HYLEIT WORKSHOP

MODELLING ELECTROCHEMICAL REACTORS & SYSTEMS IN DIFFERENT TIME AND SPATIAL SCALES

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Overview

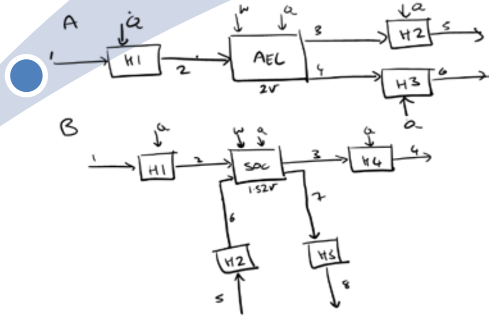
- Why we use models?
- Modelling Framework: TEMPEST
  - Reactor Modelling
  - Transient System Modelling
- Modelling Framework: CELESTE
  - Stationary System Concepting

SOC and AEL System Activities at DLR-TT-ESI

Research and Development of Solid Oxide Cell (SOC) and Alkaline Electrolysis (AEL) systems

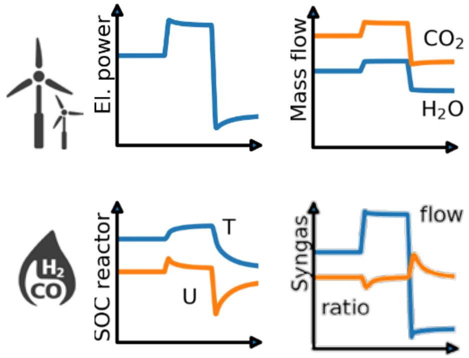
- Process engineering for systems into multi MW range
- Linking experiments with system modelling
- From concept KPIs to operation strategies

Process system concepting



Experimental reactor investigations

Transient process system simulations



Process system experiments

TEMPEST

Transient Electrochemical Models for Process and Energy SysTems

Modelling Framework TEMPEST

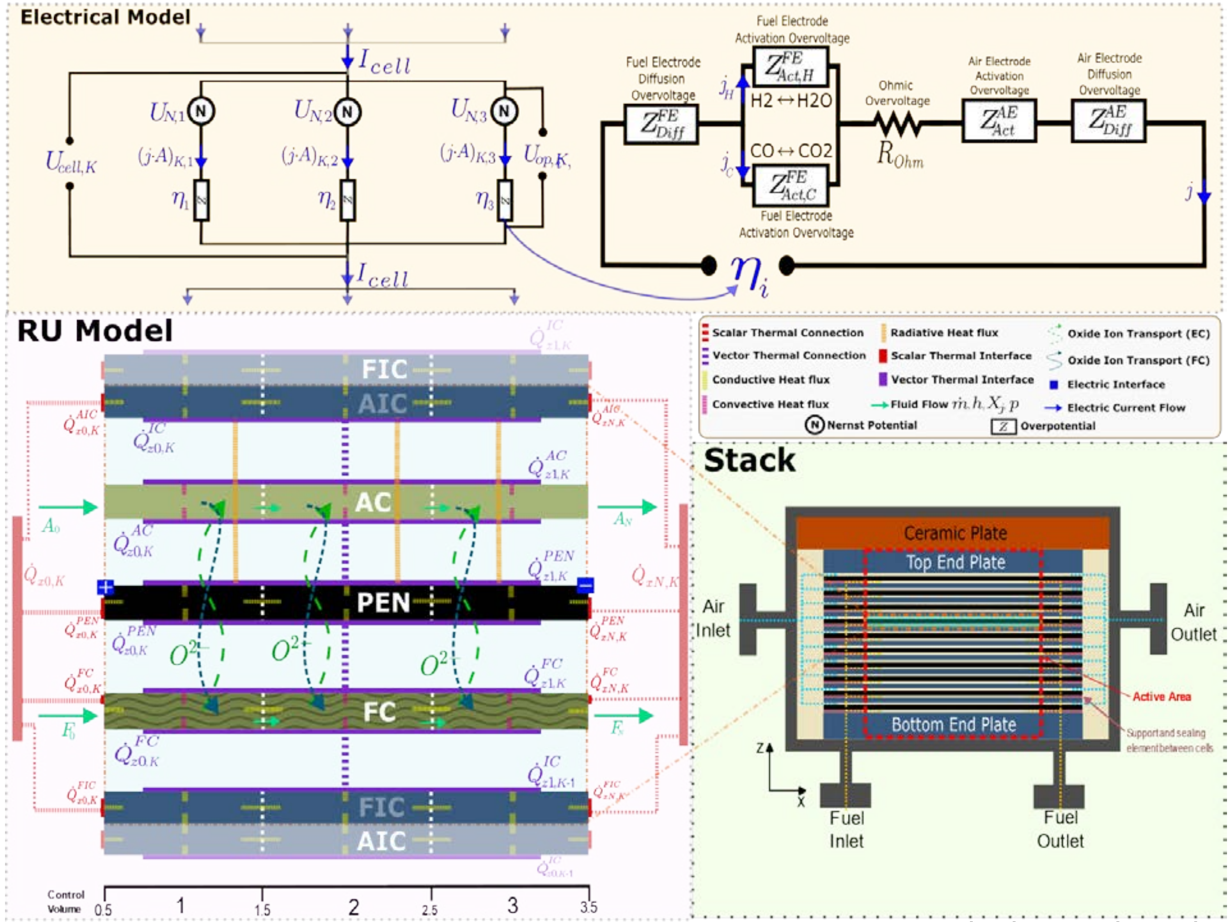
Modelling Depth and Examples

Reactor	Stack model	Loss mechanism model
Includes all stacks, manifolds and insulation	Detailed 1D+1D	Ionic conductivities, Butler-Volmer-equation, dusty gas model
Assumes all cells/stacks have the same boundary conditions	Simplified 1D+1D	Lumped ASR approach
Lumped reactors	0D/1D	

Plant simulations	SOC system simulations Focus: plant and control	SOC system simulations Focus: reactor and operation	SOC stack simulations	AEL system simulations

Modelling Solid Oxide Cell Reactors
Detailed Model

- 1D+1D Transient model of SOC reactor
- Considers the main phenomena within cell
  - Heat & mass transfer, Electro- & thermo-kinetics
- Based on in-house and opensource libraries for reusable models
- Estimate behaviour with very fast solving speed
- Can include different numerical methods and accuracies (FVM, DG, flux functions …)
- Can be adapted for different cell designs



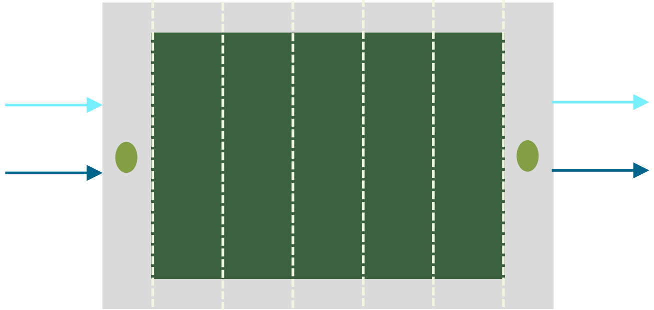
F. Sedeqi 2023, in review

System of DAEs:

$$\begin{cases} \Delta x_i A \frac{d\bar{\boldsymbol{u}}_i}{dt} = \dot{\boldsymbol{F}}_{i-\frac{1}{2}} A - \dot{\boldsymbol{F}}_{i+\frac{1}{2}} A + \dot{\boldsymbol{S}}_i \\ \dot{\boldsymbol{S}} = g(\boldsymbol{u}, t, \boldsymbol{\alpha}) \\ \dot{\boldsymbol{F}} = f(\{\boldsymbol{u}_i\}, \boldsymbol{\beta}) \end{cases}$$

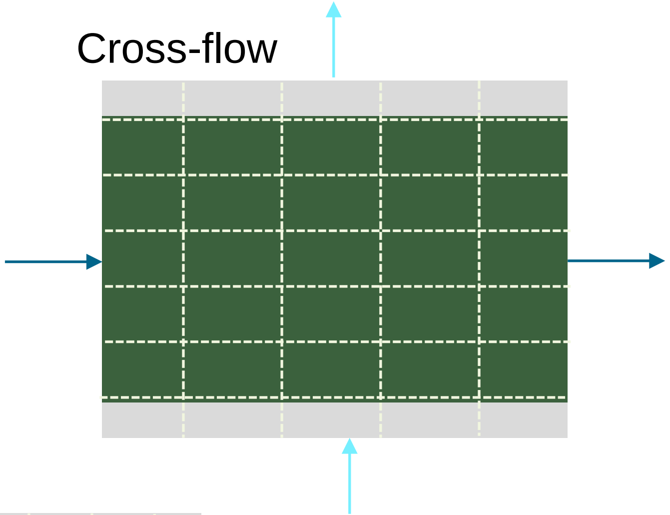
Solid Oxide Cell Designs

Planar

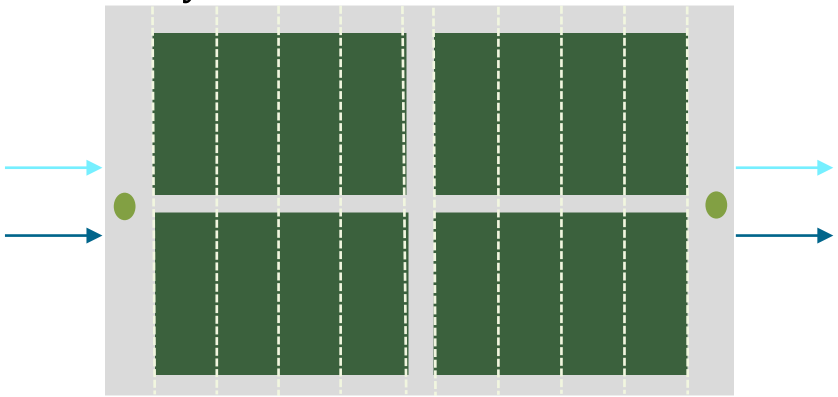


Co-flow

Cross-flow



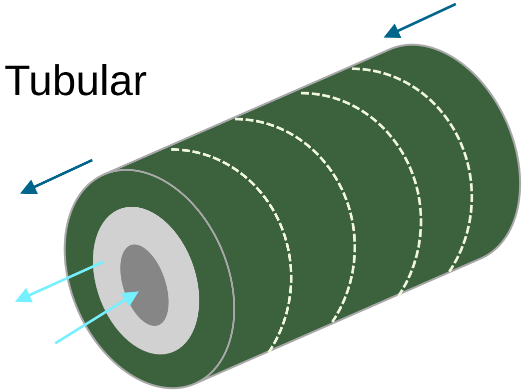
Arrayed co-flow



- ESC
- CSC/ASC
- MSC

…

Tubular



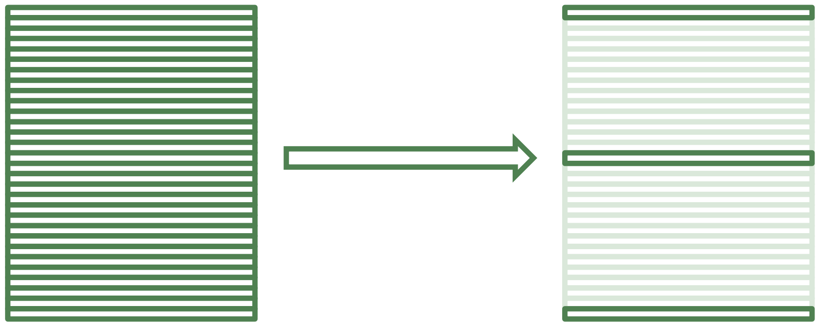
Modelling Solid Oxide Cell Reactors
Simplified Model

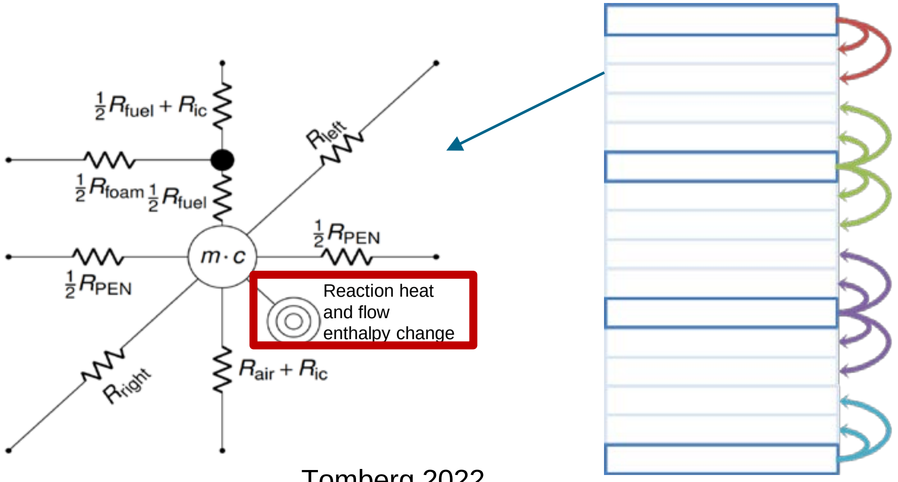
- For larger reactors, detailed modelling not feasible → Simplifications needed

- Reduce system of equations by representing multiple cells as one “block”
  - Interpolate phenomena from detailed cells
  - Represent cell block as thermal mass with internal resistances and generation

$$\frac{d\left(m_{\mathrm{Simp}}\, c_{\mathrm{Simp}}\, T\right)}{dt} = \sum \dot{Q}_i + \underbrace{\Delta\dot{H}_{\mathrm{OC}} + \Delta\dot{H}_{\mathrm{FC}} + P_{\mathrm{el}}}$$

$$P_{\mathrm{el}} = -\left(U_{\mathrm{id}}^{\mathrm{ref}} - \left(U_{\mathrm{id}}^{\mathrm{ref}} - U^{\mathrm{ref}}\right)\frac{ASR_{\mathrm{ohm}}(T)}{ASR_{\mathrm{ohm}}(\mathrm{T}^{\mathrm{ref}})}\right) \cdot I^{\mathrm{ref}}$$





Tomberg 2022,
[DOI: 10.1149/1945-7111/ac7009]

Transient process system simulations

Example: Operation strategies for SOC reactors

Development of operation and control strategies for H_2O- and co-electrolysis

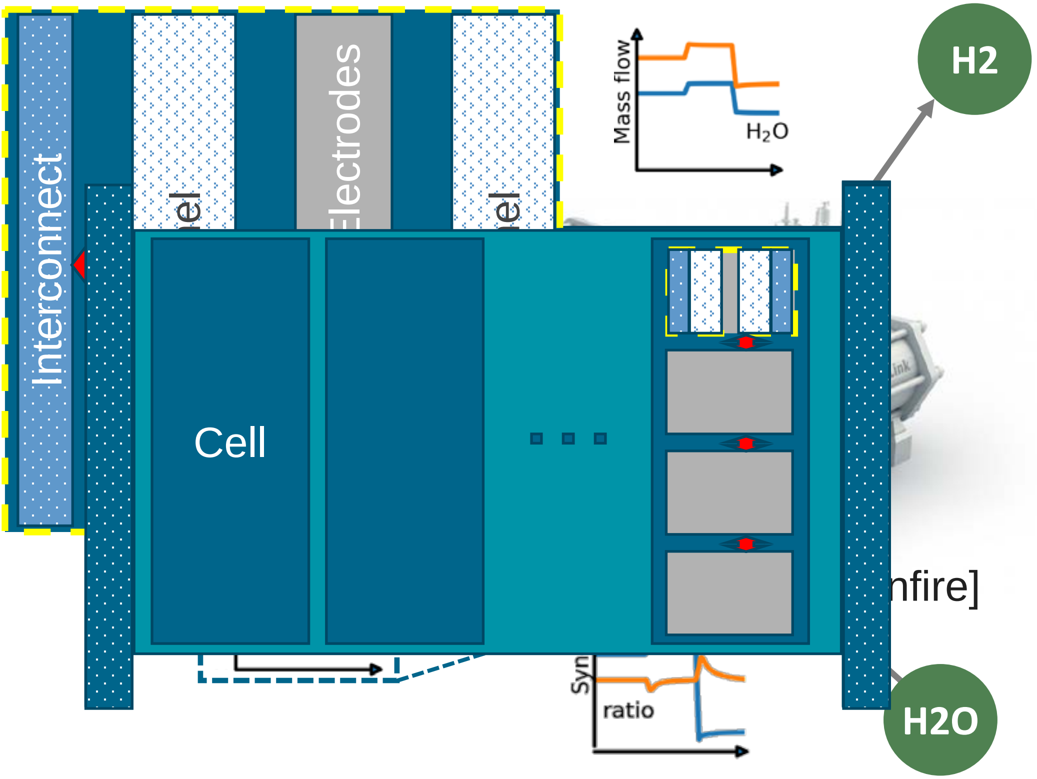
General goals

- Efficiency and robustness

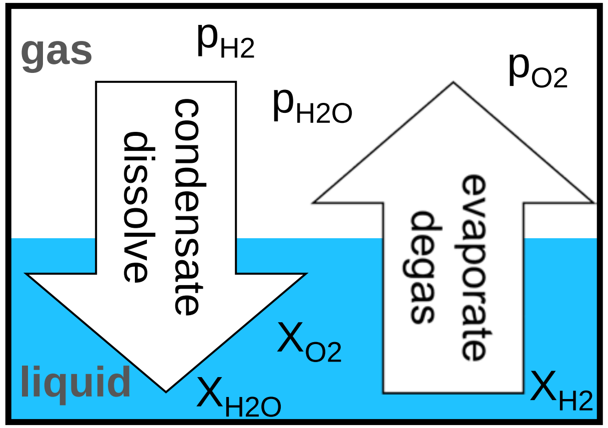
Specific goals (examples)

- Fast and safe transients
- Reactions to incidents
- Outlet composition

Modelling Alkaline Electrolysis Reactors
Current Status



- Two-phase medium is major challenge
- Kinetic approach for transient solving of equilibrium
- Coupling with CFD (Fraunhofer-IFAM) planned



TEMPEST Use Cases Summary

SOC

- Reactor-level
  - Cell technologies + operation mode
    - SOEL/SOFC/co-electrolysis/CO_2-electrolysis
- System level
  - Operation and Control strategies
  - Interaction with BoPs (also for heat integration)
- Reactor and System
  - Safe scale-up considering thermophysical behaviour
  - Synergies with synthesis process (e.g. pressurised + recirculation)
  - Coupling with renewables
  - Powering electric drivetrains (ships, planes etc.)

AEL

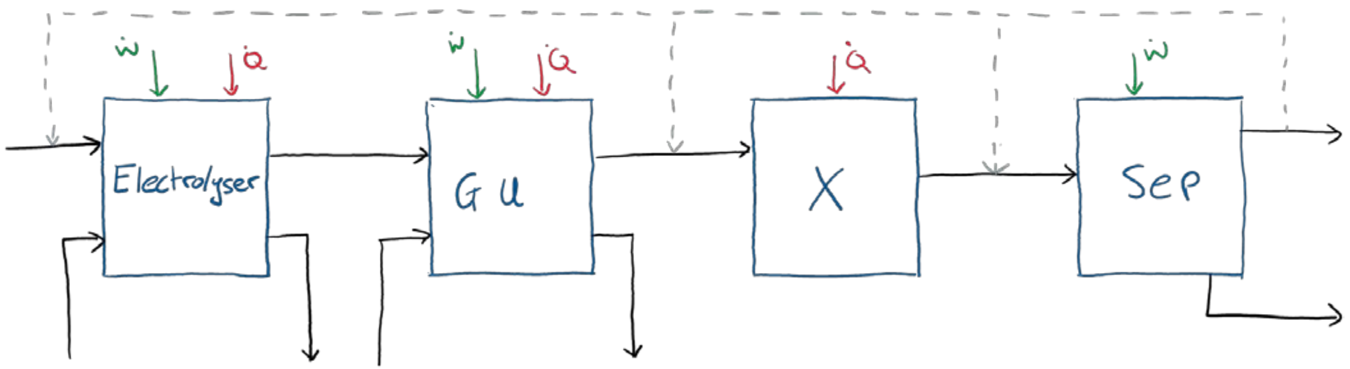
- Reactor level
  - Hot spot prediction
- System level
  - Impurities management
  - Coupling with renewables
  - Thermal management
  - Field management

CELESTE

Conceptual design of ELectrochemical procEss SysTems with Exergy analysis

Conceptual System Design With Electrochemical Reactors

- PtX Systems have many configurations
  - Need a fast way to evaluate relevant scope



Conceptual design of Power ↔ X systems

- Create stationary process system models
- Analyse KPIs e.g. efficiency, yield, exergy

Tool: CELESTE

- Component oriented concepting framework written in Python
- Modular and integrable with other libraries

Use cases

Determine mass and energy balances

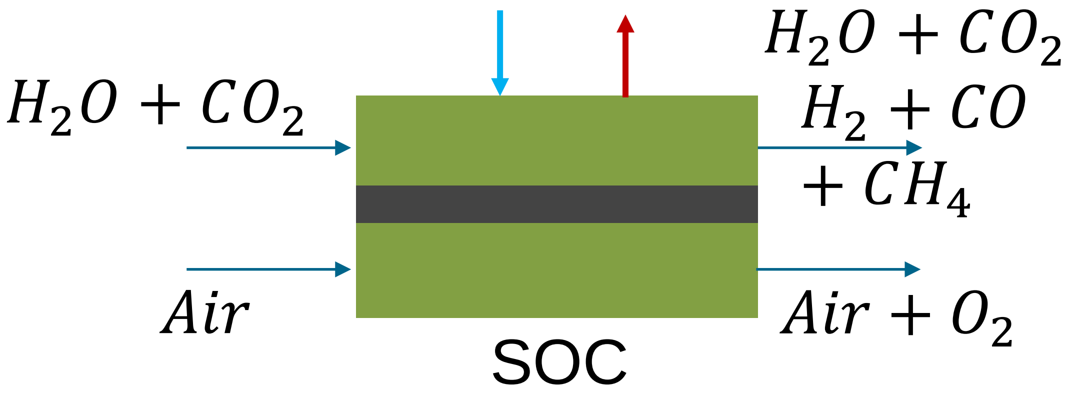
Harmful product formation study (i.e. carbon)

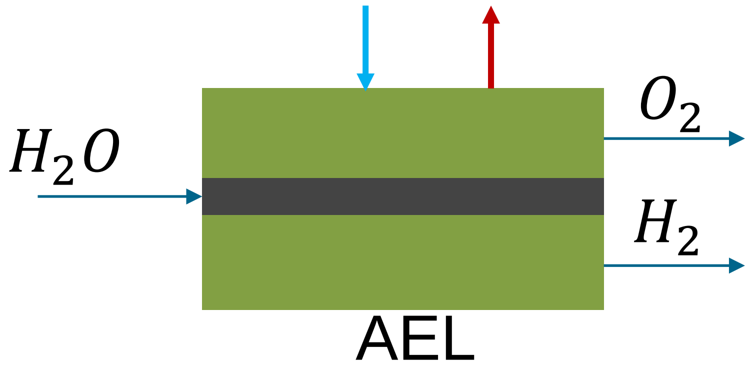
Exergy analysis

Off-gas recirculation studies

Stationary Electrolyser Models

- 0D Models
- Balance equations considering mass transfer and reactions + thermodynamics
- ASR model for voltage loss (experimentally derived)
- Additional models for heat losses can be added on top



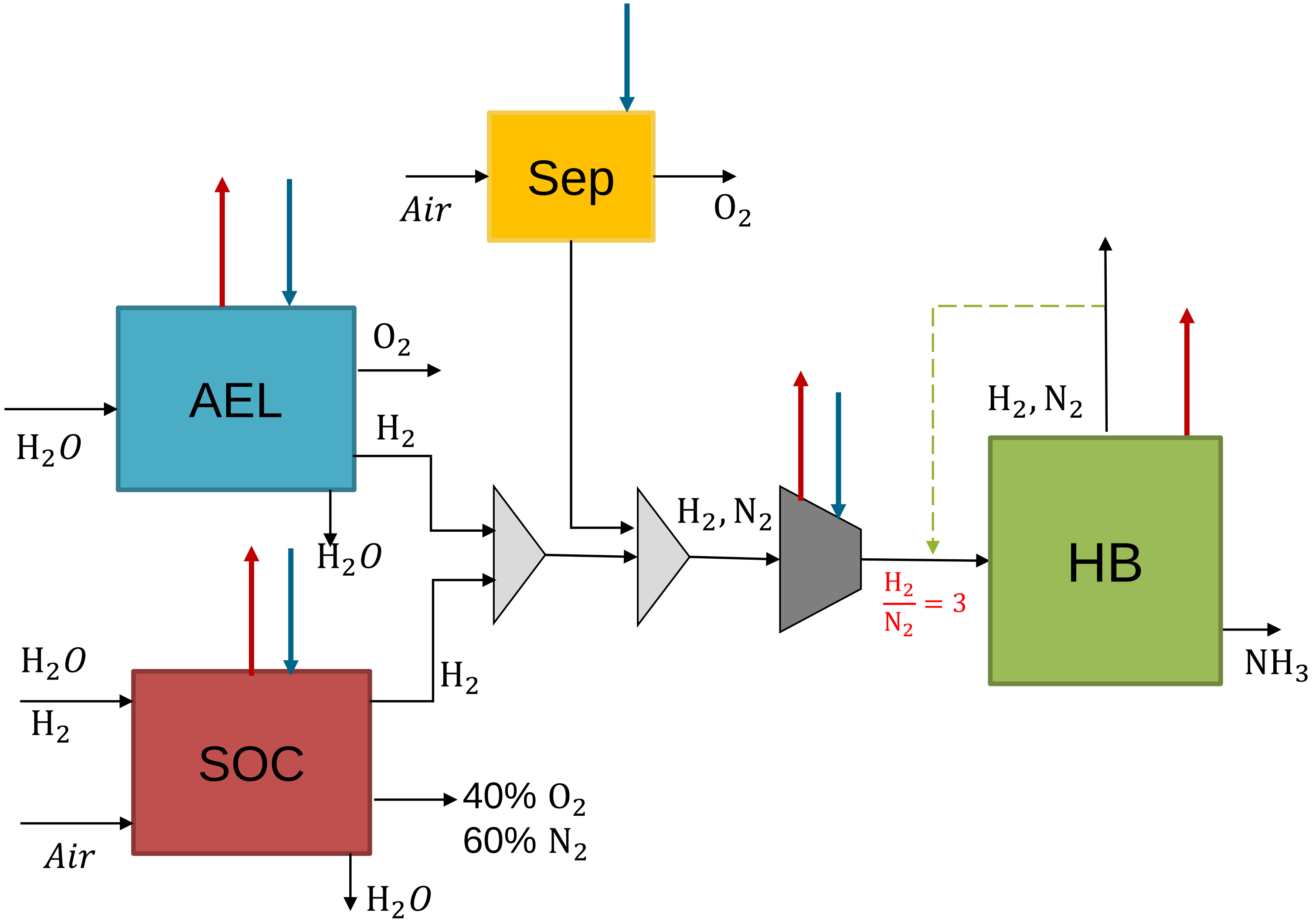


System Modelling Example

Basic Concept for >100MW Plant

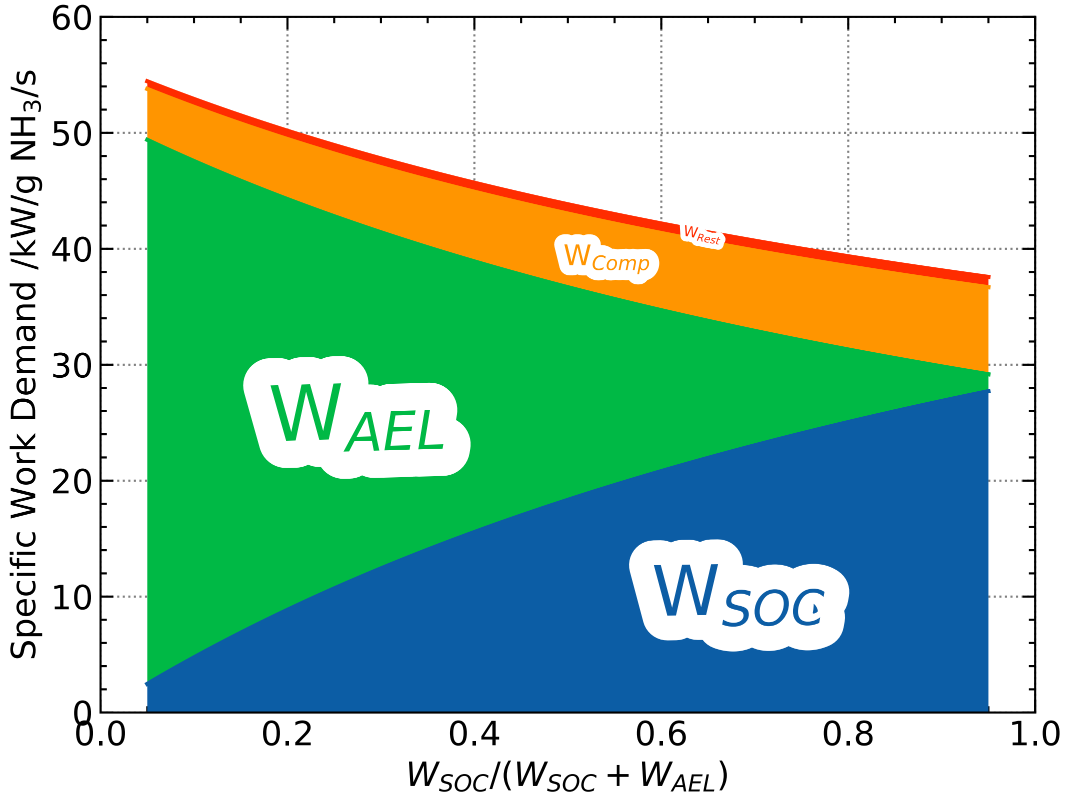
- Simplified model for hybrid SOC-AEL H_2synthesis for NH_3 production
- Simplified air separation model (exergy based)
- Kinetic HB reactor model

- Optimiser used to solve inverse problem to find feed considions to meet desired operating point



Varying SOC and AEL Reactor Size

- Electrolysis majority of work demand for process
- Higher SOC share, lowers total specific work demand
- Increased compression work demand, less than drop in total work demand
- Will analyse impact of Pressurised AEL
- Thermal demand increases with SOC, but rate of increase smaller
  - Will lower with thermal integration
  - Net thermal Exergy negative throughout



Thank you!

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