Embracing Uncertainty: Unleashing Value in the Evolving Industry Landscape

Driving Innovation and Sustainability toward Net-Zero World with Engineering Simulation Technology Spotlight on Hydrogen applications

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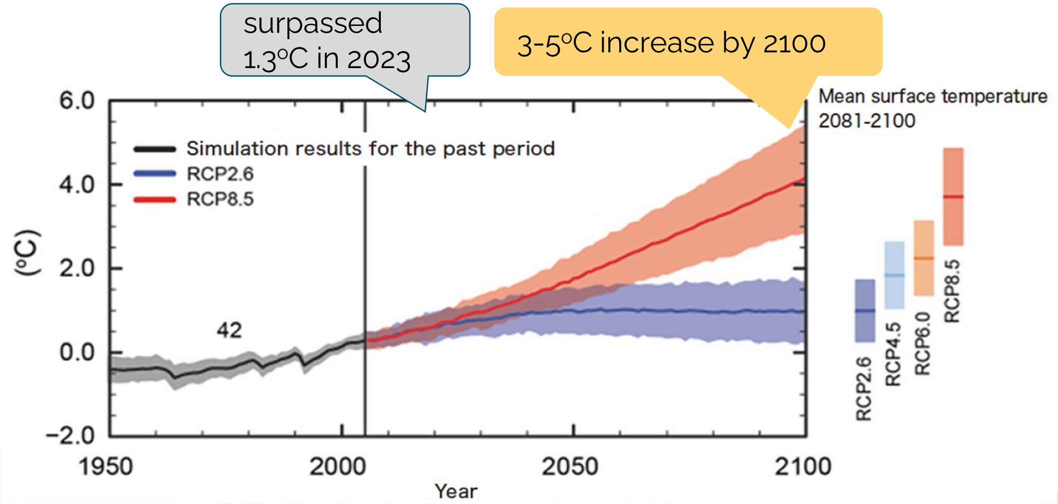
CADIT (Thailand) Co., Ltd.

The Urgency of Net-Zero



Global surface temperature continue to increase

Decarbonization

Achieve **Net Zero** CO_2 emission by 2050

- Removal of ~ 25Gt/year of carbon emissions | Close to $50Trillions investments

Initiatives

- Renewable Energy | **Carbon Capture & Storage** | Biofuel | Electric Vehicles | **Hydrogen Energy**

Mega-trends in Energy sectors

- Hydrogen/Alternate Fuel/Renewable
- Sustainability
- Emission reduction; Carbon capture
- Digitalization/Automation

Hydrogen: Key Enabler for Decarbonization

3x	0
More Energy Density than Hydrocarbons	Carbon Emission at Point of Utilization

Ansys / CERTIFIED ELITE CHANNEL PARTNER

CAD-IT

CADIT Global

Company Profile 2025

Found since 1991

Vision

To Lead the global shift to Industry 4.0 by delivering digital transformation solutions that create exceptional value for our customers, keeping industry best practices in mind & a God centered culture at heart.

Mission

To Empower companies to achieve greater innovation and efficiency through digital transformation solutions & helping clients across the globe reduce costs and time-to-market as your key global partner.

Engineering Simulation

Industry 4.0

Digital Twin

Engineering Simulation with Ansys Technology

SIMULATION PLATFORM
- MATERIALS
- CLOUD / HPC
- OPTIMIZATION
- PROCESS & DATA MANAGEMENT
- MULTIPHYSICS

SYSTEM OF SYSTEMS
- DIGITAL MISSION ENGINEERING

SOFTWARE & SYSTEMS SIMULATION
- DIGITAL TWIN
- SYSTEMS
- EMBEDDED SOFTWARE
- SAFETY ANALYSIS

PHYSICS-BASED SIMULATION
- STRUCTURES
- FLUIDS
- ELECTRONICS
- SEMICONDUCTOR
- OPTICAL
- 3D DESIGN
- PHOTONICS

CAE

STRUCTURES	FLUIDS
FEA	**CFD**
Mechanical	Fluent
LS-DYNA	**DEM**
	Rocky

Mixing Process and Flow in Pipe

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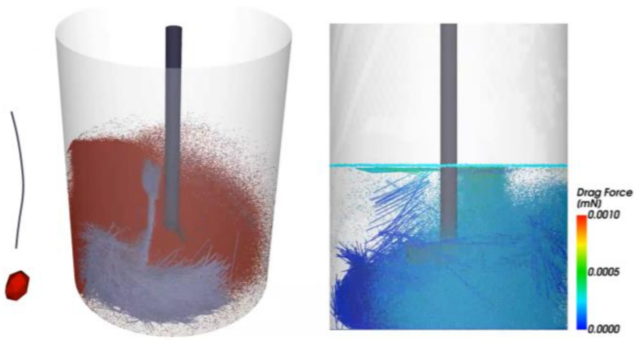
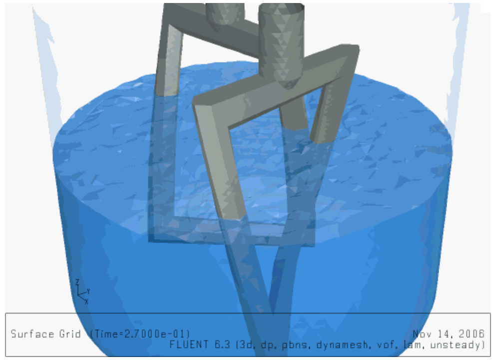
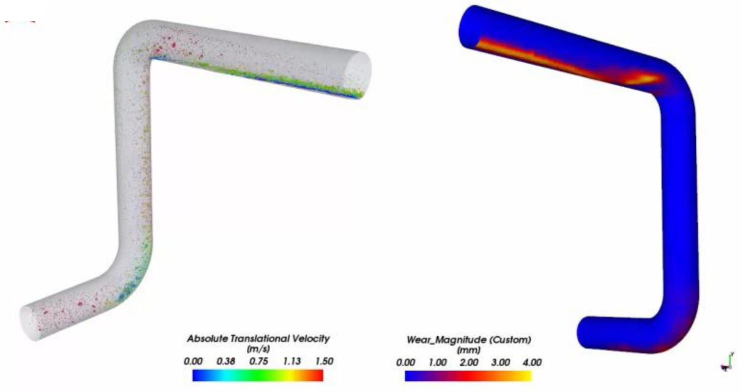
Process industry



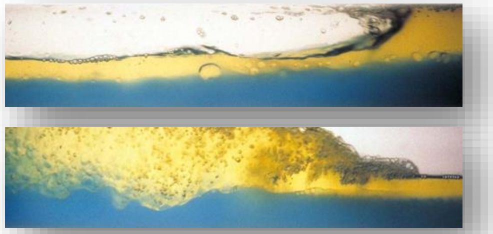
Powder and Fiber Dispersion



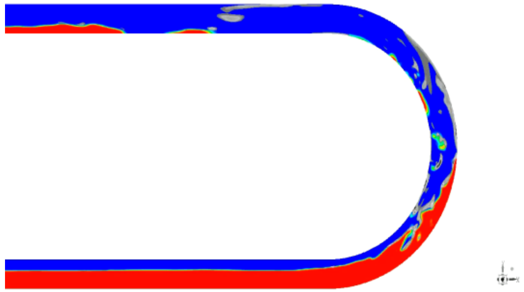
Newtonian Fluid-mixing

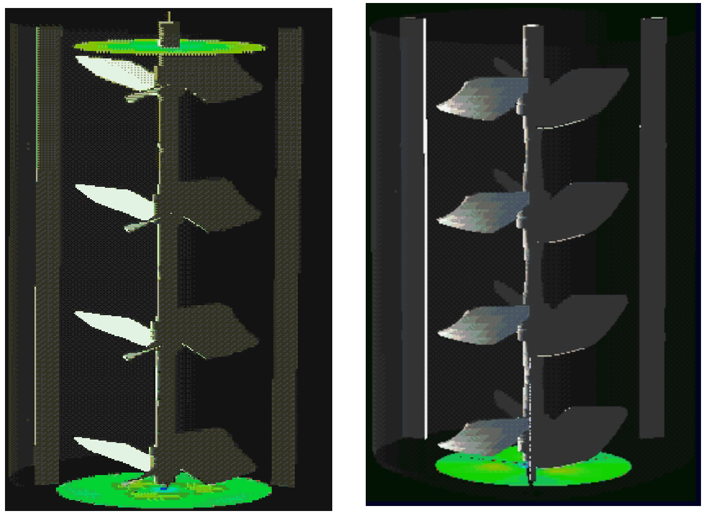


Pipe Bend Erosion

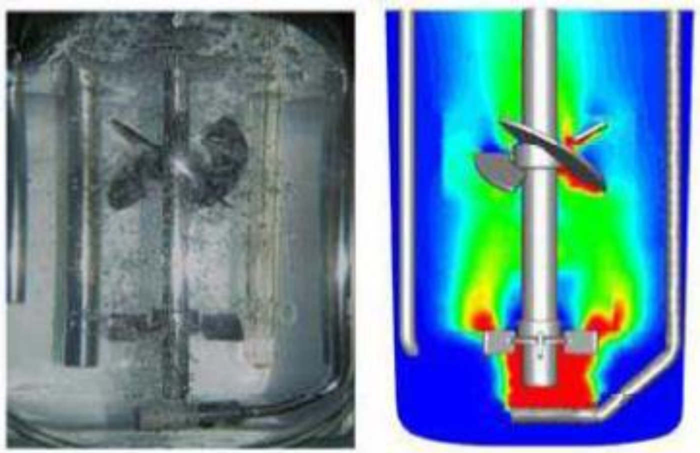


Flow Assurance – Slug flow induce Vibration

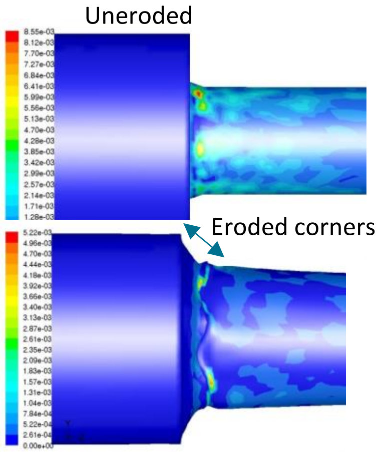




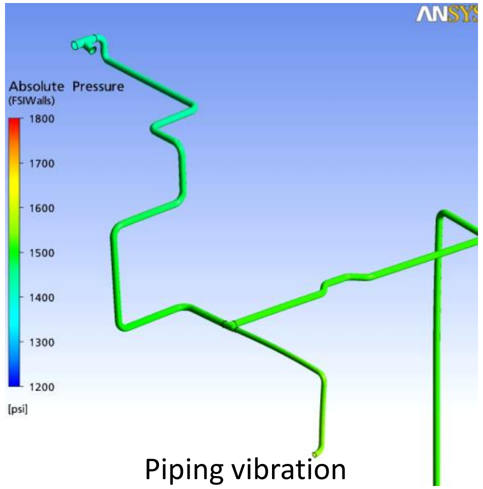
Agitator-comparison



Bubble distribution



Pipe Conjunction Erosion



Piping vibration

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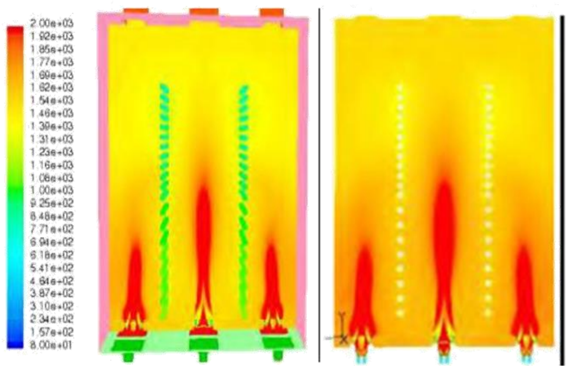
Furnace, Heat Exchanger, Combustion & Reaction

Process industry

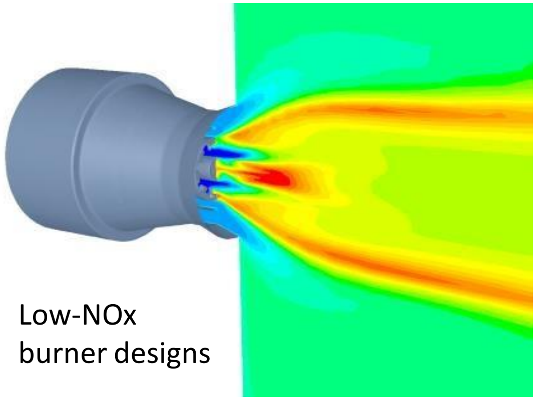


Temperature profile during Start of Run

Temperature profile during End of Run

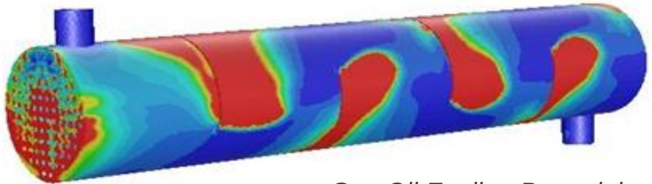
Coker furnace modeling

Burner Design

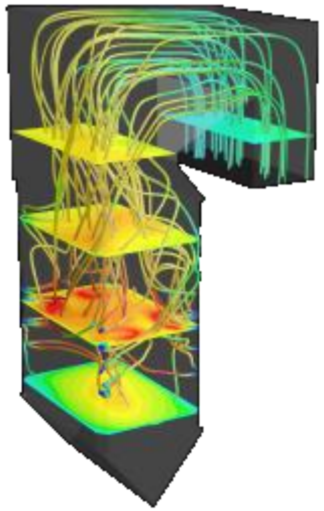


Low-NOx burner designs

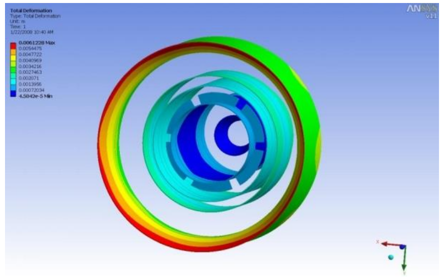
Courtesy Of: GE Energy and Environmental Research Corporation

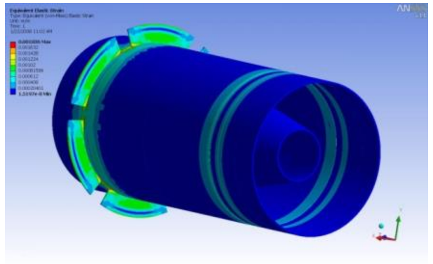


Gas Oil Fouling Potential

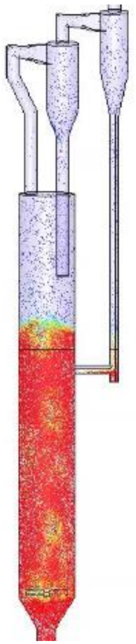


Boilers

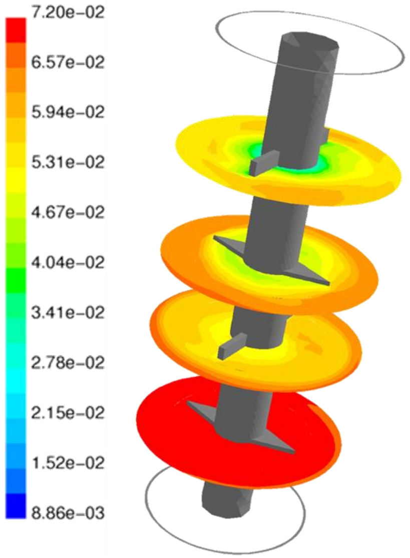




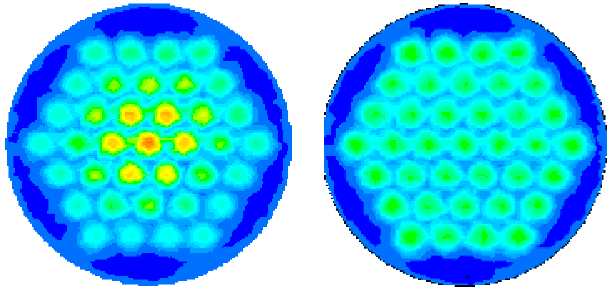
Total deformation due to thermal stresses of burner



Fluidized bed reactor



Polymerization reaction



Maldistributed

Improved

Axial velocity at the inlet to the tubes; no "hot spots" visible for the improved design

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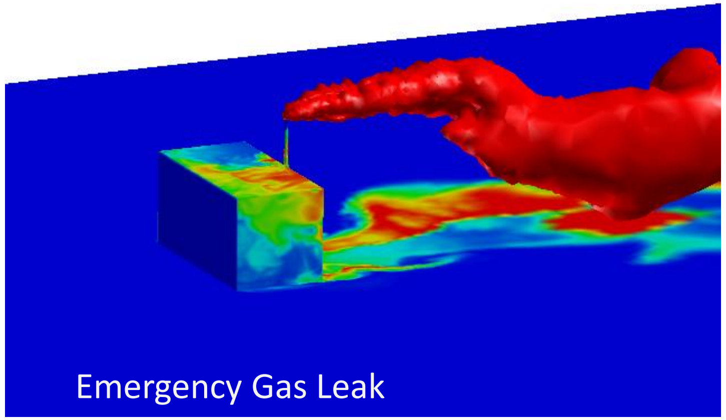
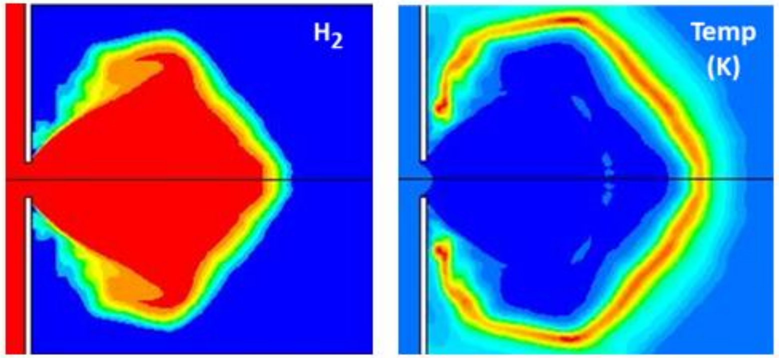
Safety, Maintenance equipment

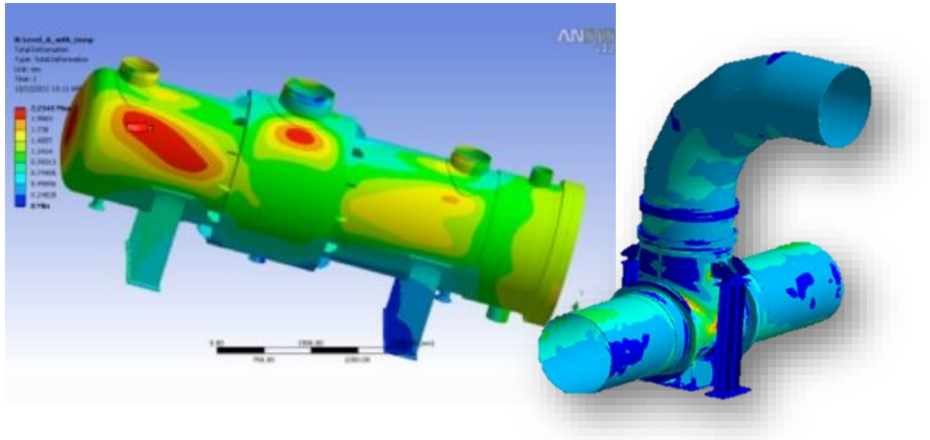
Process industry



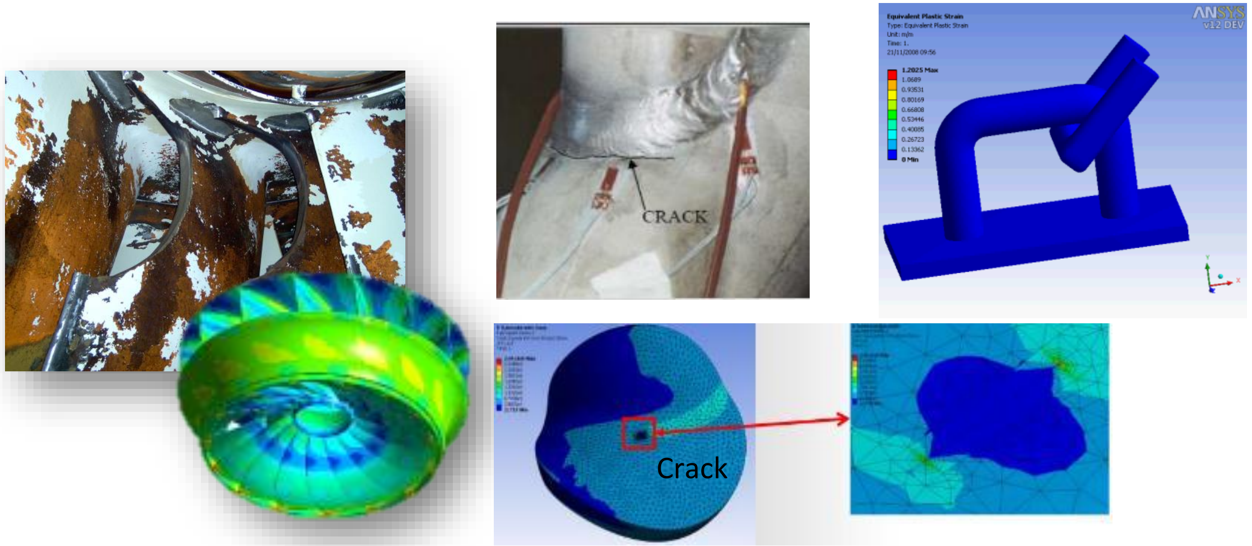
Emergency Gas Leak



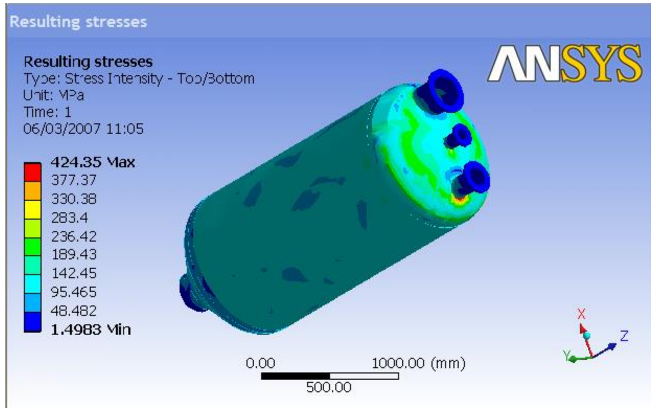
Predict leakage auto ignition & flame propagation



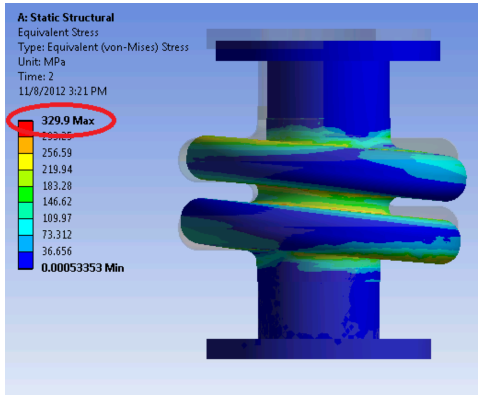
Strength analysis for Maintenance and services



Equipment/component Life prediction



Pressure vessel

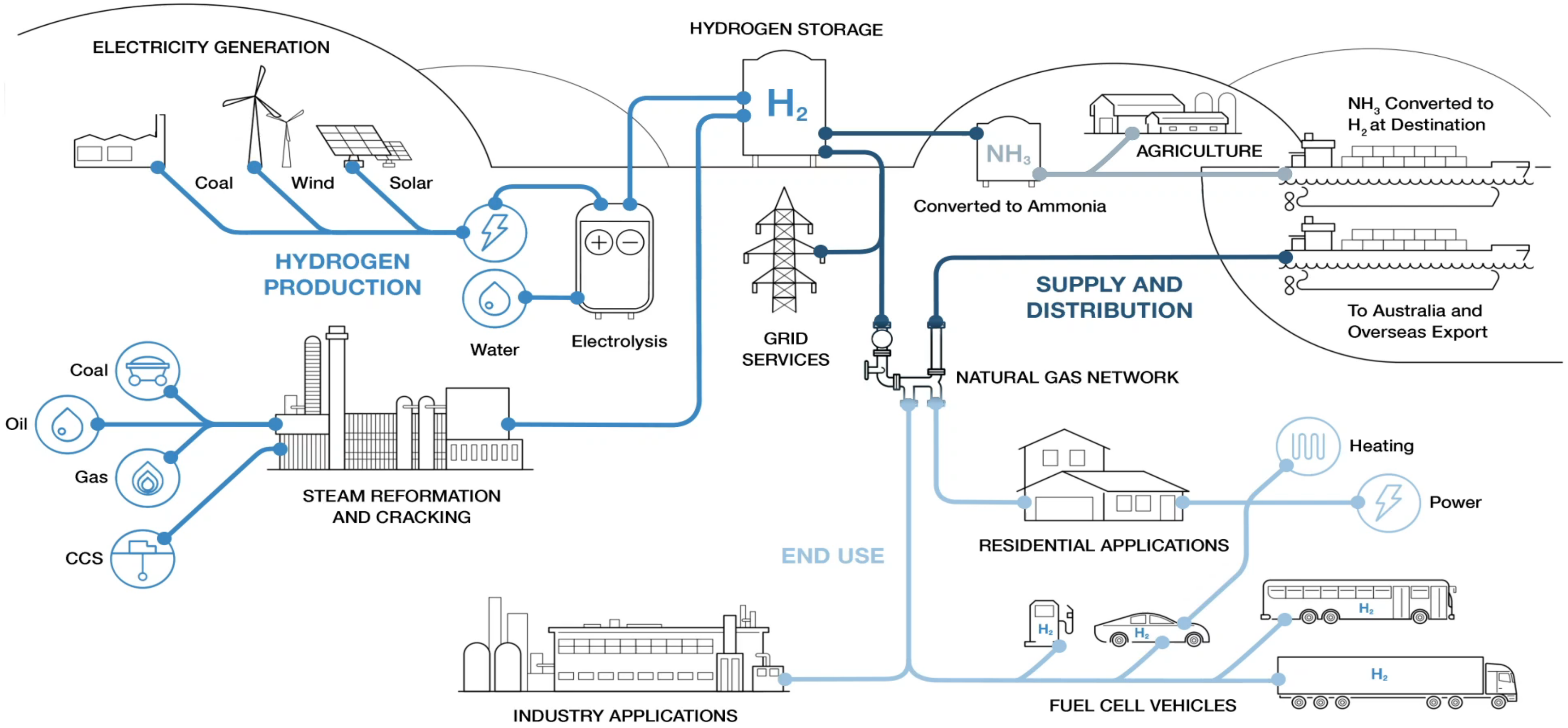


Simulation Empowers Hydrogen Innovation

Driving Innovation and Sustainability toward Net-Zero World with Engineering Simulation Technology
Spotlight on Hydrogen applications

Challenges in Hydrogen Value Chain

Production and Purifier	Storage	Transport	Utilization
• Modeling SMR • Modeling electrolysis • Integration of CCUS with reformer	• Design of cryo-coolers • Liquefaction • Storage tank design	• Auto-ignition • Hydrogen embrittlement • Adsorption in hydrides • Ammonia Conversion	• H2 combustion • Flashback | NOx | H2-Blends | NH3- Blends • Fuel cell design
Main Challenges			
Efficiency | CO_2	**Compression | Liquefaction**	**Safety | Embrittlement**	**NOx | Flashback**



Hydrogen Characteristics

57x
Lighter than gasoline vapor. Prone to leak

15x
Smaller ignition energy requirement

4-70
Vol% in air flammability limit

8x
Higher flame speed than methane

Hydrogen Production: Steam Methane Reforming

Objective

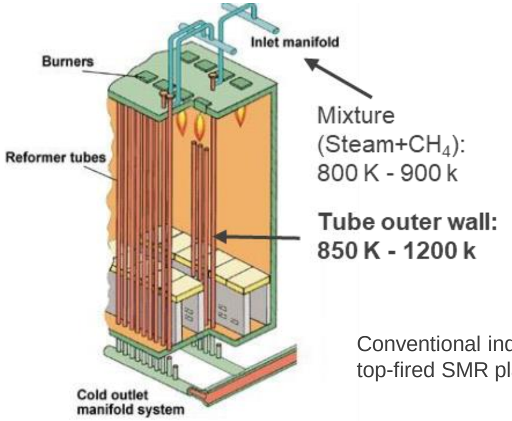
- To **improve hydrogen yield** and **thermal efficiency** in a Steam Methane Reforming (SMR) process

Ansys Solution

- Use CFD to optimize burner layout and **flame profiles**, including radiative and convective heat transfer in the furnace. *(Fluent)*
- Use **reacting flow models** help tune catalyst performance using:
  - **1D plug flow models** (detailed chemistry)
  - **Porous media** model to represent the catalyst bed
  - **Coupled with 3D models** to capture heat distribution within the furnace chamber

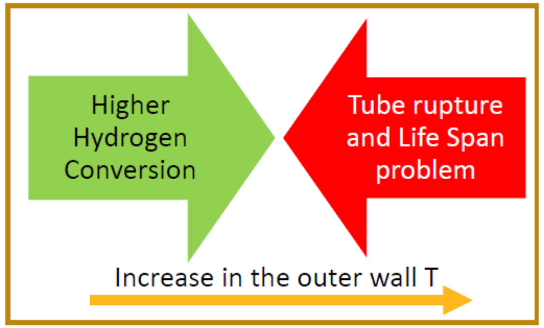
Outcome

- Better insights in virtual environment to ensure uniform heat distribution and flame interaction **to avoid hotspots or cold zones** that reduce reforming efficiency.
- Apply **1D–3D Coupled Models to reduces simulation cost** while maintaining accuracy for scale-up.
- Balance high-temperature performance with long-term **structural integrity.**



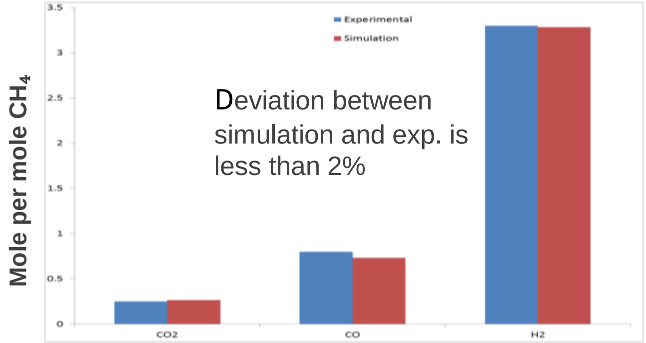
Conventional industrial top-fired SMR plant

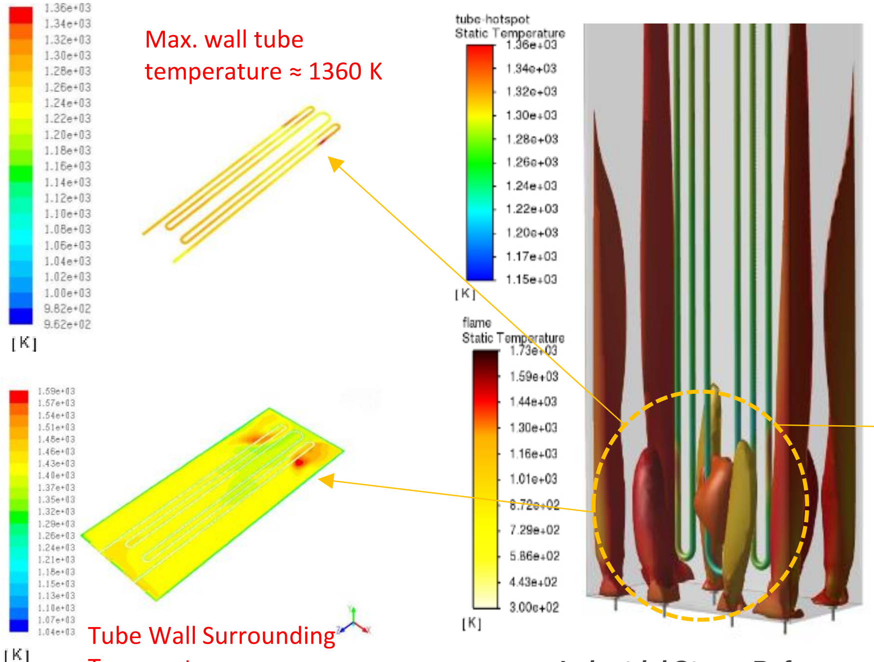
Kevin Bakey (2015), ENGL 202C "The Production of Hydrogen Gas: Steam Methane Reforming" – Process Description.



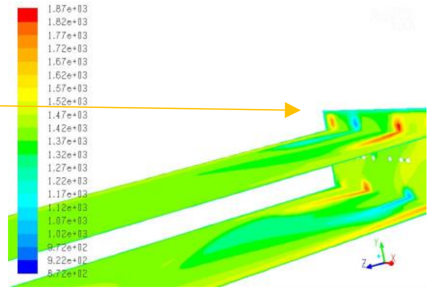
Aguirre, A. (2017). Computational Fluid Dynamics Modeling and Simulation of Steam Methane Reforming Reactors and Furnaces (Doctoral dissertation, UCLA).

- Temperature of the furnace-side wall of the reforming tube
- **50 K increase results in a 50% reduction of tube life**





Industrial Steam Reformer



Hydrogen Purification: Post-Combustion - Carbon Capturing Using MOFs

Objective

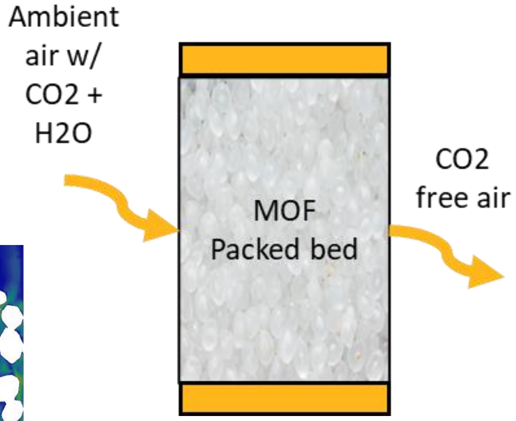
- Evaluate the performance of **Metal-Organic Frameworks (MOFs) on adsorption of carbon dioxide** from ambient air
- Predict **particle bed porosity and permeability.**
- Evaluate effects of particle **swelling/deswelling** on pressure drop and porosity.

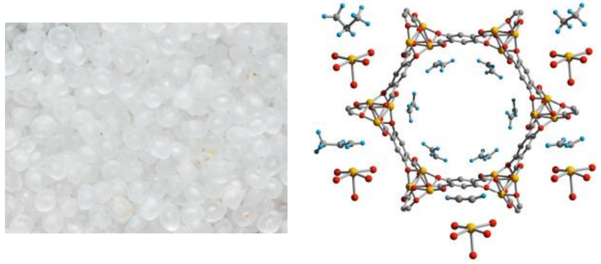
Ansys Solution

- Particle bed generation with **real particle shape** of the MOF. (Rocky, Fluent)
- **Custom model** for adsorption/swelling in DEM-CFD coupled simulations.
(Rocky, Fluent)

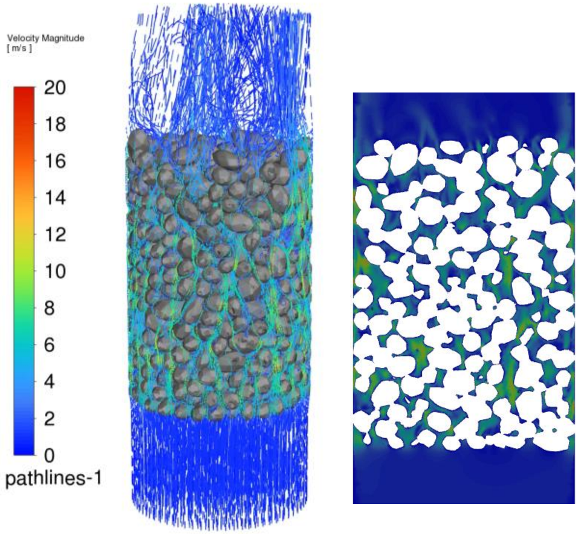
Outcome

- The DEM-CFD approach enables **analyzing species concentration** for each particle in the domain, as well as **volume and mass change** of the particles.
- Find the **particle shape and size distribution** that provides the desired **pressure drop** and **porosity conditions.**

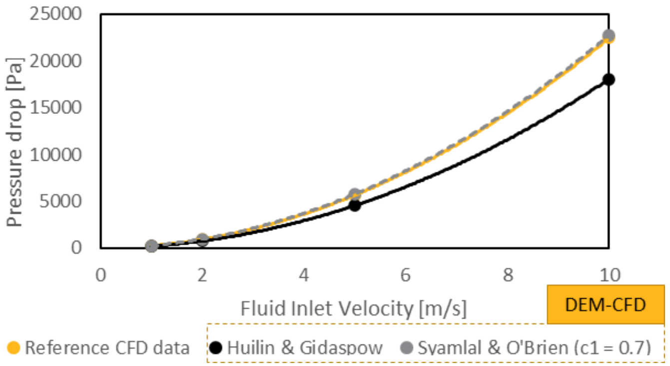




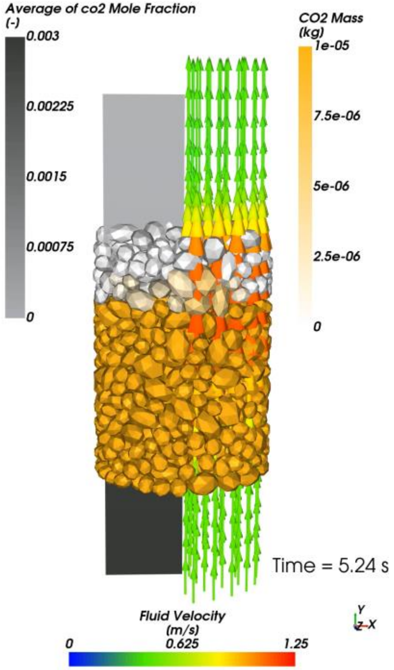
Metal-organic-framework materials act as a sponge to capture the CO2 chemically

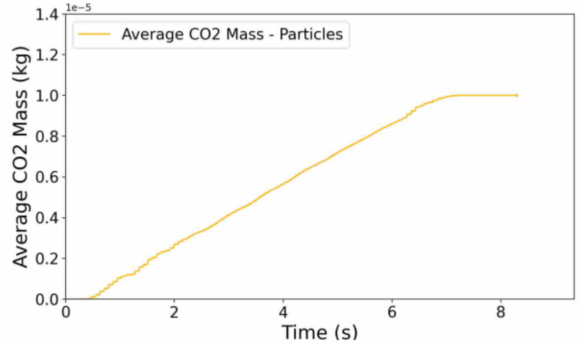


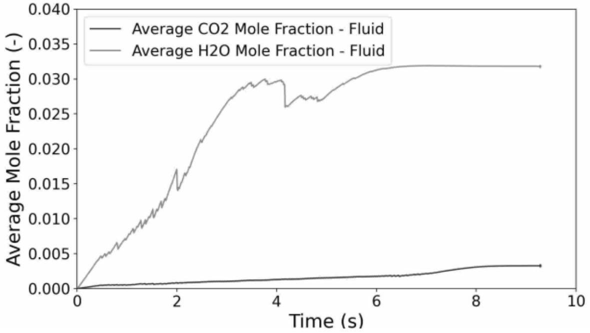
Velocity profile from **standalone CFD**



DEM-CFD Drag law calibration







Adsorption Results of **CFD-DEM**

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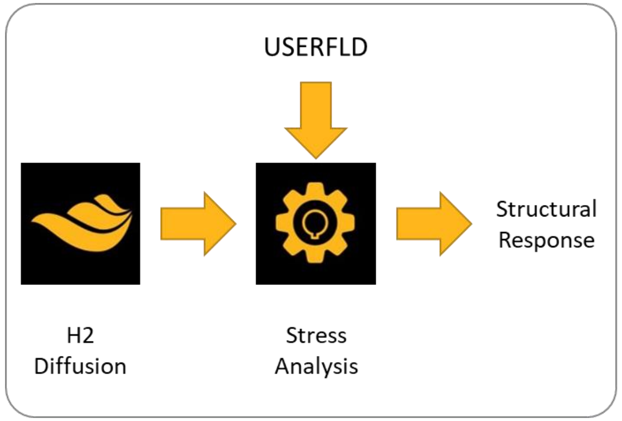
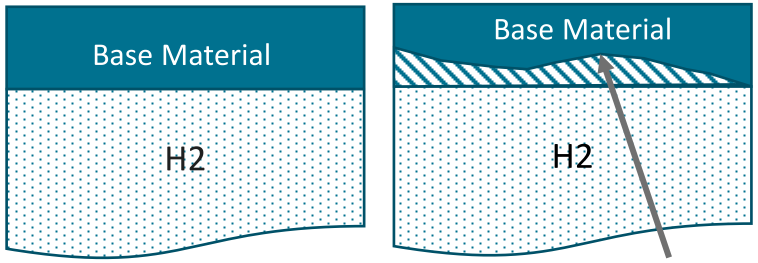
Hydrogen Storage & Transportation: Embrittlement

Challenges

- **Hydrogen atoms diffuse into high-strength steels**, causing brittleness and sudden failure.
- **Lack of standardized testing** of material properties as a function of hydrogen concentration
- Prediction is complex due to **material microstructure, stress states**, and **hydrogen diffusion**.





Material Selection

Environmental Loads (temperature, Stress, Hydrogen Conc)

Granta

Material Selection Tool/Database

Alloy/ Polymer Composition

Current Status
- Test data in National Lab databases
- H-Mat consortia stores data internally in Granta-MI
- Collaboration with DoE, Sandia for database

Granta

Safety: Catastrophic failure in presence of Hydrogen

Granta

Material Database

Fluids

Diffusion Simulation

Mechanical

Stress Simulation

Mechanical

Calculate Fracture Toughness/ SIF

Extract Limiting Loads for Catastrophic Failure in the presence of Hydrogen

Current Status
- Stress simulation with material properties as a function of H2 conc.
- SIF as a function of H_2 concentration maybe possible with scripting

Workbench /pyAnsys

PHM: Fatigue Life

H_2 spatial distribution

Mechanical

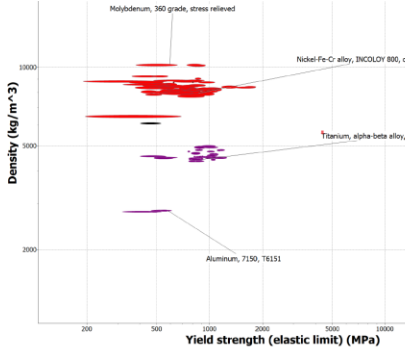
Stress + Crack Propagation Simulation

Mechanical/nCode/

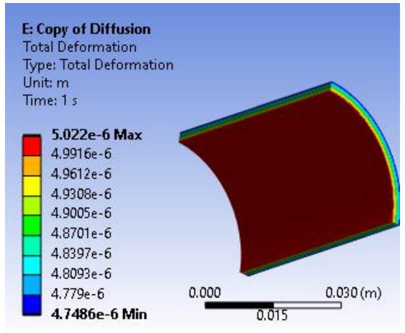
Fatigue Life compromised by Hydrogen Presence

TwinDeployer

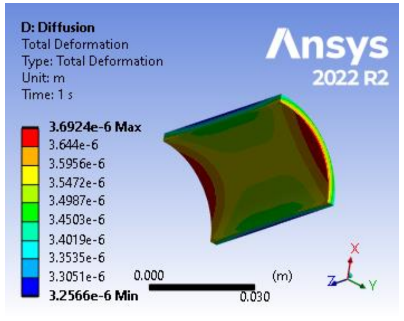
Current Status
- Fatigue Law may be made H2 conc. Dependent by mapping the concentration field as temperature



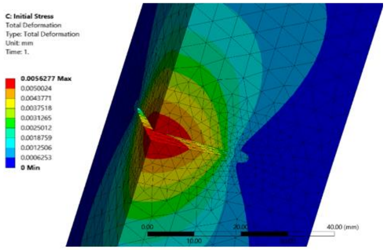
Granta Selector for light, brittle resistant and cost-effective material identification



Deformation without Diffusion



Deformation with Diffusion



Crack propagation

H2 Utilization:
Ammonia Combustion

Objective

Predict Change in flame shape with the increase in cracking ratio (represented H2-N2 percentage, KAUST Flame)

Challenge

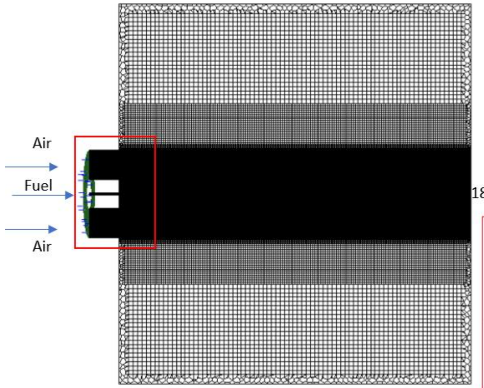
- Utilize ammonia effectively to produce hydrogen through thermal cracking
- Manage low reactivity of ammonia (NH3)
- Control NOx emission and avoid ammonia slip (unburnt Ammonia)

Solution

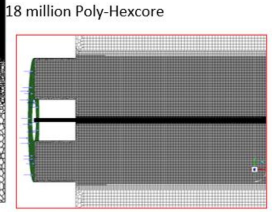
- Accurate combustion simulations using finite rate (FR) and Flamelet-Generated Manifold (FGM) combustion models|Ability to include larger reaction mechanisms in the simulations. (Fluent)
- Fast solves using the highly scalable CFD solver on hundreds of thousands of cores for faster design iterations. (Fluent, HPC)

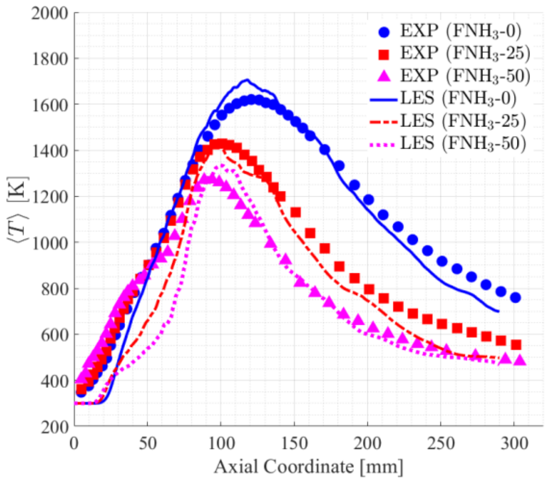
Benefits

- **Understand flame characteristics** of ammonia and ammonia blended fuels | ammonia slip | stable operating points.

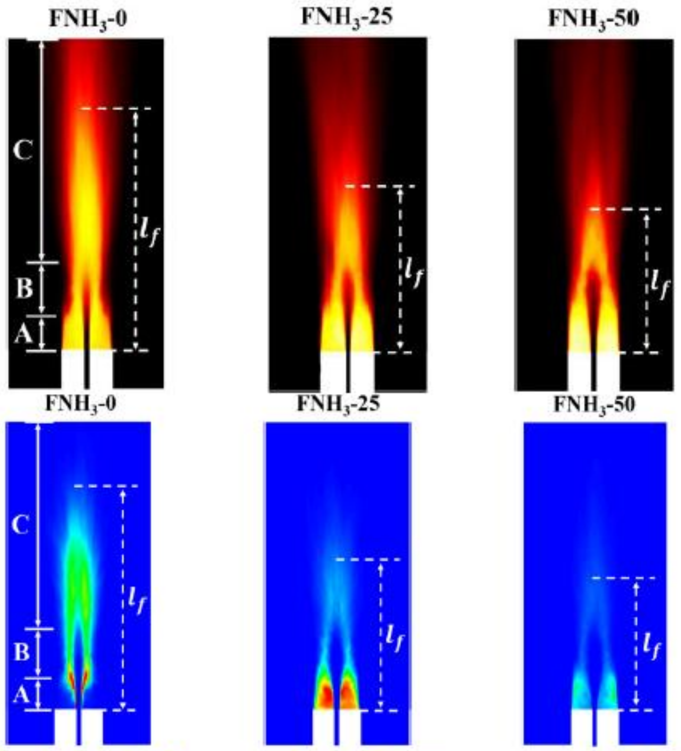


- External dia. = 50 mm
- Jet outlet dia. = 4.6mm.
- Co-flow air : 150 mm air contractor.
- Air flowrate : 12.9 m/s2





Adamu A., Ayman M. E., Jiajun L., Suliman A., Hong G. Im, Bassam D., Combustion and Flame, Volume 258, Part 2, 2023,



Fuel vol.: 0% NH3, 72% H2, 25% N2	Fuel vol.: 25% NH3, 56.25% H2, 18.75% N2	Fuel vol.: 50% NH3, 37.5% H2, 12.5% N2

lf: effective flame length, **Zone A:** mixing & recirculation, **Zone B:** “neck” zone, **Zone C:** expanded jet flame

Flame length decreases as NH3 increases, and the global mixture reactivity reduces

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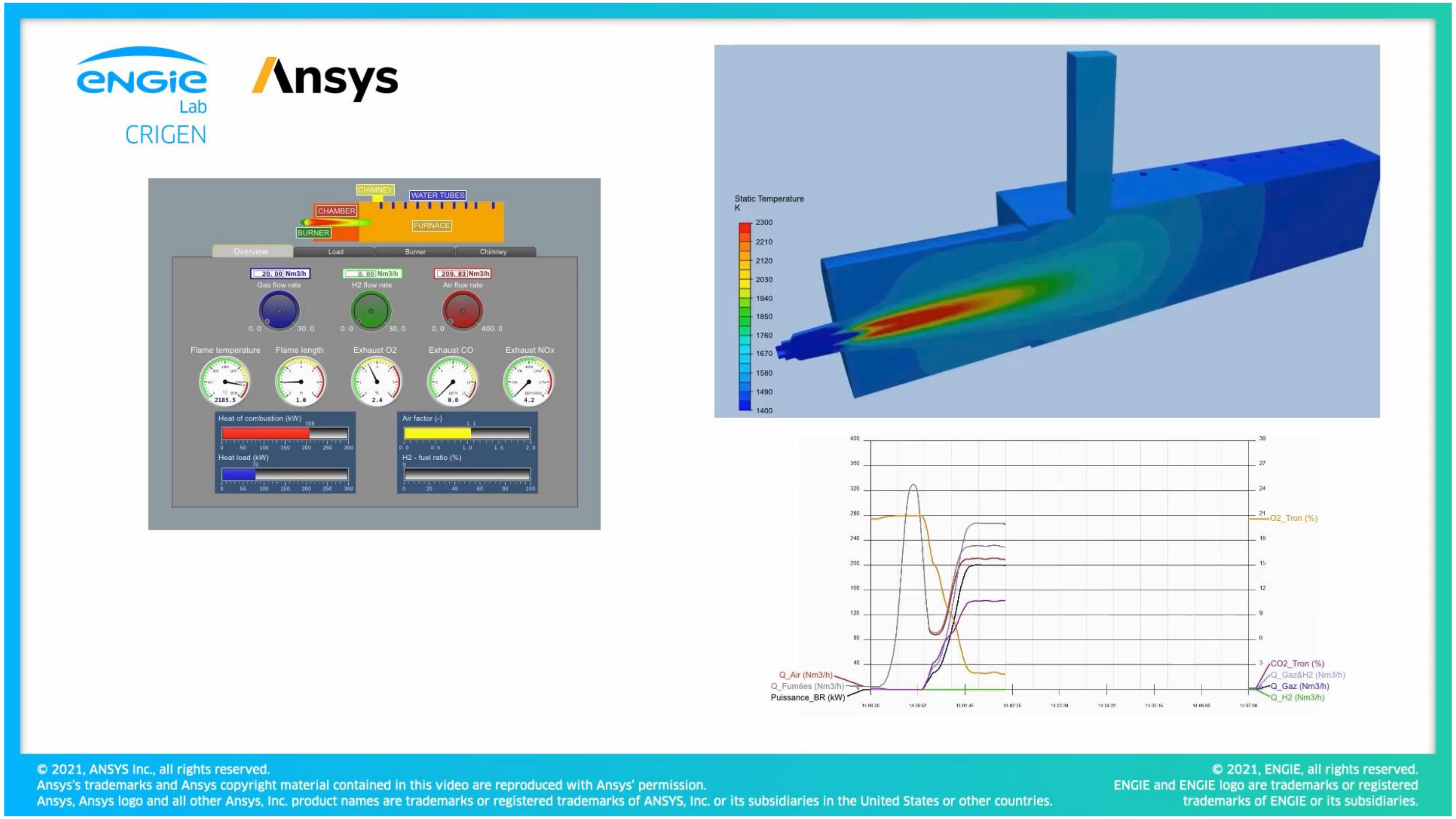
Accelerating Hydrogen adoption with Digital Twin

Objective

- ENGINE is helping their customers **accelerate the transition to zero carbon**.
- To achieve this, they need to **optimize combustion system, operation, reduce system failure risk, and reduce maintenance cost**

Solution & Value

- Through its collaboration with Ansys, ENGIE Lab CRIGEN – the ENGIE Group’s corporate center for R&D and high-level expertise is developing an **<u>ultrafast and high-fidelity simulation based digital twin to:</u>**
  - Maximize the **efficiency**
  - Make industrial equipment sustainable by boosting **product reliability**
  - Help evaluate **new concepts** in energy production (hydrogen etc.)
  - Improve **product performance** during operation through **predictive maintenance** and asset performance management decisions.
  - Control industrial processes, anticipate **carbon reduction** challenges and **lower maintenance costs**



Energy’s Sustainability Pillars

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Low-Carbon Energy Solutions

- **Hydrogen value chain**
- **Carbon capture**
- Renewable energy
- Nuclear energy
- Electrification
- Material circularity

Efficiency Improvements

- Fuel production
  - Up/ Mid/ Downstream
- Energy conversion
  - Electricity/ Heat/ Motion
- Operational efficiencies, assets & processes

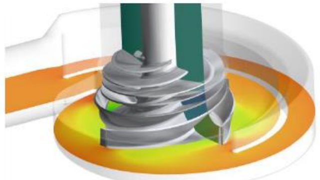
Advancing Energy Reliability and Affordability

- Safe and reliable energy production and transmission
- Energy storage solutions
- Integrated energy systems
- Life and performance prediction

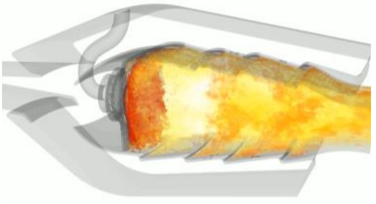
Acceleration Through Digital Transformation

- Digital assets, simulation
- Digital twins
- System simulations
- AI/ML applications
- Additive manufacturing
- AR/VR
- Internet of Things (IoT)
- Edge computing

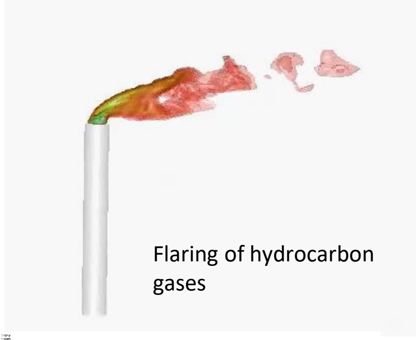
Fluidized beds



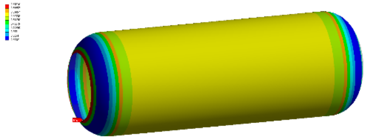
Cryogenic pumps



Gas turbine



Flaring of hydrocarbon gases



Identify critical location and failure mode

Simulation is playing a vital role in helping industries transformation to green energy effectively

THANK YOU

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