COBIA Implementation of the Quantum Converter Multi-Stream Heat Exchanger for Hydrogen Liquefaction Processes

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Liquid Hydrogen

Overview

Liquid Hydrogen

Primary usages

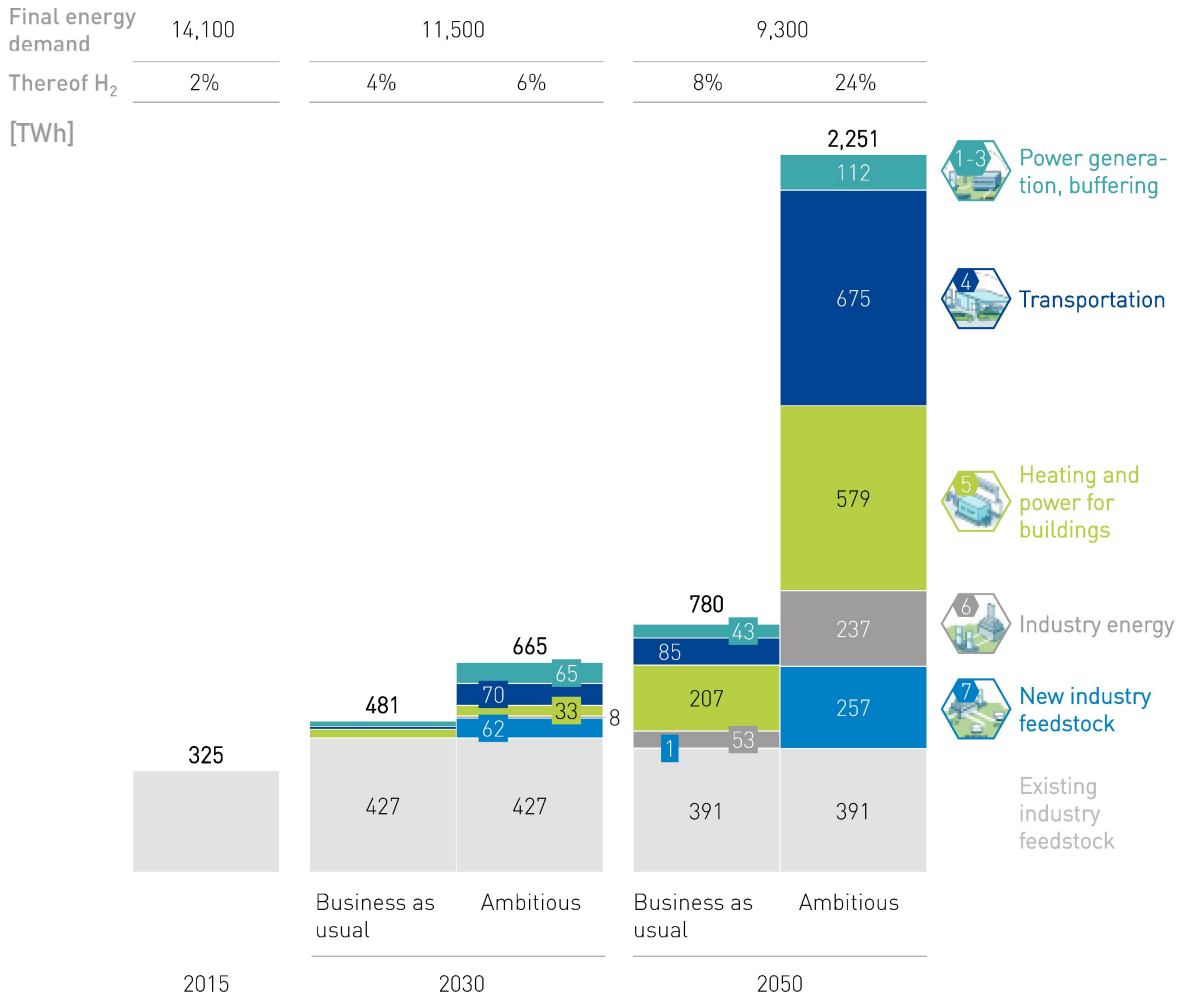
- Storage
- Transportation

Hydrogen Market

EU Ambitions

Conservative scenario (2050):
+6% (+455 TWh)

Ambitious scenario (2050):
+22% (+1926 TWh)



Source: Fuel Cells and Hydrogen 2 Joint Undertaking, 2019

Hydrogen Market

Current Production (North America & Europe)

Operational plants in **North America** and **Europe** until 2009

Continent/Country	Location	Operated by	Capacity (TPD)	Commissioned in
Canada	Sarnia	Air Products	30	1982
Canada	Montreal	Air Liquide, Canada Inc.	10	1986
Canada	Becancour	Air Liquide	12	1988
Canada	Magog, Quebec	BOC	15	1989
Canada	Montreal	BOC	14	1990
French Guyane	Kourou	Air Liquide	5	1990
USA	Ontario	Praxair	20	1962
USA	New Orleans	Air Products	34	1977
USA	New Orleans	Air Products	34	1978
USA	Niagara Falls	Praxair	18	1981
USA	Sacramento	Air Products	6	1986
USA	Niagara Falls	Praxair	18	1989
USA	Pace	Air Products	30	1994
USA	McIntosh	Praxair	24	1995
USA	East Chicago, IN	Praxair	30	1997
France	Lille	Air Liquide	10	1987
Germany	Ingolstadt	Linde	4.4	1991
Germany	Leuna	Linde	5	2008
Netherlands	Rosenburg	Air Products	5	1987

Source: Krease-in et al. 2010

NA mean: 20 TPD

EU mean: 6.1 TPD

Hydrogen Market

EU Ambitions (perspective)

Consider 100% liquid hydrogen request for transportation in 2050 with conservative scenario (85 TWh):

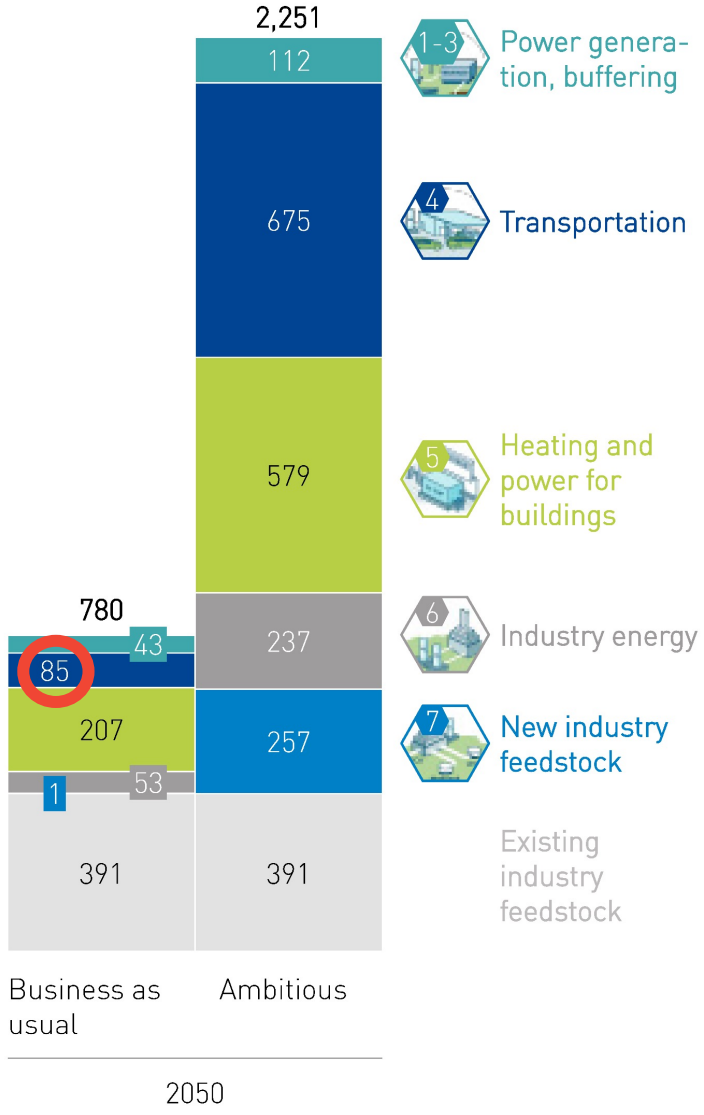
$$LHV_{H_2} = 120\ MJ/kg$$

$$Mass_{H_2} = \frac{Energy_{H_2}}{LHV_{H_2}} = 2.55\ Mt$$

$$DailyProduction_{H_2} = \frac{Mass_{H_2}}{Annual\ Operativity_{90\%}} = 7763\ TPD$$

Calculation for new plants request with average European production of 6.1 TPD:

$$NewPlants_{EU} = \frac{DailyProduction_{H_2}}{PlantProduction_{H_2}} \approx \mathbf{1200\ new\ plants}$$

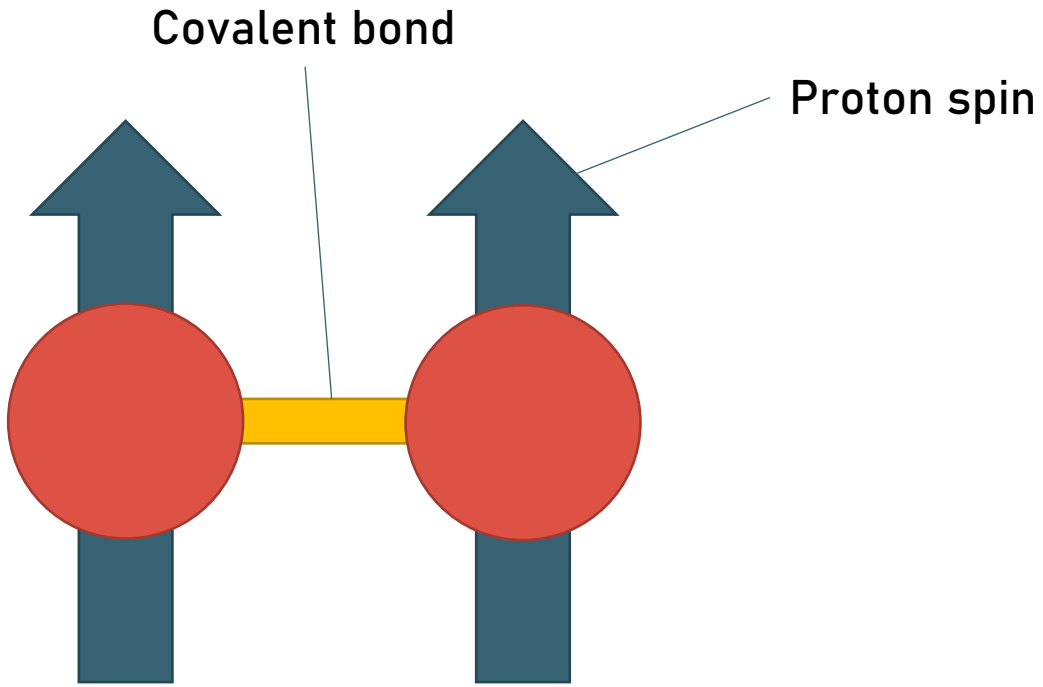


Hydrogen Liquefaction

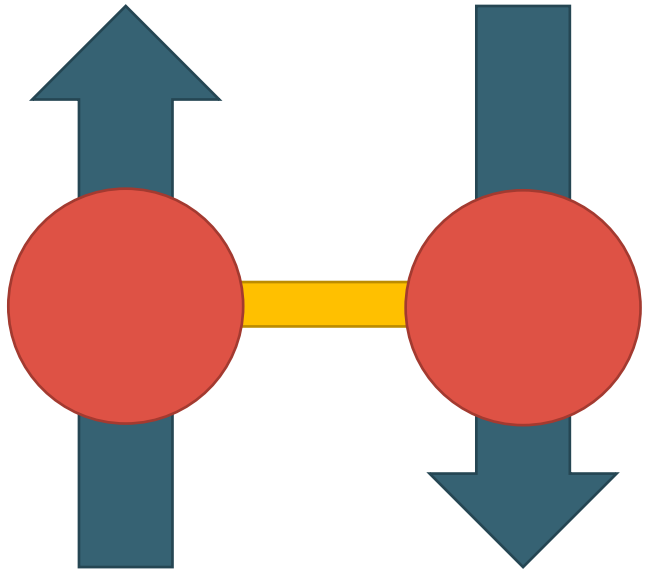
Process

Hydrogen

Spin isomers



Ortho hydrogen

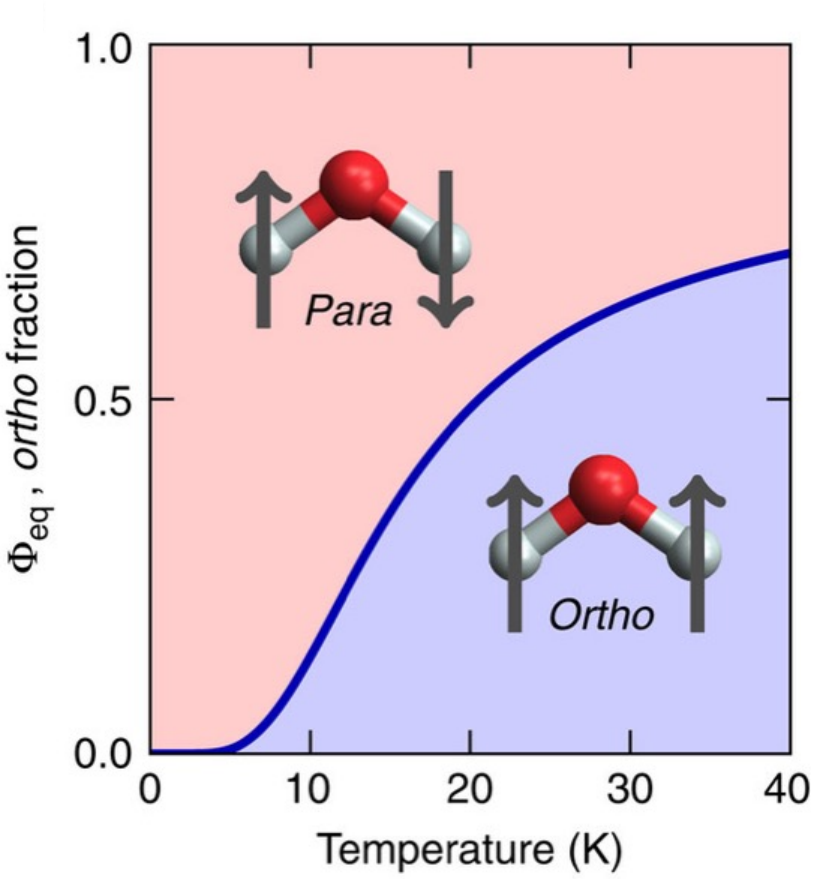


Para hydrogen

Hydrogen Isomers

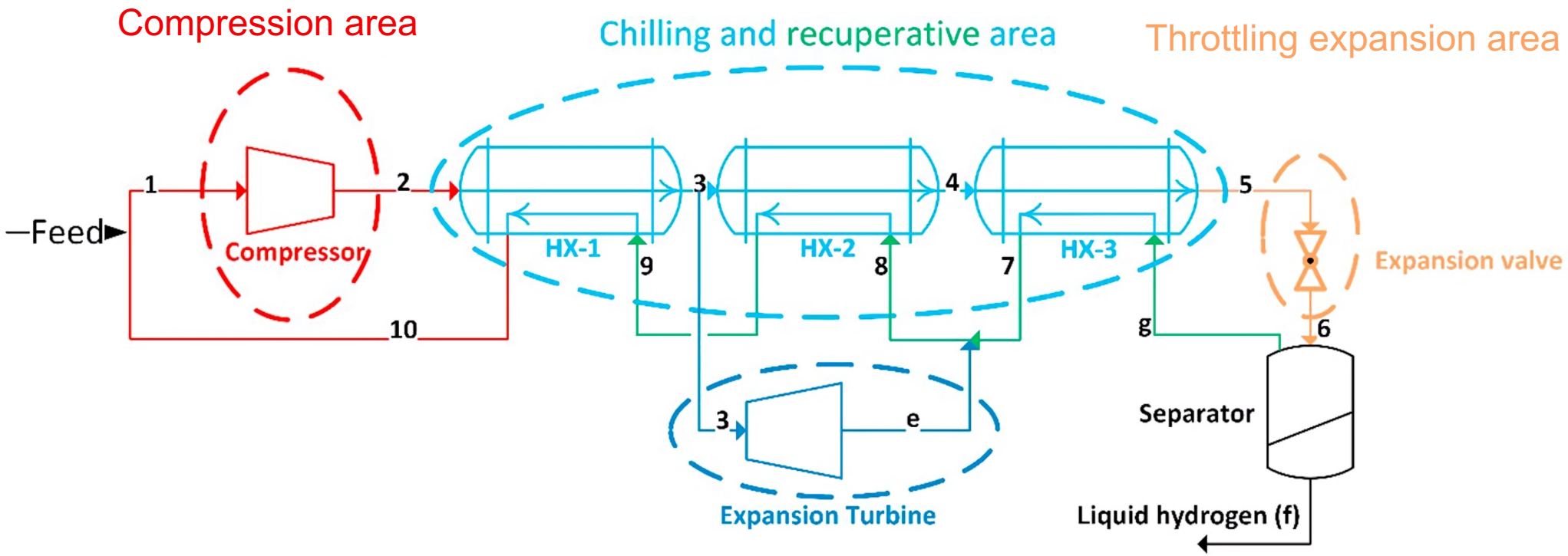
Ortho-para equilibrium

- **Para-Hydrogen** is the only stable specie for liquid Hydrogen storage
- If **Ortho-Hydrogen** is stored at low-temperatures it reaches the equilibrium composition (99+% of p-H_2) with heat generation
- **Equilibrium Hydrogen** is defined as the most stable o/p composition at any temperature
- **Normal Hydrogen** (75/25, ortho/para) is the hydrogen existing at high temperatures



Liquefaction process

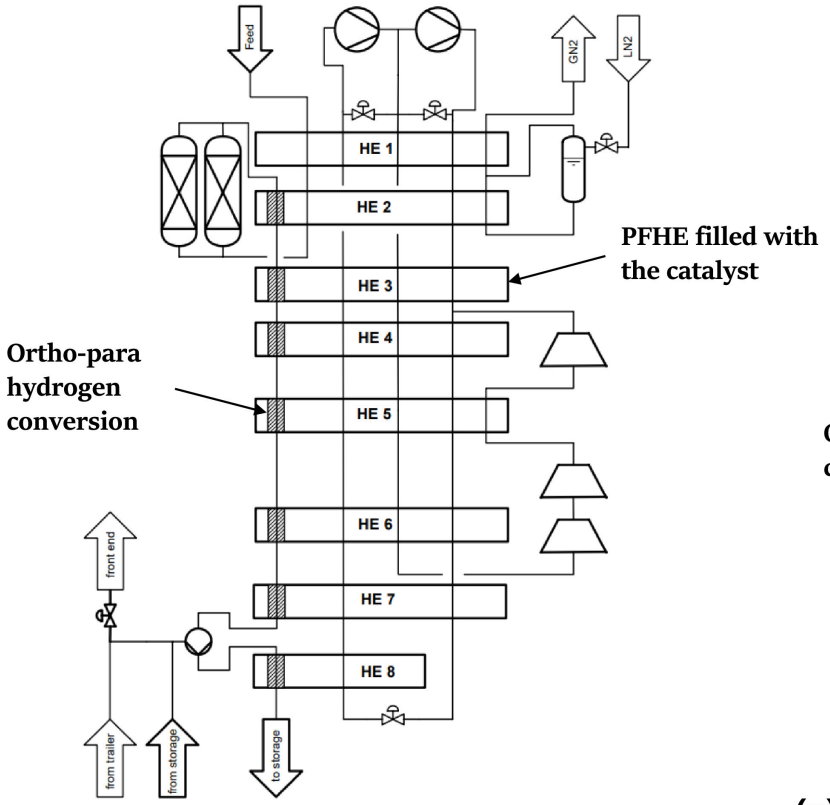
Traditional Claude process



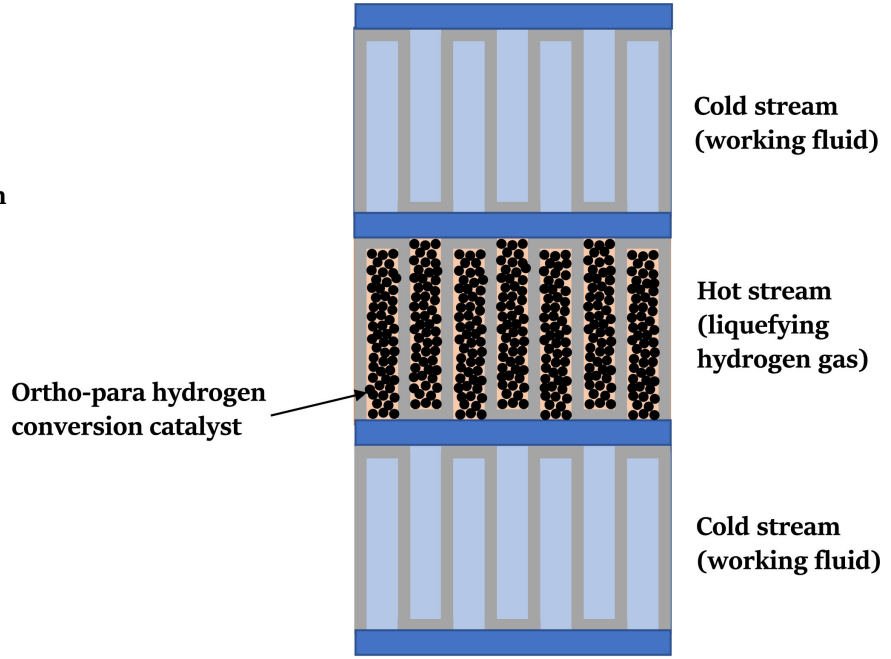
Source: Aasadnia et al. 2018

Core unit

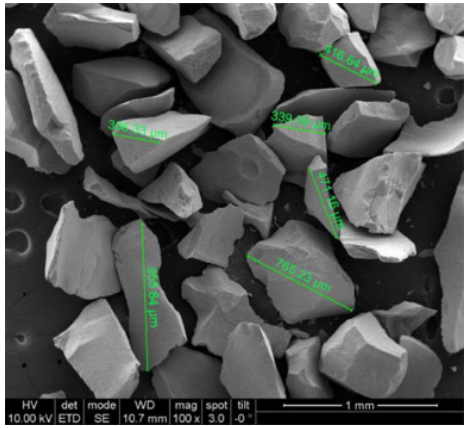
Catalytic Plate Fin Heat Exchanger (PFHE)



(a)



(b)

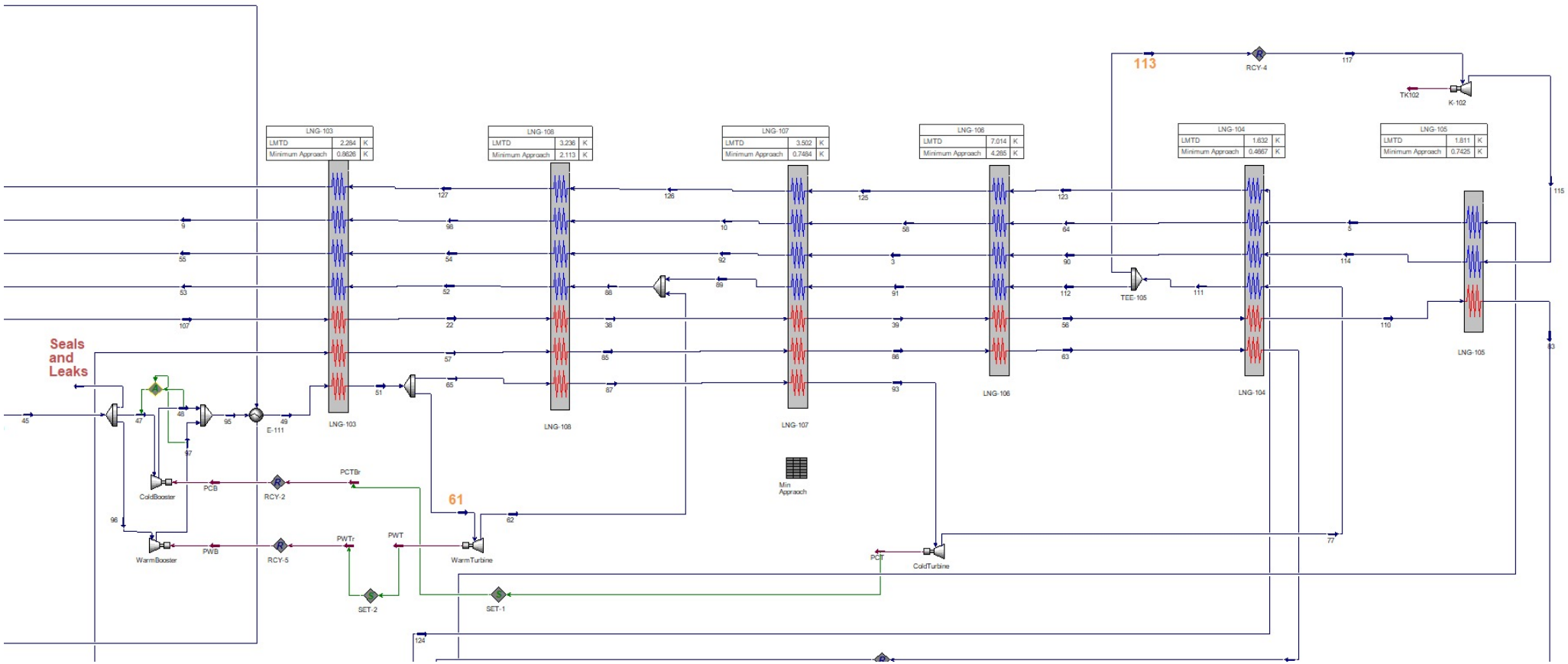


Hydrous Ferric Oxide Catalyst

Source: Park et al. 2021

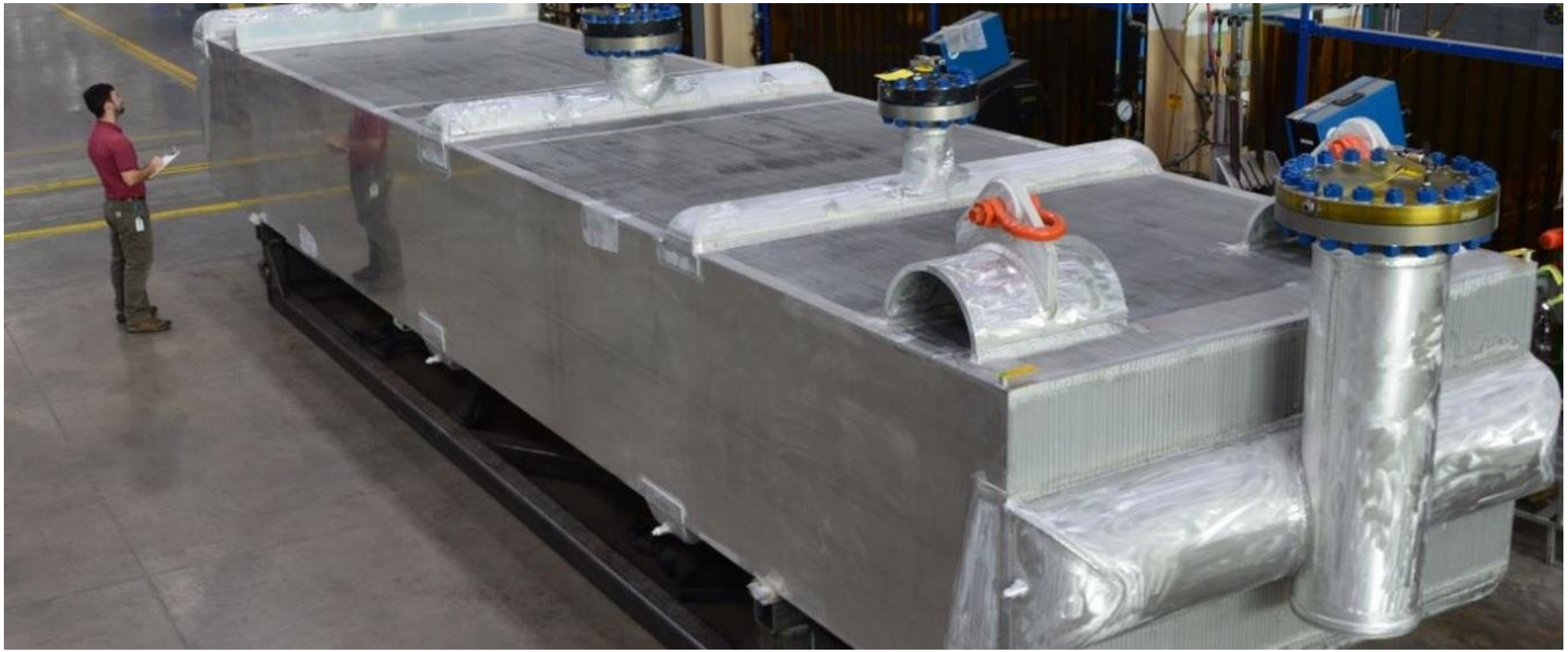
Core unit

PFHE – simulation



Core unit

PFHE – in reality (single unit)



Brazed Aluminum Heat Exchanger

Source: Chart industries

Heat Exchanger Simulation

Current Methods and Proposed CAPE-OPEN Solution

Simulation Methods

Current solutions

1. Heat of reaction is added at the end of each heat exchanger
   – Non rigorous method with inaccurate results

2. Equilibrium hydrogen is modelled as a **pseudo-component** and used only inside the reactive heat exchangers
   – Requires thermodynamic modelling with a pseudo heat capacity which includes the equilibrium heat of reaction

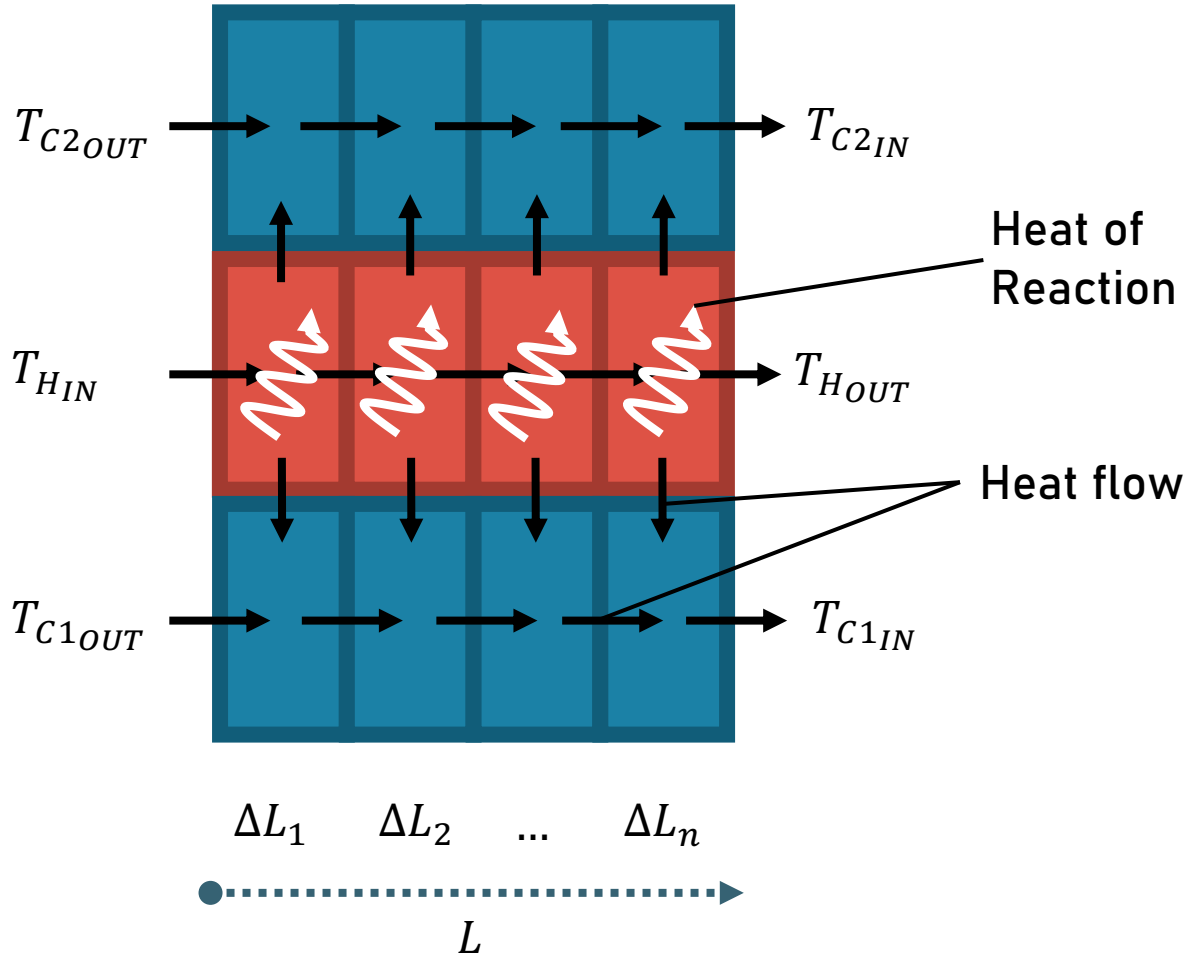
3. Linkage to **external tools** like Excel for calculation of heat exchanger
   – Cumbersome method with possibly accurate result

Proposed Solution

Rigorous reactive PFHE - CAPE-OPEN Unit Operation

- Finite difference method with **heat exchange** and additional **heat of reaction** at in-out differential temperatures

- Final inlet-outlet unknown temperatures are calculated through a **convergence** cycle



Proposed Solution

Why use COBIA interface

- Lower entry barrier thanks to **class wizard**
- Easier customizability and features addition
- Better forward/backward compatibility with platform independence

Conclusion

And prospects

Conclusion

- Solve the problem of simulating the ortho-to-para hydrogen conversion
- **CAPE-OPEN** is a valid tool for simulating **unconventional unit operations** without compromises or tricks
- **COBIA** is the desired interface in order to build new solution **efficiently**

Future Developments

- Use the **integrated UI** over the **ICapeUtilities** Interface to extend the unconventional unit to user-defined processes

- Implement a simulation-wide reaction system for oH_2-pH_2 using the Chemical Reactions interface specification in COBIA once it is released

Thank you for your kind attention

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