow diagram of SOC system.

- SOC dynamic flowsheet model (Fig. 1) was developed in open-source, equation-oriented **IDAES modeling framework**.
- First-principles non-isothermal planar SOC model** uses 1D channel sub-models with 2D electrode, electrolyte, and interconnect sub-models. (Fig. 2)
- Dynamic system behavior is dominated by **thermal holdup in metal mass** of SOC, heat exchangers, and trim heaters.

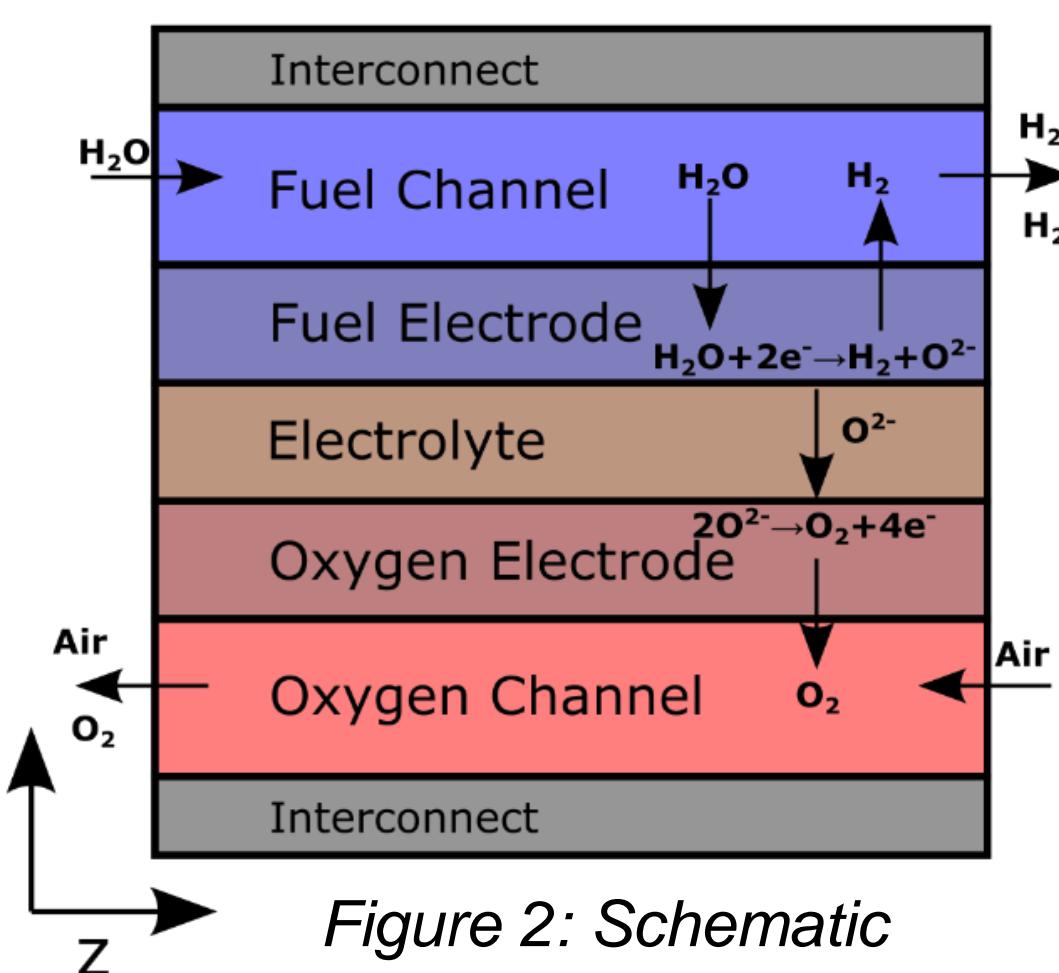


Figure 2: Schematic of SOC model.

System Performance Constraints

- Cell potential** lies between 0.7 V and 1.4 V to prevent unintended electrolysis.
- H₂ concentration in feed** remains no less than 5 mol% to avoid degradation.
- O₂ concentration in sweep outlet** remains below 35 mol% to prevent oxidation of process components.
- Fuel electrode temperature** is kept below 1023.15 K and **inlet-outlet temperature difference** below 75 K to avoid stack thermal stress.

Classical Process Control

Table 1. Manipulated variables and their pairings in classical control. Artificial variables marked with *.

Controller Type	Manipulated Variable (MV)	Controlled Variable (CV)
PI	Cell potential	SOC fuel outlet H ₂ mole fraction
P	Makeup feed rate	Hydrogen production rate
P	Sweep feed rate	SOC stack core temperature
PI (C1I)	Steam heater duty	Steam heater outlet temperature
PI (C2I)	Sweep heater duty	Sweep heater outlet temperature
P (C1O)	Steam heater outlet temperature setpoint*	SOC feed outlet temperature
P (C2O)	Sweep heater outlet temperature setpoint*	SOC sweep outlet temperature
None	Feed and sweep recycle ratios, makeup H ₂ and H ₂ O mole fractions, condenser vapor outlet temperature, condenser recycle ratio (for NMPC only)	

Nonlinear Model Predictive Control (NMPC)

- NMPC** was developed for setpoint transition using 8 non-artificial MVs in Table 1.
- Objective function** (eqn. 1) contains weighted sum of squared errors of:
 - trajectory tracking of H₂ production rate** y_i (1st term);
 - deviations of MVs (excluding trim heater duties and condenser vapor outlet temperature), u_{ij} (2nd term) and CVs, x_{ik} (3rd term) from reference values.
 - Rate of change penalty on trim heater duties** v_i (4th term) to prevent oscillations.
 - To prevent thermal degradation over time, the magnitude of **positive-electrolyte-negative (PEN) temperature mixed spatial-temporal partial derivatives (curvatures)** along cell length (z-direction), $\partial^2 T / \partial z \partial t$, is penalized (5th term).

$$f_{\text{obj}} = \sum_{i=0}^N \rho_{H_2} (y_i - y_i^R)^2 + \sum_{i=0}^N \sum_{j \in J} \rho_j (u_{ij} - u_{ij}^R)^2 + \sum_{i=0}^N \sum_{k \in K} \rho_k (x_{ik} - x_{ik}^R)^2 + \sum_{i=1}^N \rho' (v_i - v_{i-1})^2 + \sum_{i=0}^N \sum_{z=1}^{z_L} \rho_M \left(\frac{\partial^2 T_{iz}}{\partial z \partial t} \right)^2 \quad (1)$$

Dynamic Simulations

- Case Study: Hydrogen-Power Mode Switching**
 - Maximum H₂ production to power generation and back to maximum H₂.
 - Hydrogen-power ramp performed over 5 min. followed by 5 h of settling time.
- Solution Approach**
 - Classical: PETSc variable-step implicit Euler DAE solver.
 - NMPC: Full-discretization NLP with IPOPT solver.

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Classical Control and NMPC Results

- Both classical control and NMPC reach target **H₂ production rates** by the end of the 5-min ramps with **NMPC not overshooting** (3a).
- NMPC** produces different trim heater duty profiles than classical control does (3b) but retains **near-identical power usage** to that of the latter (3a).
- NMPC affords longer SOC temperature settling times (3d, 3f) but **smaller temperature gradients and curvatures** as well as **less oscillation** (3c, 3e).

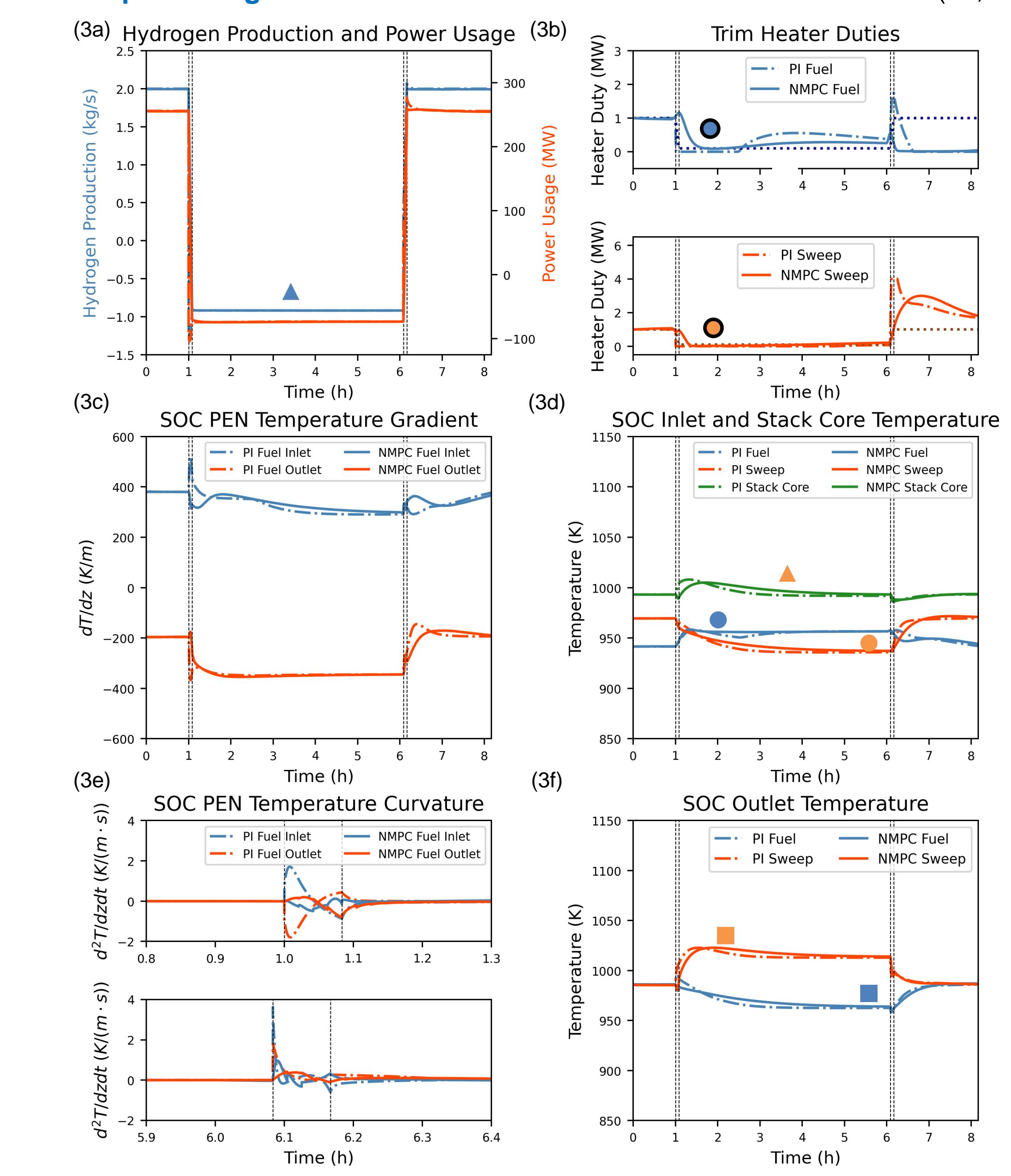


Figure 3. Comparison of classical control with NMPC.

Conclusions and Future Work

- IDAES simulation results show that while both control methods attain similar performance in a few areas, **NMPC reduces SOC temperature gradients and mixed partial derivatives more effectively during mode switching**.
- Future work
 - State estimation through **moving horizon estimation**.
 - Maximize mode-switching performance in fluctuating **locational marginal prices** of electricity markets.
 - Manage **trade-off** between **operating performance and cell degradation** over **long-term system operation** and mode switching.