PUBLIC

Model-based Balance of Operations for Carbon Capture and Storage

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ABB Process Automation, Energy Industries

Introduction

Facts & Figures

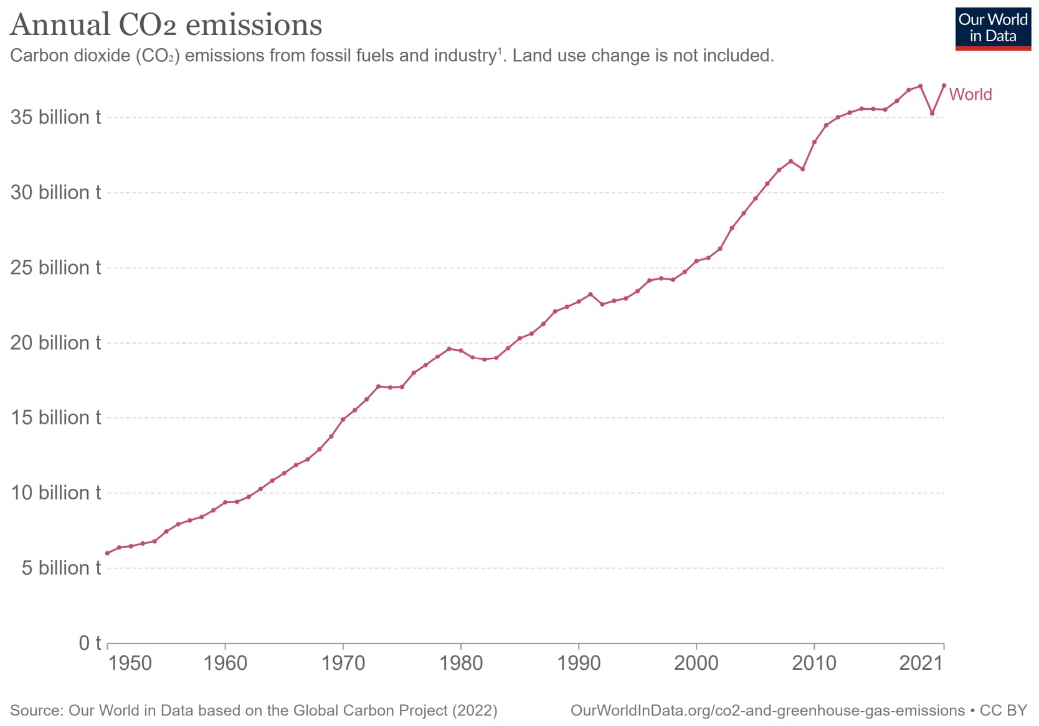
How much CO_2 do we generate?

- 36.8 Gt in 2022, all time high, further increased by 1.1% in 2023!

How are we doing?

- 1.5°C limit – CO2 to reduce 43% by 2030 (from 2019 levels), 60% by 2035, net zero by 2050

Our World in Data



"Without CCS, net-zero is practically impossible" - IEA

https://www.mckinsey.com/industries/oil-and-gas/our-insights/global-energy-perspective-2023-co2-emissions-outlook

Carbon Capture and Storage (CCS)

CCS Value Chain

Capture

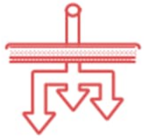
CO_2 is separated from other gases at industrial facilities – cement, steel, power plant, etc

Proven and effective capture methods applied based on emission source

Transport

CO_2 is dehydrated and may be compressed for transportation in liquid state or free gas flow.

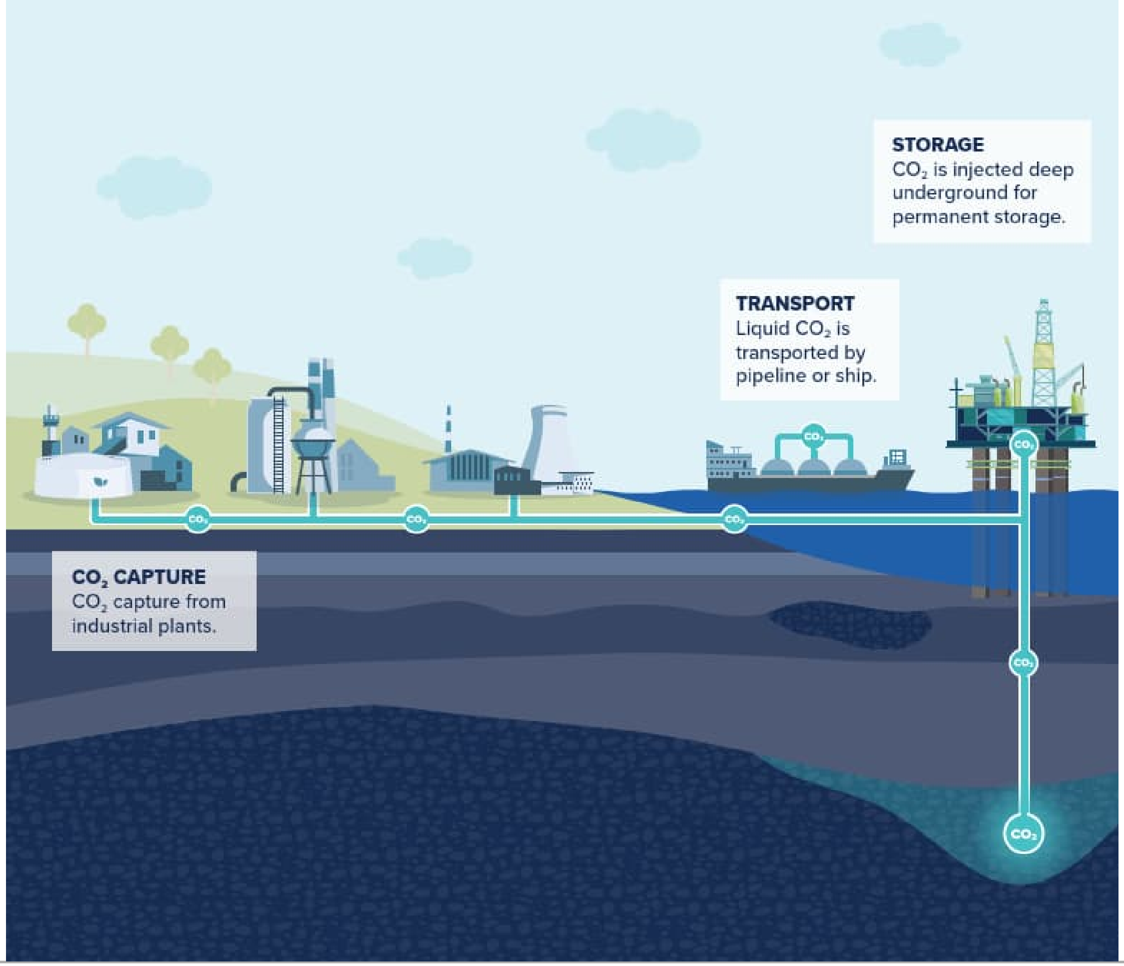
Pipelines and ships are two most common modes of transport



Storage

CO_2 is injected into deep rock formations, often at depths of >1km

High subsurface pressures keep CO_2 in dense or supercritical phase



Example of a CCS Cluster Project

Investment is phased as the cluster grows

Trunk pipelines

Export pipelines

Power

Compression / Booster pumps

Blue hydrogen & new industry

Storage reservoirs / aquifers

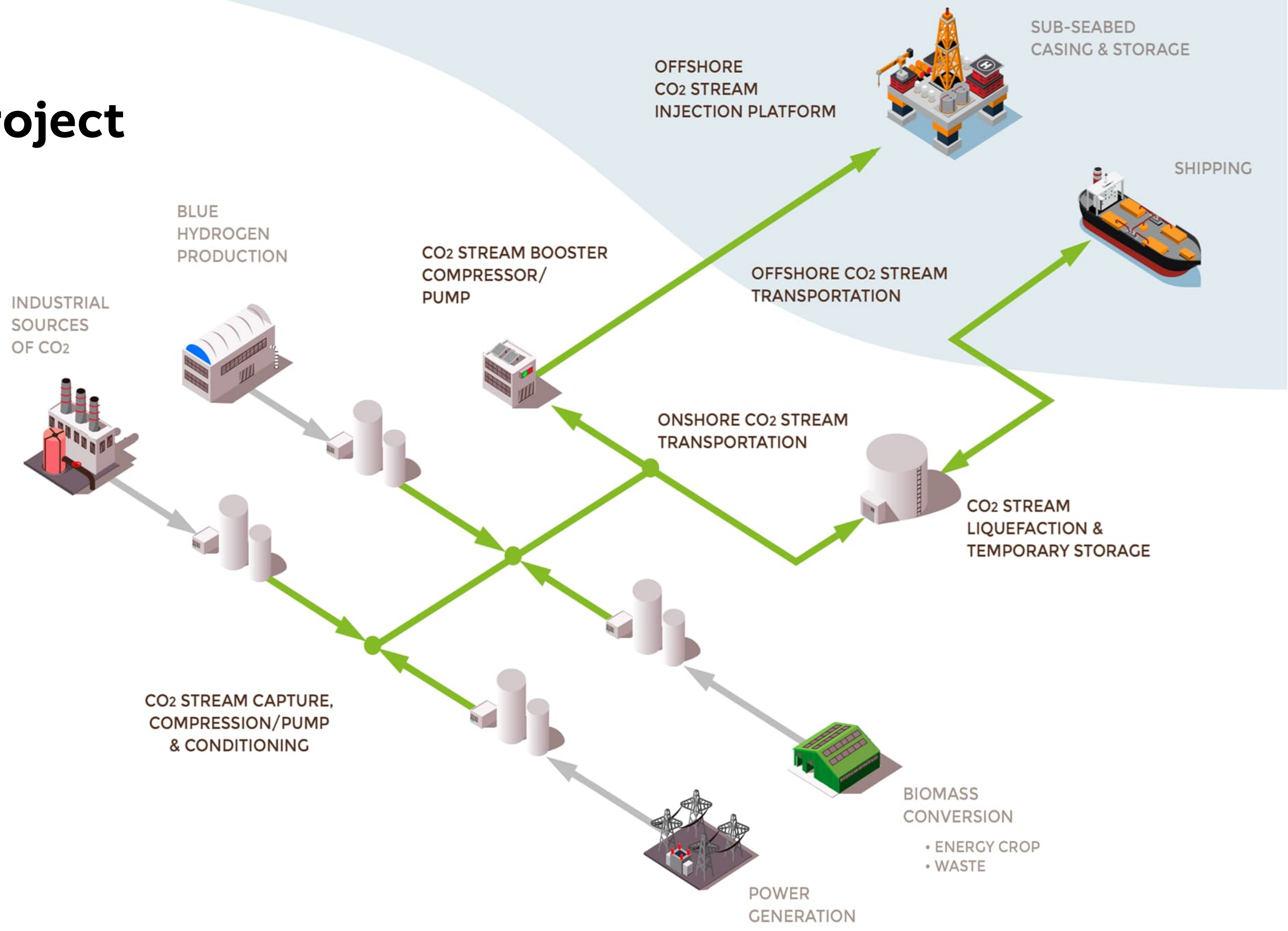
Wells & injection capacity

Re-use of infrastructure

Midstream and oil & gas pipelines

Re-purposed platforms

Re-purposed wells



CCS Cluster Projects: Operational Challenges

- Complex overall CCS infrastructure with various components
- Captured CO_2 contains impurities, which can react to create corrosive compounds
- Storage capacity, integrity & lifetime
- CO_2 states vary through lifetime of plant from gas phase to supercritical
- Operational costs (compression, pumps, heating, cooling)

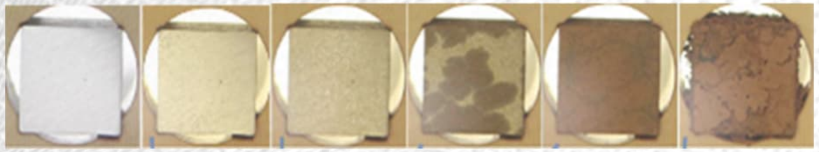


Figure: Carbon steel corrosion in CO_2, caused by typical CCS impurities

- 100 bar / 1500 psi & ambient temperature
- 99+ % CO_2
- Impurities are NO_x & H_2O at <100 ppm

Building partnerships to tackle the challenges

Current challenge of CCS industrial cluster projects: **Transition from design to operations**

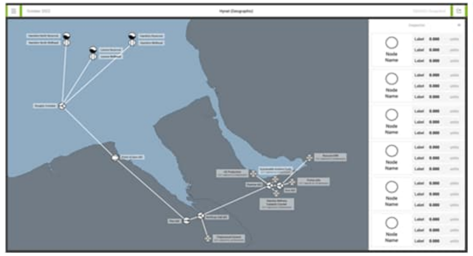
Need for a **full-chain** model/digital twin of the entire CCS network during entire project lifecycle

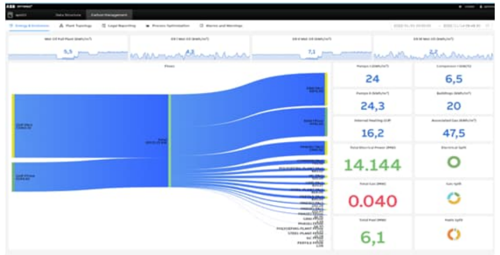
ABB + PACECCS

- ✓ ABB is **global market leader in distributed control systems** and process optimization
- ✓ Pace CCS is **market leading in early design and FEED studies** of CCS HUB projects

ABB OPTIMAX® Balance of Operations

Carbon Capture and Storage (CCS) Digital Twin: Features



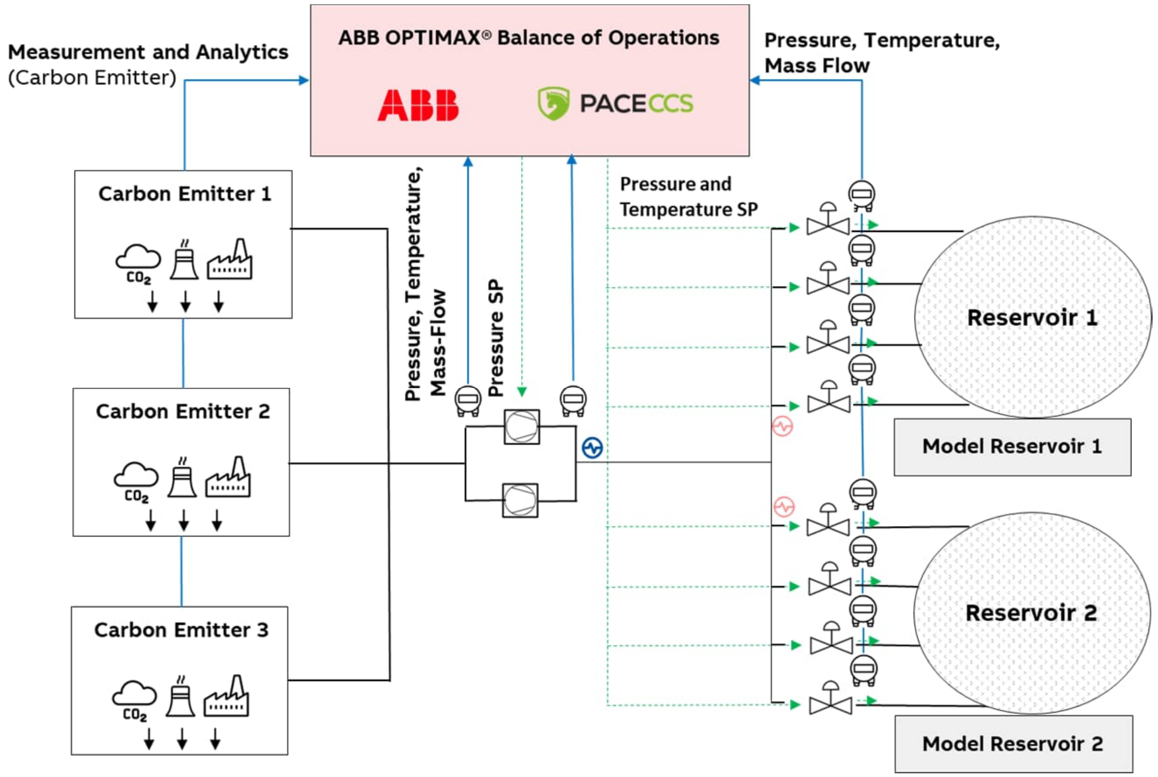


- ✓ **End-to-end CCS solution:** The collaboration between our partner Pace CCS and ABB ensures safety, reliability, and efficiency from the emitters to the reservoirs and the full system lifecycle

- ✓ **Leading-Edge modelling of CO2 processes and impurities:** Combined expertise in complex thermodynamic fluid systems, including compositional tracking, enhancing our product's capabilities

- ✓ **Training, Simulation, and Scenario Analysis:** Facilitates understanding and application through exploratory scenarios and offline simulations.

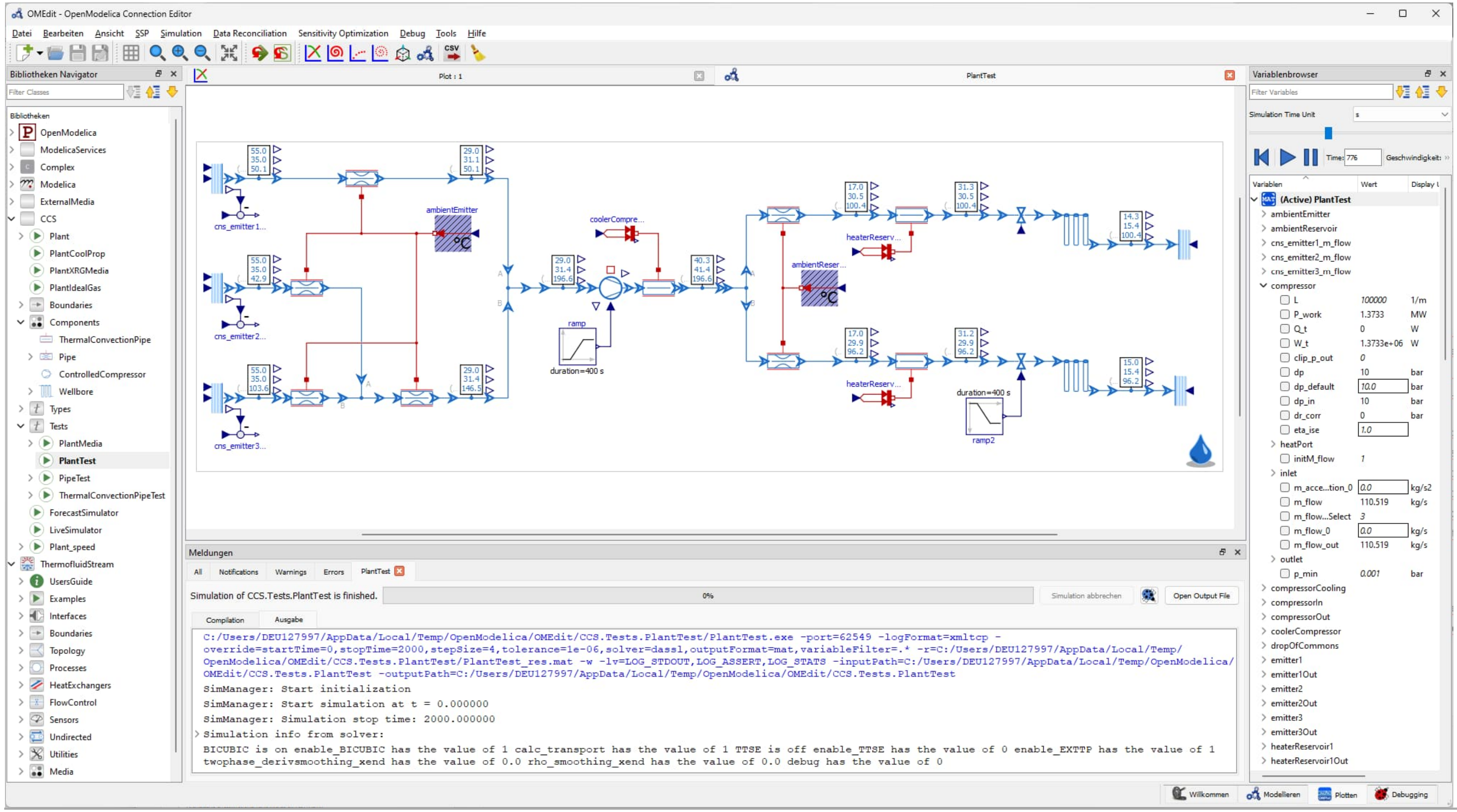
- ✓ **AI-Enhanced Monitoring & Optimization:** Hybrid integration of AI and physical process optimization, enabling autonomous operations, enhanced by advanced monitoring and reporting. Our solution places a special focus on real-time (e.g. APC) as well as predictive optimization for
  - Efficient Compressor Control
  - Smart Heating and Cooling
  - Optimal injection into reservoirs or aquifers
  - Integrity supervision / management



Maximize Availability and Efficiency

Exemplary CCS plant: Modelica system model

Basing on ThermofluidStream and ExternalMedia libraries



Model characteristics

- Equations/Variables: 2445
- Number of dynamic states: 4
- 1 linear core equation system: 5 (36)
- Model inputs: 19
- Model outputs: 47

Model-based predictive optimization

- Export FMU ME using C++ runtime
- Optimize balance of plant over K time steps, e.g. 96 steps for 15min intervals of one day
- Option: solve time steps in parallel

New model features

ExternalMedia library

- Access to general purpose libraries for media properties, in particular CoolProp

ThermofluidStream library

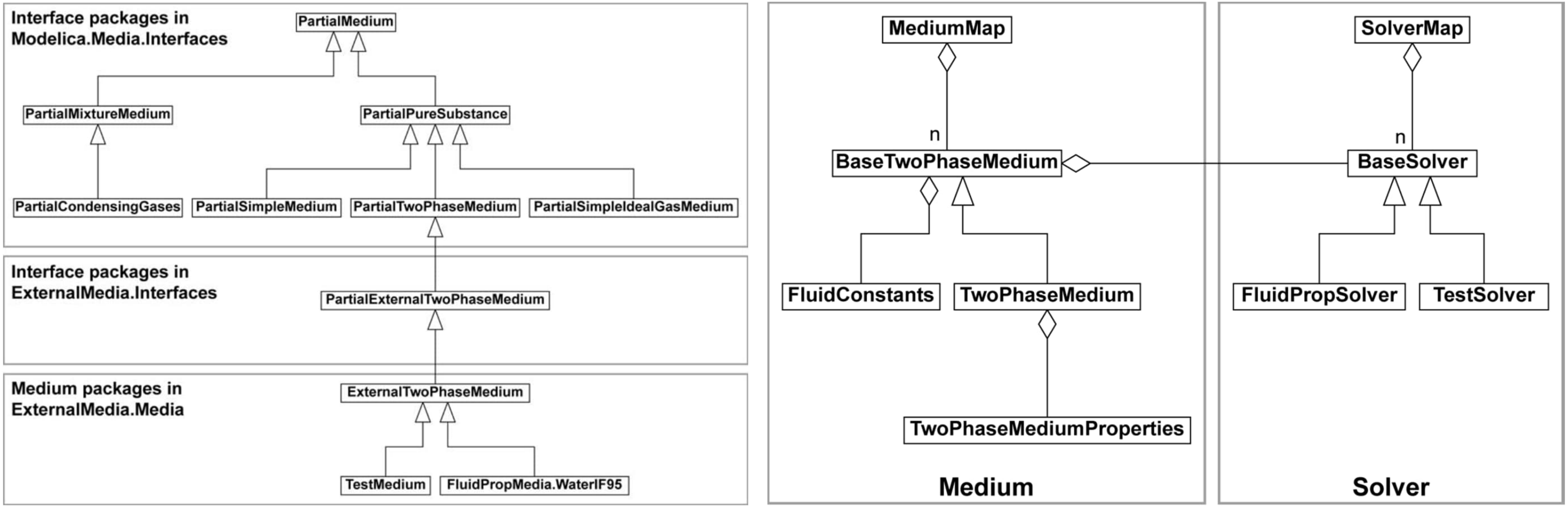
- Robust modeling of complex thermo-fluid systems
- Novel concept, separating steady mass flow pressure from inertial pressure

FMI export exposing local IOs

- Easier path from simulation model to optimization model
- No need to create additional connectors at top level before model export
- Translator exposes unconnected IOs of component models

ExternalMedia

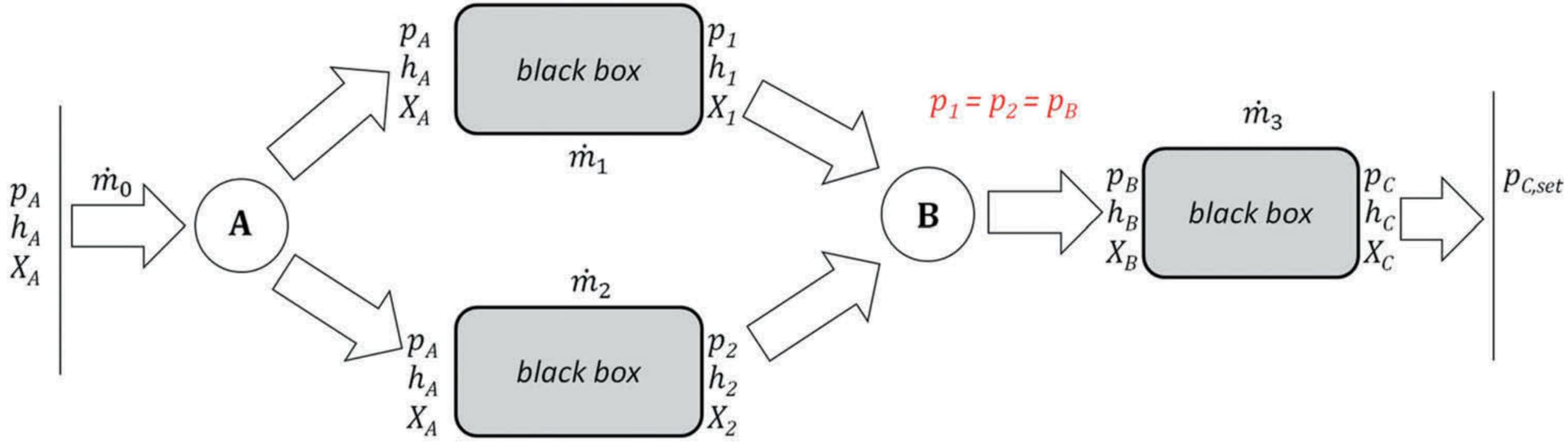
A Library for Use of External Fluid Property Code in Modelica



Francesco Casella, Christoph Ricter: ExternalMedia: A Library for Easy Re-Use of External Fluid Property Code in Modelica, 6th International Modelica Conference, Bielefeld, 2008.

Robust object-oriented formulation of directed thermofluid stream networks

Root cause: Mixing flows generate non-linear equation systems: $p_{1/2}$ = f($m_{1/2\_flow}$), $m_{1/2\_flow}$ = g($p_{1/2}$), $p_1 = p_2$



Dirk Zimmer (2020) Robust object-oriented formulation of directed thermofluid stream networks, Mathematical and Computer Modelling of Dynamical Systems, 26:3, 204-233, DOI: 10.1080/13873954.2020.1757726.
https://www.tandfonline.com/doi/full/10.1080/13873954.2020.1757726

ABB

Introduction of Inertance L, inertial pressure r and steady mass flow pressure p^

Derived from one-dimensional Euler equation for a stream

$$\rho \frac{\partial v_s}{\partial t} + \rho v_s \frac{\partial v_s}{\partial s} = -\frac{\partial p}{\partial s} - \frac{\partial p_{ext}}{\partial s}$$

$$\int_{s_1}^{s_2} \rho \frac{\partial v_s}{\partial t} ds + \rho \bar{v} \Delta v = -\Delta p - \Delta p_{ext} \qquad v_s = \frac{\dot{m}}{\rho A_s} \qquad \Delta q = \rho \bar{v} \Delta v$$

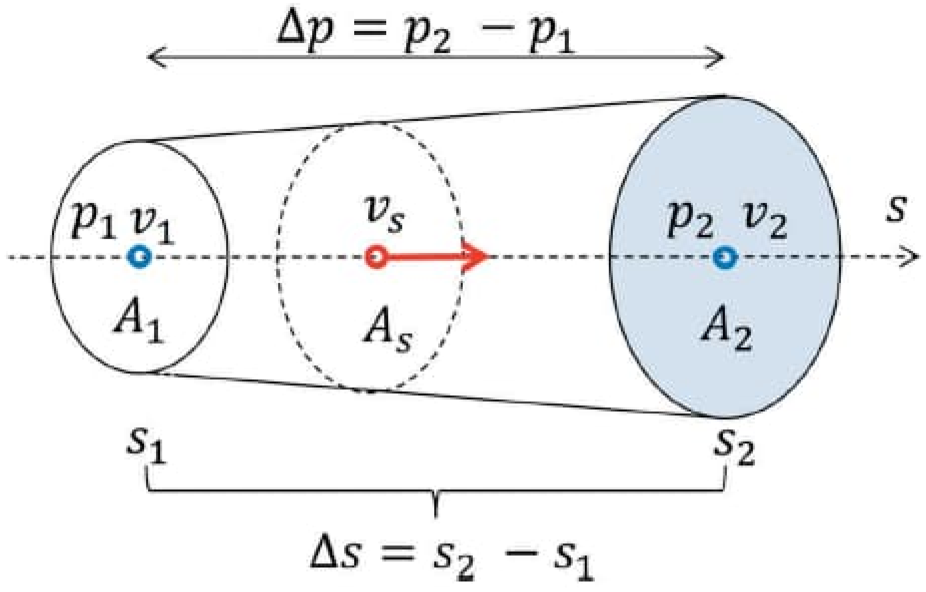
$$\frac{d\dot{m}}{dt} \int_{s_1}^{s_2} \frac{1}{A_s} ds + \Delta q = -\Delta p - \Delta p_{ext} \qquad L = \Delta s / A$$

Inertance

$$p = \hat{p} + r$$

Steady mass flow pressure

Inertial pressure during transients



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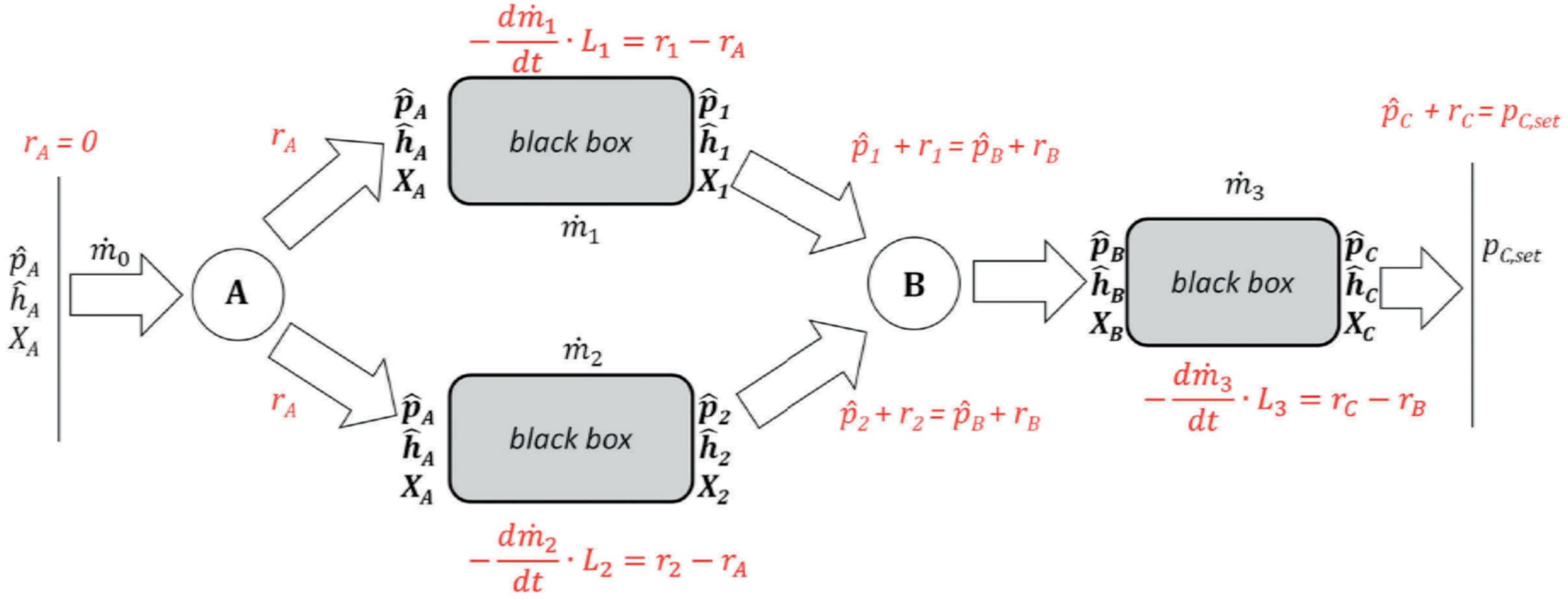
Robust object-oriented formulation of directed thermofluid stream networks

Idea: separate steady mass flow pressure p^ from inertial pressure r – get rid of non-linear $m_{1/2\_flow}$ = $g(p_{1/2})$



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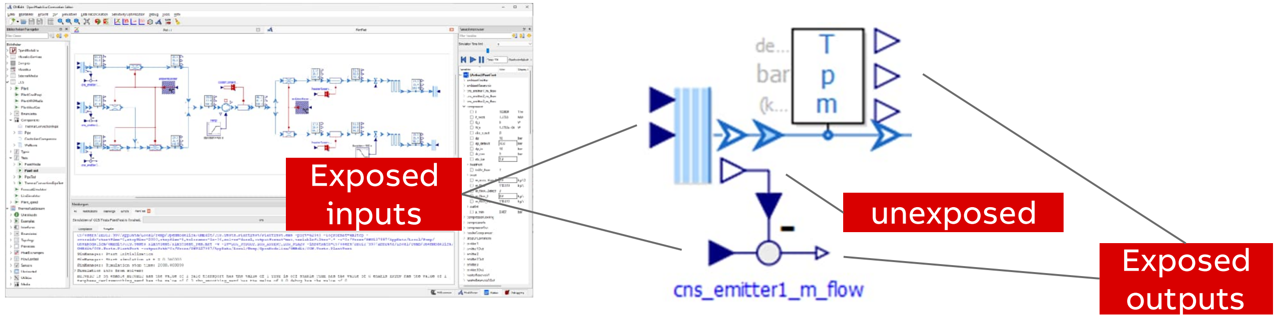
Expose local IOs as toplevel IOs

New omc flag: --nonStdExposeLocalIOs = <level>



Idea

- Many models, such as boundaries or sensors, provide conditional input and output connectors
- Automatically promote them to toplevel IOs, particularly for FMI export – 19 inputs and 47 outputs in the example

Why only connectors instead of any input/output?

- input/output is used for many things (e.g. binding equations, time varying "parameters")
- connector is intended for connections; unconnected connectors are likely to be exposed, e.g. RealInput of a boundary model

Why configurable level?

- Can exclude unconnected connectors at deeper model levels; nice: filter out unconnected outputs of submodels
- Critical: `Modelica.Media.Interfaces.PartialMedium.BaseProperties.p/h/Xi` are defined as input connectors to get balanced models without need to define binding equations – connectors not intended for connections :~|
- Cf. approach of ThermofluidStream avoiding generic medium model by using specific state record with generic access functions instead – use `specificEnthalpy(state)` instead of `medium.h`
- A medium model is typically at model level 2 or higher, e.g. component.medium.p

ABB Dynamic Optimization

Treat optimal control programs basing on simulation models

For dynamic system model and sample time points t_k , $t_0 < t_1 < \ldots < t_K$

find control u (and/or initial states x(0)) that minimize criterion J

subject to model behavior, initial conditions

and further constraints g

FMU ME

$$J = \sum_{k=0}^{K} f_0[k, x_c(t_k), u_c(t_k)] \quad \rightarrow \quad \min_{x_c(t_0),\, u_c(t)}$$

$$\frac{dx_c(t)}{dt} = f_c[t, x_c(t), u_c(t)], \qquad x_c(t_0) = x_{c0}, \qquad t \in [t_0, t_K]$$

$$y(k) = h[k, x_c(t_k), u_c(t)], \qquad k = 0,1,\ldots,K$$

$$g[y(k), u_c(t_k)] \geq 0$$

Model Predictive Control for CCS hub networks

Always ensures safe operation in complex and dynamic conditions

Statistical forecasts based on historical data

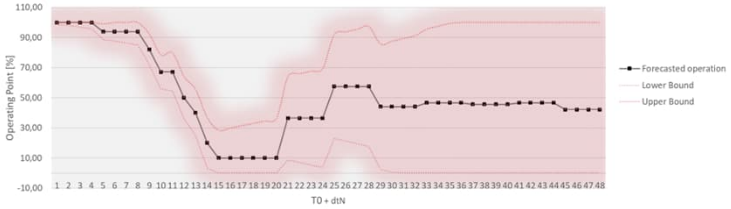
Input: Historical process data

Output Forecasts:

- Emitter operation
  - CO2 massflows
  - Impurities
- Ambient temperatures

Predictive optimization with process model

Input: Forecasts (Step 1) + reservoir simulation CMG

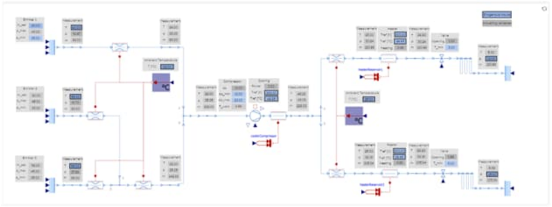


Output Schedules:

- Compressors/pumps
- Heaters & coolers
- Injection Management (well head valves)

Realtime operation & safety constraints

Input: Schedules (Step 2) + reservoir simulation CMG



Output Setpoints (advisory or automatic):

- Compressors/pumps
- Heaters & coolers
- Injection Management (well head valves)

Monitoring & Alarming

Input: Live measurements and calculations

Output Alarms & Notifications:

- Thresholds/Limits
- Worst case scenario
- Infeasiblilty

AutoML/AI model

CCS Network Model (MPC) Modelica

100% CO2 model, optional with impurities

CCS Network Model (segmented) PACECCS

Mixed composition model, including impurities

External CO2 media model:

Fluid properites based on **Equation of State**

Production forecast and scheduling

Every day – every 15 minutes ⟷ **Next hour – next 3 days**

Realtime control under safety constraints

Every 1s – 5s ⟷ **Next single timestep**

Conclusions

Carbon Capture and Storage reduces CO2 emissions to the atmosphere that cause global warming

- Can use depleted oil and gas reservoirs, to some extend re-purposing platforms and wells
- Even larger potential when building new aquifer storages

Promising applications for CCS

- Cement industries
- “blue” hydrogen (generated from natural gas) until “green” hydrogen will be available at scale

Modelica proved well suited for modeling and optimization of CCS processes – the open Modelica community rocks!

- ThermofluidStream library for robust fluid modeling
- ExternalMedia library for using CoolProp
- OpenModelica with new frontend and instance-based graphical editing for treatment of fluid models in OMEdit
- Extension with –nonStdExposeLocalIOs simplifying export of simulation models for optimization
  e.g. don’t mess up exemplary CCS model with additional 19 toplevel inputs and 47 toplevel outputs
- Further work: efficient multiphase CO2 media models, including impurities – AI for Model-Based Systems Engineering?

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