# NMPC for Mode-Switching Operation of Reversible Solid Oxide Cell Systems

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## 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

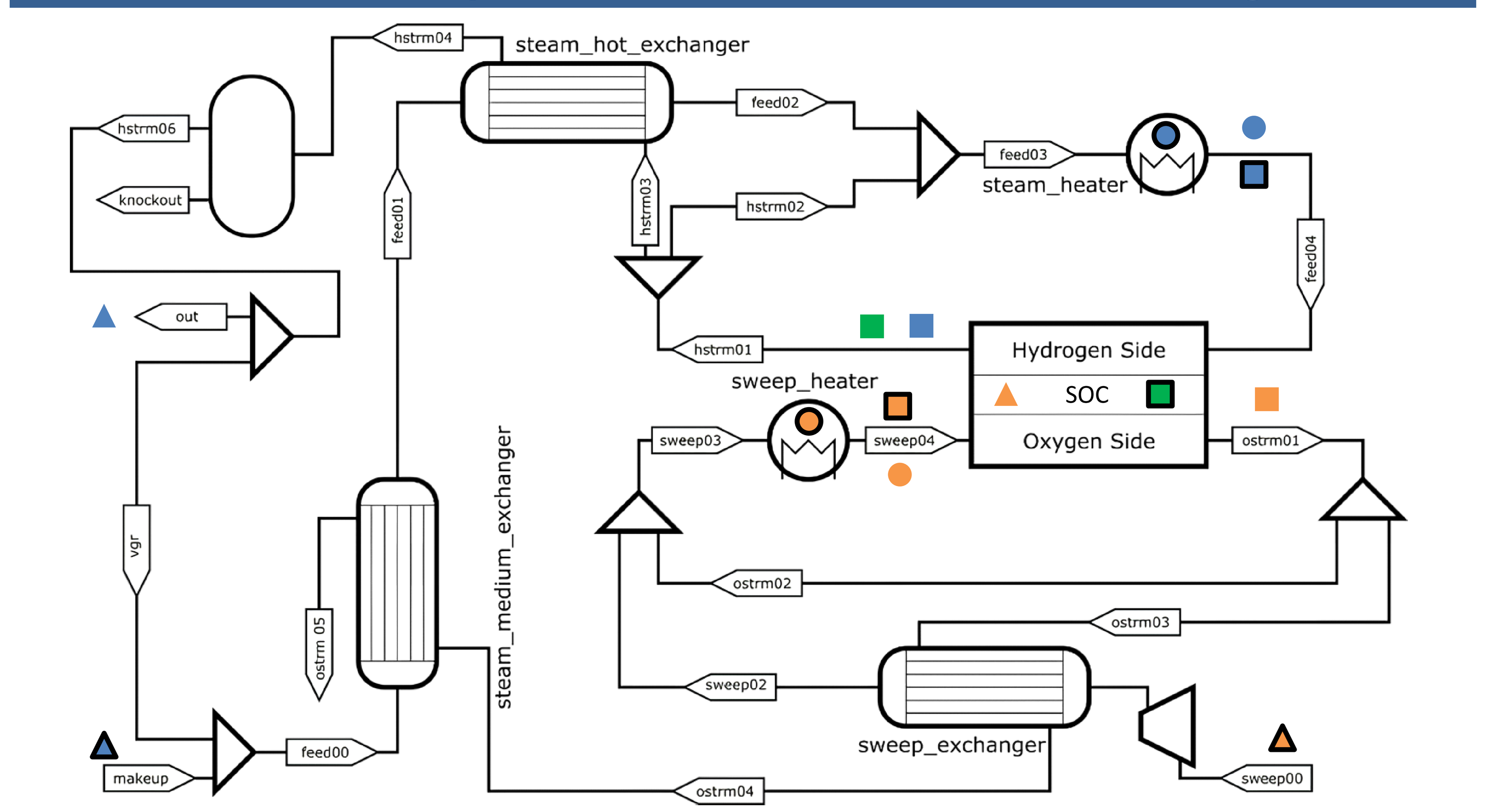


*Figure 1: Process flow diagram of SOC system.*

- 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.

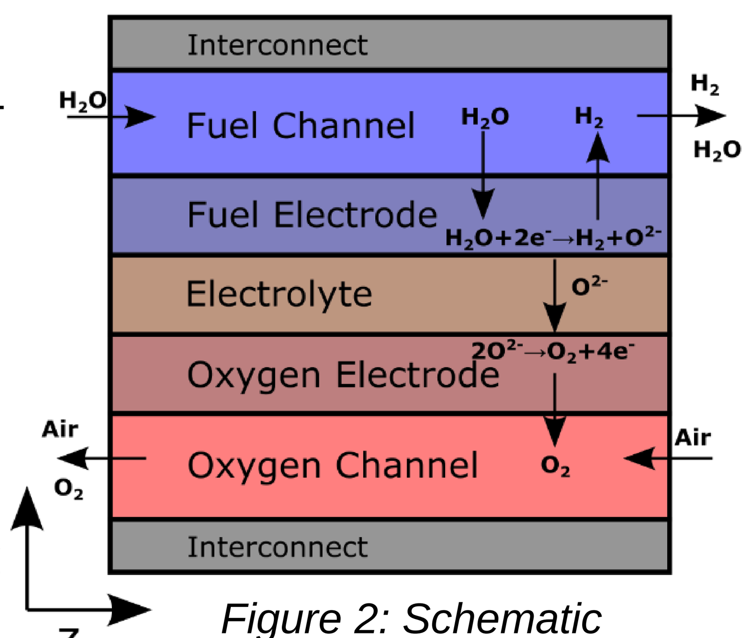


*Figure 2: Schematic of SOC model.*

## System Performance Constraints

- **Cell potential** lies between 0.7 V and 1.4 V to prevent unintended electrolysis.
- **$H_2$ concentration in feed** remains no less than 5 mol% to avoid degradation.
- **$O_2$ 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 & sweep recycle ratios, makeup $H_2$ & $H_2O$ 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 $H_2$ 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, 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).

$$f_{\text{obj}} = \sum_{i=0}^{N} \rho_{\text{H}_2}\left(y_i - y_i^R\right)^2 + \sum_{i=0}^{N}\sum_{j\in J} \rho_j\left(u_{ij} - u_{ij}^R\right)^2 + \sum_{i=0}^{N}\sum_{k\in K} \rho_k\left(x_{ik} - x_{ik}^R\right)^2$$
$$+ \sum_{i=1}^{N} \rho'\left(v_i - v_{i-1}\right)^2 + \sum_{i=0}^{N}\sum_{z=1}^{z_L} \rho_M\left(\frac{\partial^2 T_{iz}}{\partial z \partial t}\right)^2 \quad (1)$$

## Dynamic Simulations

- **Case Study: Hydrogen-Power Mode Switching**
  - Maximum $H_2$ production to power generation and back to maximum $H_2$.
  - 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 **$H_2$ 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).

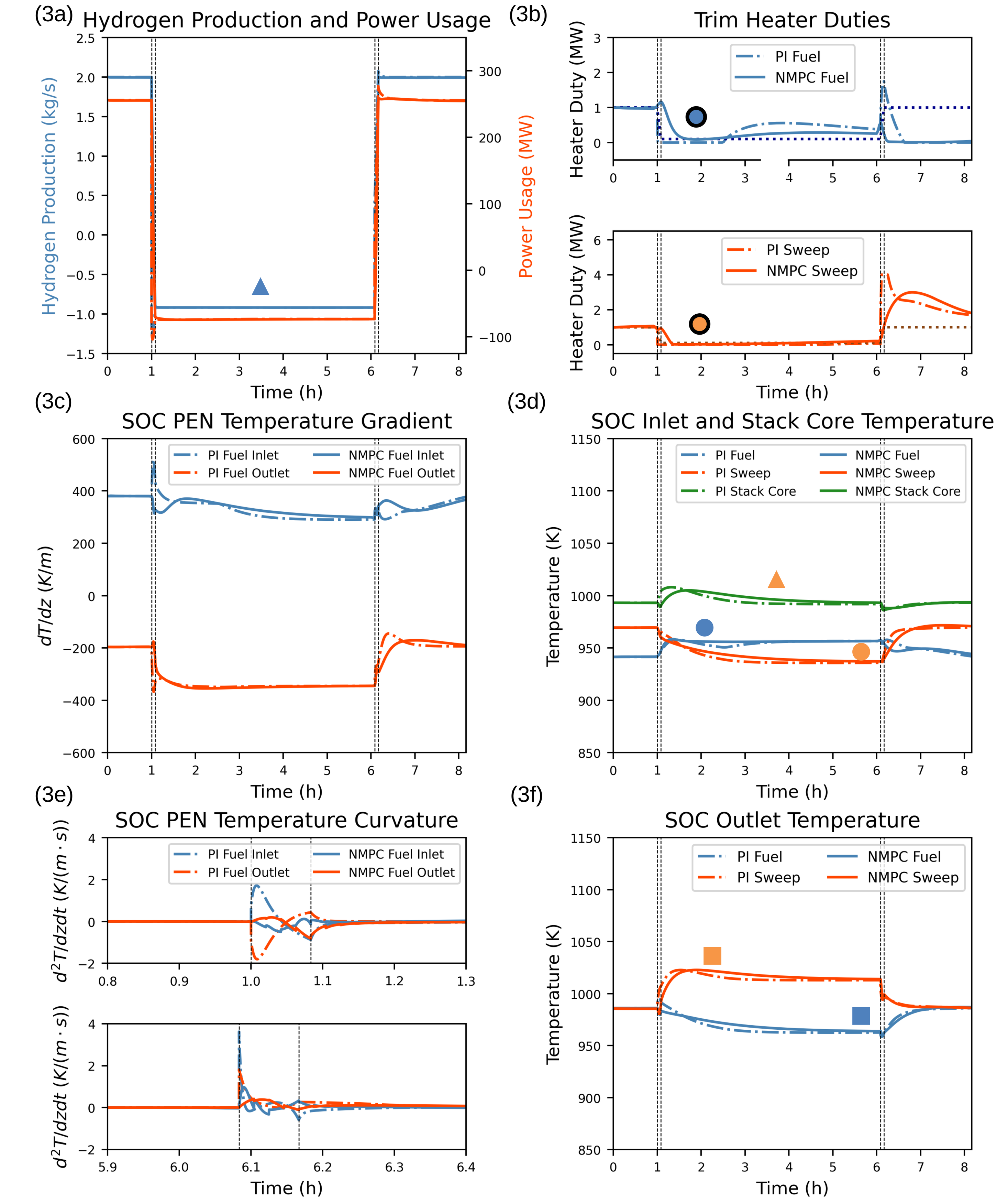


*Figure 3: Comparison of classical control with NMPC*

## 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
  - Mitigate model-plant mismatch through **moving horizon estimation (MHE)**.
  - Maximize mode-switching performance in fluctuating **locational marginal prices (LMPs)** of electricity markets.
  - Manage **trade-off** between **operating performance and cell degradation** over **long-term system operation** and mode switching.