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Simulation in the modern refinery

Renewable Diesel Process Synthesis and Optimization using AVEVA PRO/II Simulation

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Renewable Diesel Process Synthesis and Optimization using PRO/II

Kirtan Trivedi
ExxonMobil Global Projects

Energy lives here

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Transport sector emissions

Transportation

Road (Passenger)	Road (Freight)	Aviation	Shipping	Rail	Other
45.1%	29.4%	11.6%	10.6%	1%	2.2%
CO_2 emissions	CO_2 emissions	CO_2 emissions	CO_2 emissions	CO_2 emissions	CO_2 emissions

~25%

of global energy related direct CO_2 emissions

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Source: IEA (2020), Energy Technology Perspectives 2020, IEA, Paris.

Lead industry in the energy transition

Leveraging centralized expertise and capabilities to grow the portfolio

UPSTREAM	PRODUCT SOLUTIONS	LOW CARBON SOLUTIONS
• Strengthening portfolio competitiveness	• Growing high-value products	• Growing biofuels
• Executing industry-leading development portfolio	• Leveraging integrated facilities, supply chains, and markets	• Delivering CCS and hydrogen solutions
• Lowest cost of supply	• Lowest cost of production	• Lowest industry cost

Improving safety and reliability; Reducing emissions; Driving efficiencies

Technology and Engineering | Global Projects | Global Operations and Sustainability | Global Services | Corporate Functions

Scale | Integration | Technology | Functional Excellence | Talent

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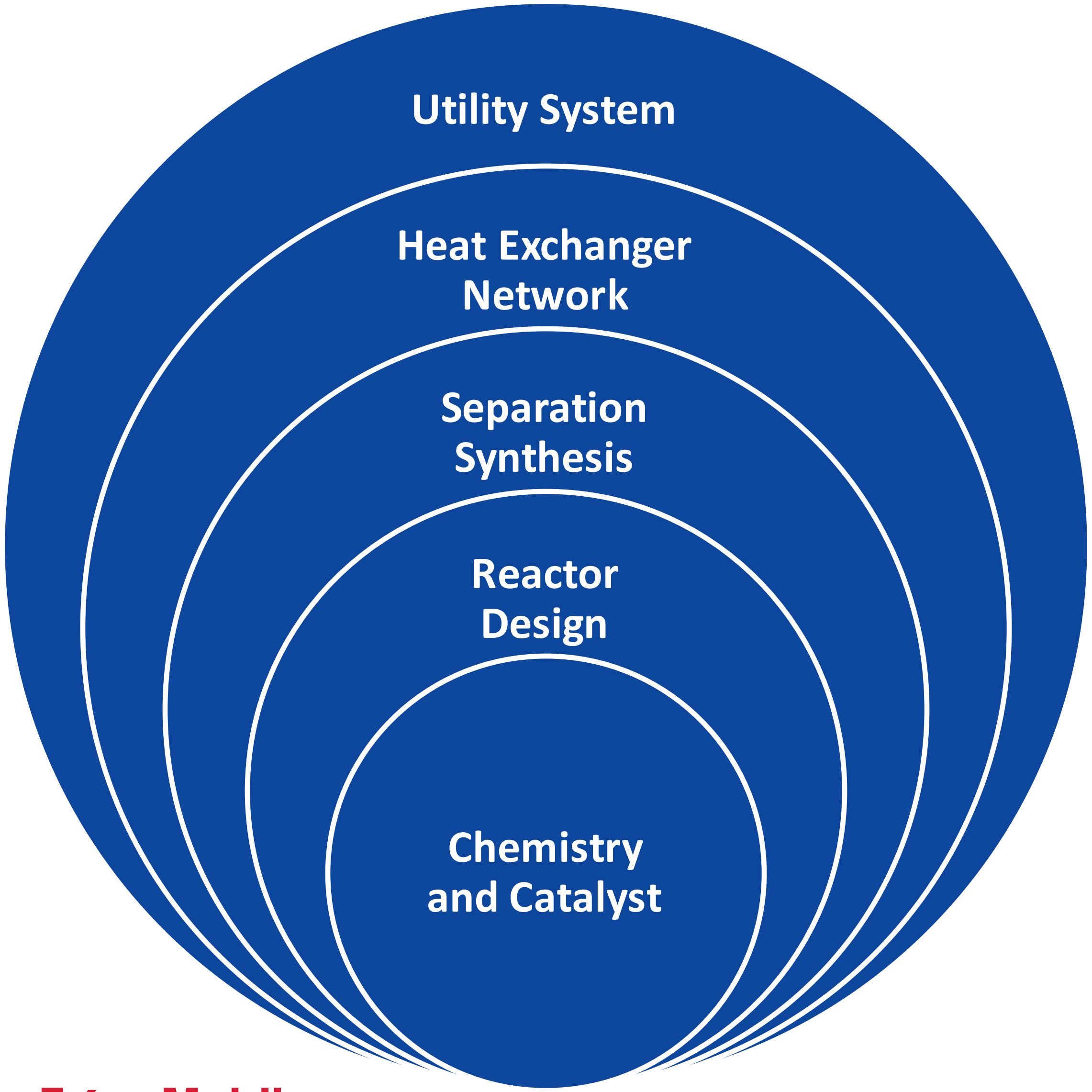
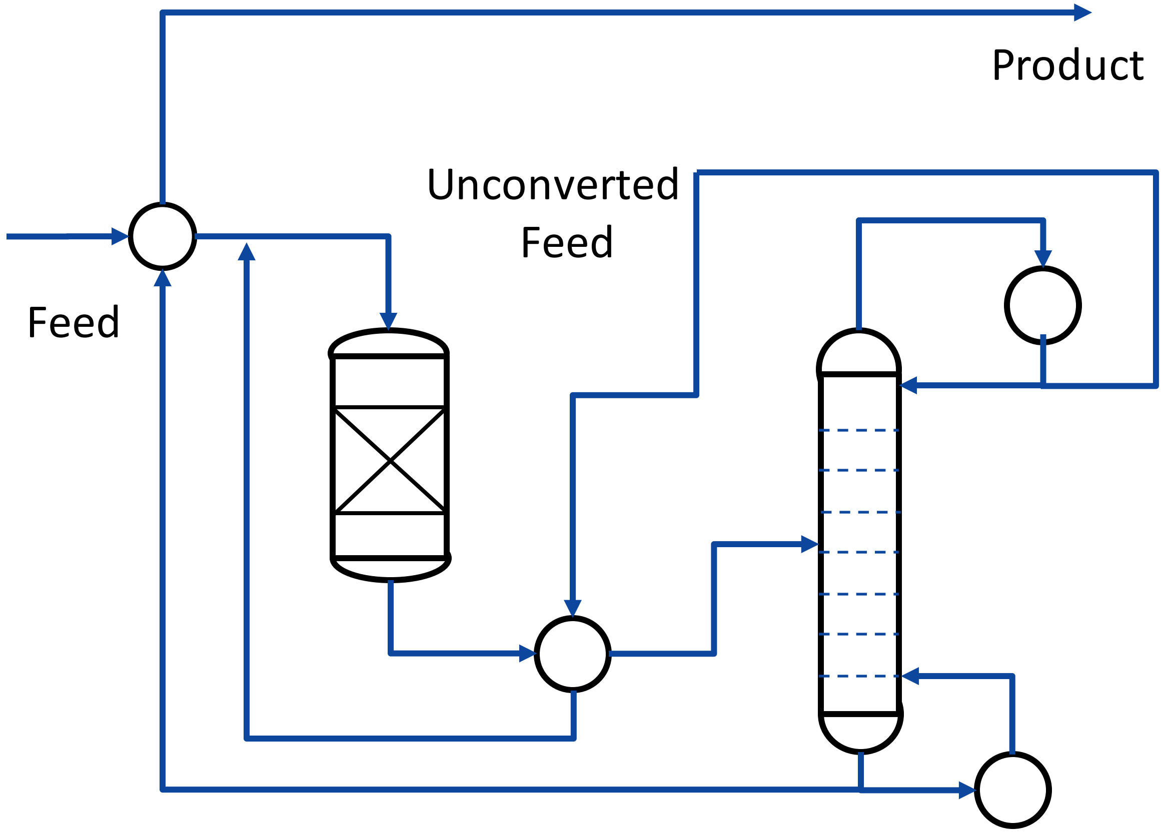
Source: 2022 ExxonMobil Investor Day Presentation. See Supplemental Information for definitions.

Process Synthesis





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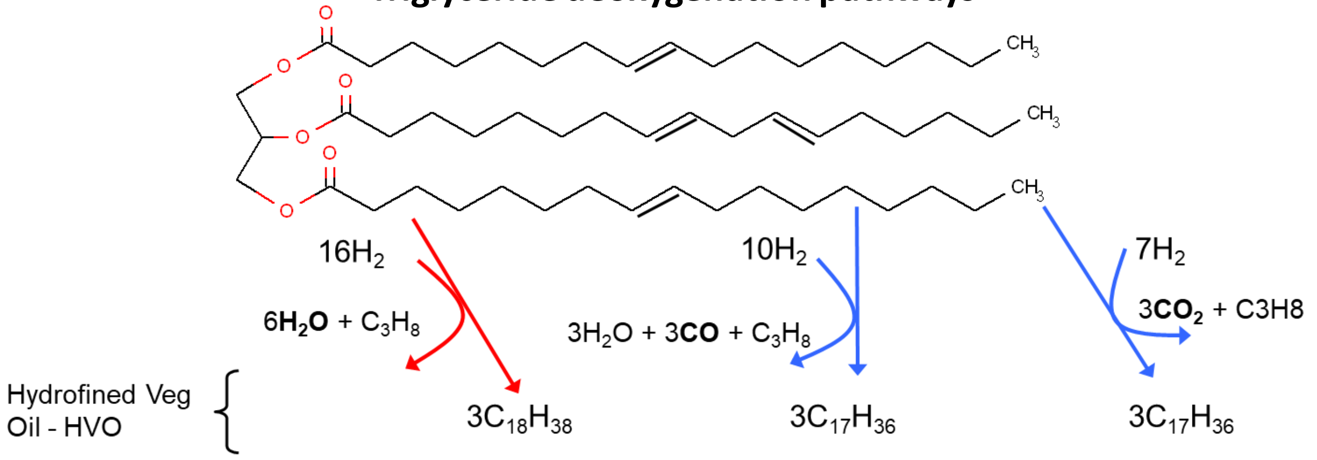
Based on: B. Linnhoff etal., User Guide on Process Integration for the Efficient Use of Energy, IChemE, 1983

Renewable diesel chemistry is well known and understood

Triglycerides + H_2 → n-paraffins + Propane + H_2O + CO + CO_2

- Bio feeds contain triglycerides with oxygen, rather than the aromatics, nitrogen, and sulfur of conventional feeds
- Oxygen can be removed via three different pathways
  - Selectivity is tunable by catalyst and process conditions
  - Additional reactions include methanation and water-gas shift

Triglyceride deoxygenation pathways



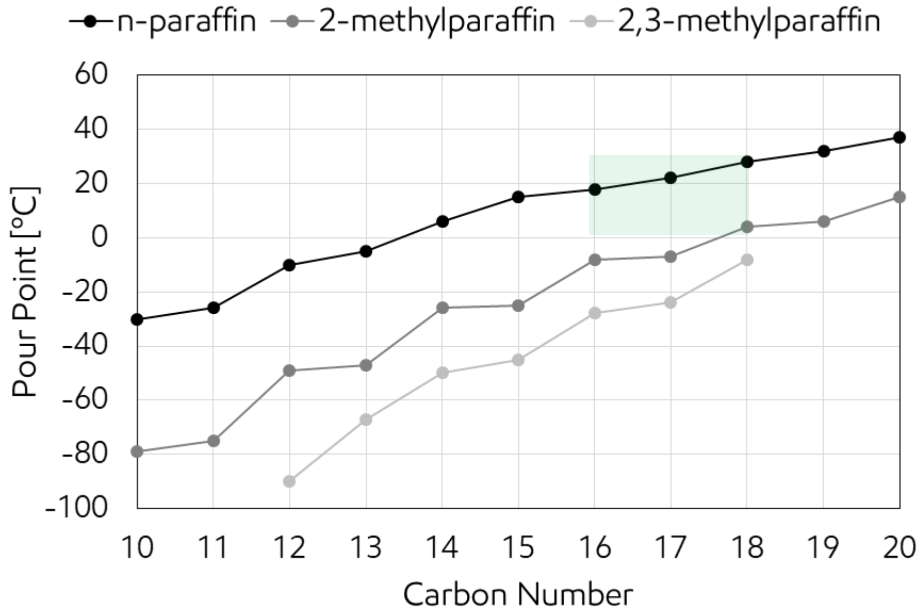
Hydrodeoxygenation HDO
Highest diesel yield

Decarbonylation DCN

Decarboxylation DCX

n-paraffins $\xrightarrow{H_2}$ iso-paraffins

- n-paraffins have poor cold flow properties
- Hydrotreated bio has a higher concentration of n-paraffins than conventional diesel
- Selective isomerization improves cloud point while retaining molecules in the diesel boiling range



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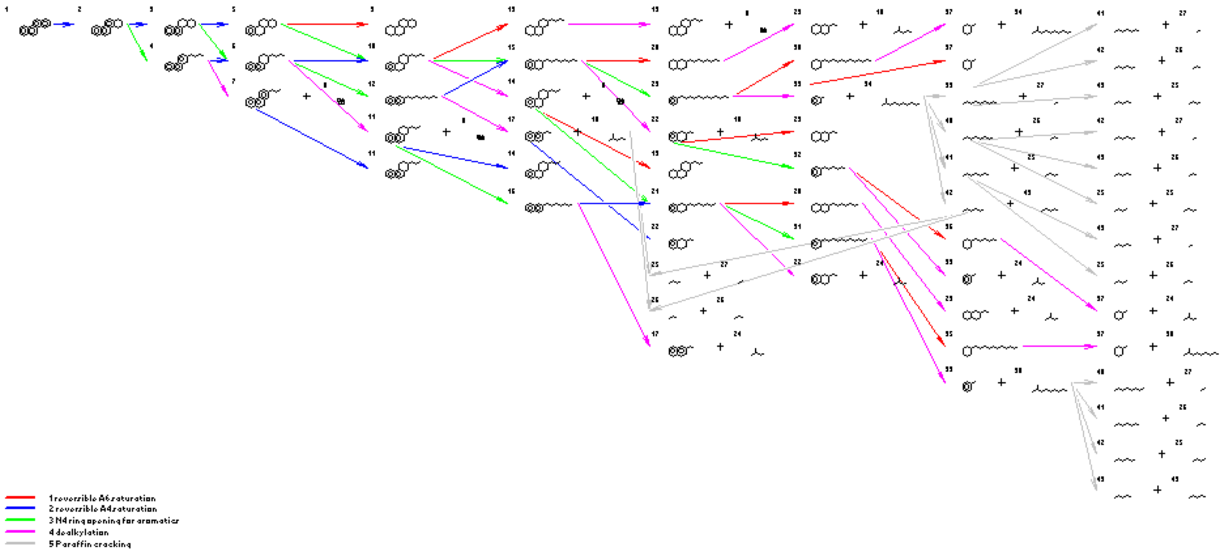
Source: Green, S and Trivedi, K., "How to enable high yields from bio-feedstocks with ExxonMobil Renewable Diesel (EMRD™) Process Technology, AIChE Spring Meeting, April , 2022

Reaction Kinetics Modeling Structure Oriented Lumping (SOL)

- SOL describes composition, reactions and properties of complex hydrocarbon mixtures
- Individual molecules and isomers represented as vectors of incremental structural features
- Components defined by functional groups instead of bulk properties
- Vector representation used for developing reaction networks and kinetics
- Molecular based property correlations
  - Physical – Boiling point, MW, SG
  - Engineering – Critical properties, VLE
  - Quality – Cloud Pt, RVP, Flash Point, VI

A6	A4	A2	N6	N5	N4	N3	N2	N1	R	br	me	IH	AA	NS	RS	AN	NN	RN	NO	RO	KO
1	0	0	0	0	1	0	0	0	10	0	0	0	0	0	0	0	0	0	0	0	0



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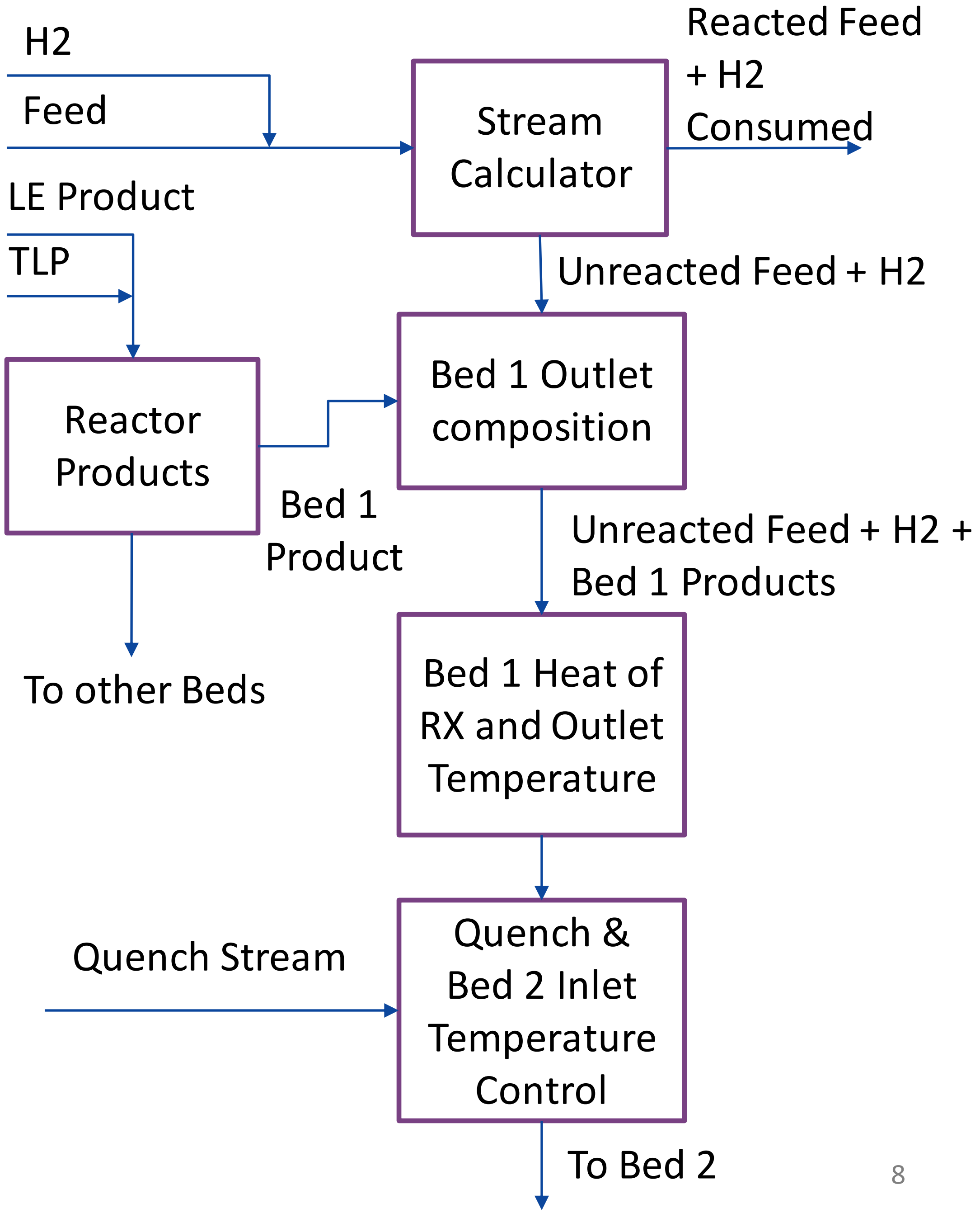
Based on: R. J. Quann and S. B. Jaffe, " Structure Oriented Lumping – Describing the chemistry of complex hydrocarbons mixtures", Ind. Eng. Chem. Res. 1992, 31, 2483-2497
Kushnerick, J. D., " Modeling Petroleum Chemistry with Structured Oriented Lumping", IBM AFM Group Seminar, IBM Zurich Labs, April, 2016

Reactor Simulation

- SOL provides
  - Hydrogen Consumption
  - Reactor yields
  - Heat of Reaction
  - Product composition
- Model in PRO/II uses
  - Calculator / Stream Calculator
  - Heat Exchanger / Flash Drum
  - Controllers
- Quench system optimization
- Control Philosophy
  - Equal bed inlet temp, Equal bed outlet temp, Ascending profile, WABT



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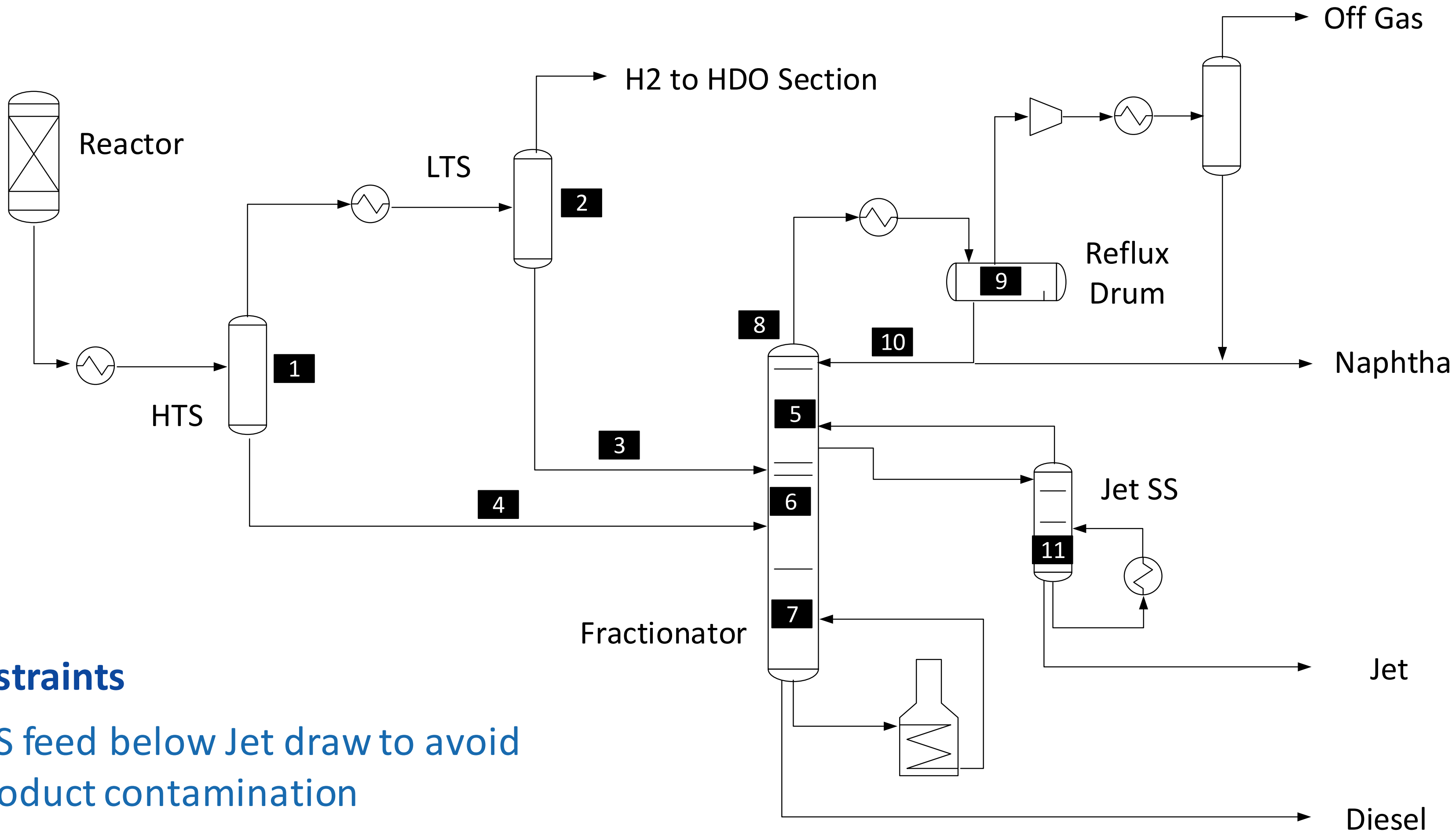
Separation Synthesis and Optimization

Optimization Variables

1. HTS Temperature
2. LTS Temperature
3. LTS liquid to fractionator – Temperature, Feed Stage location
4. HTS liquid to fractionator – Temperature, Feed Stage location
5. No of stages between top and Jet draw
6. No of stages between LTS feed and HTS
7. No of stages between HTS feed and reboiler
8. Top stage pressure



Constraints

- LTS feed below Jet draw to avoid product contamination
- Reflux drum pressure set by reboiler temperature – 650F max
- Ensure stages do not dry up in the tower
- Product specs

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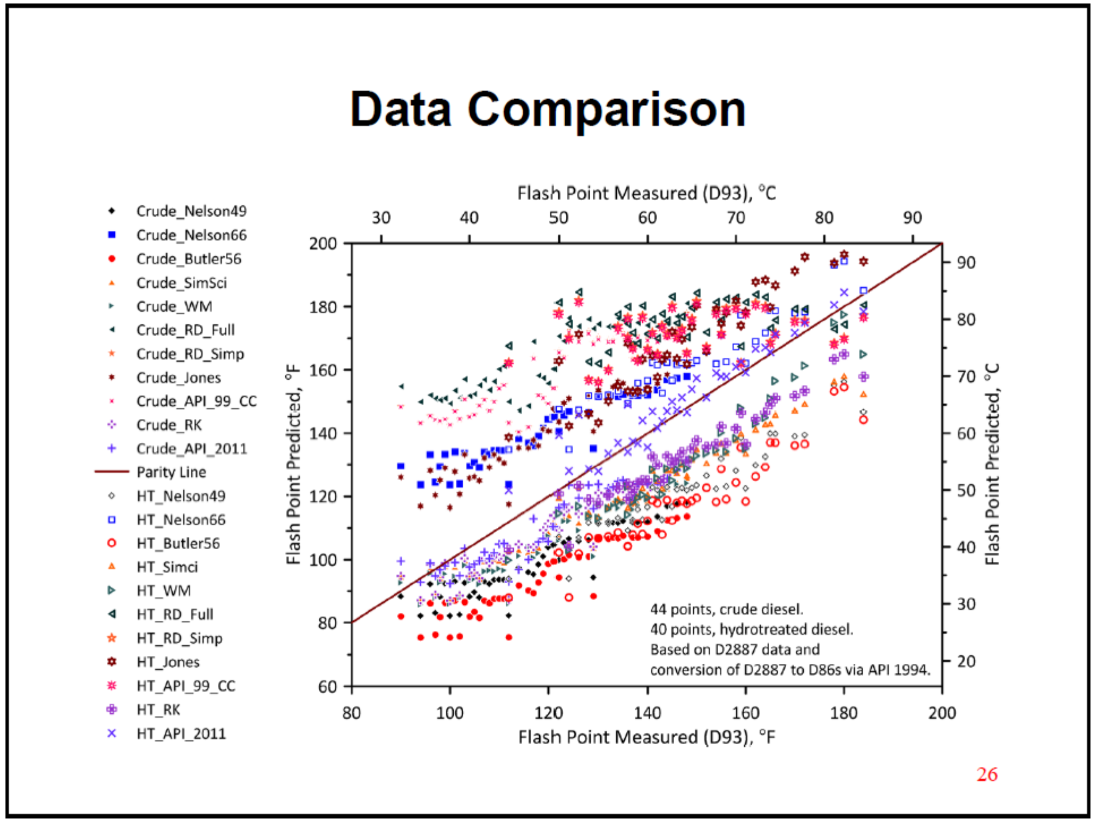
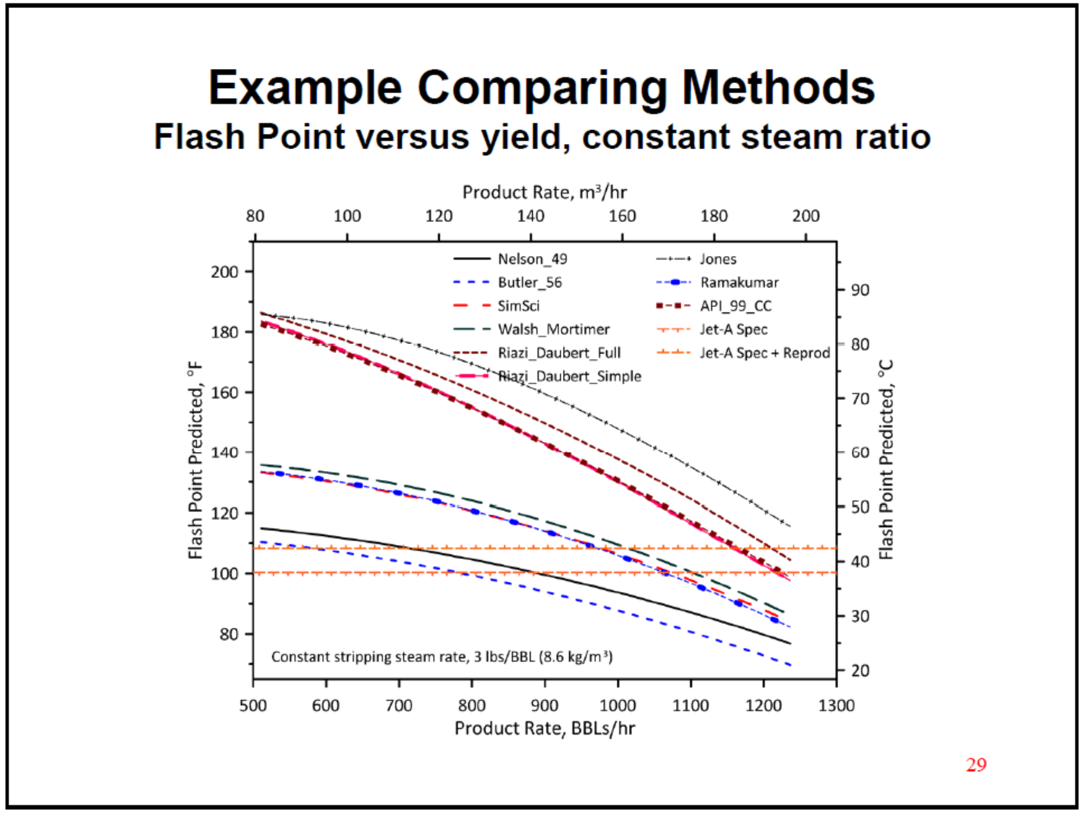
Flash Point Sensitivity

- Yields will depend on flash point calculation method
- From: Andrew Sloley, "Composition Proxies in Refinery Distillation", AIChE Spring Mtg, 2022





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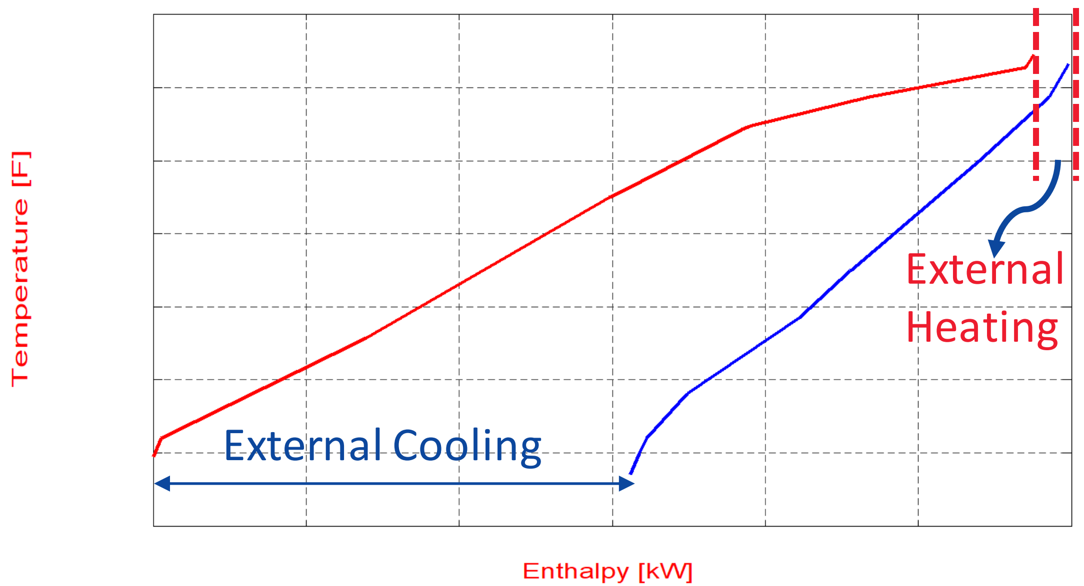
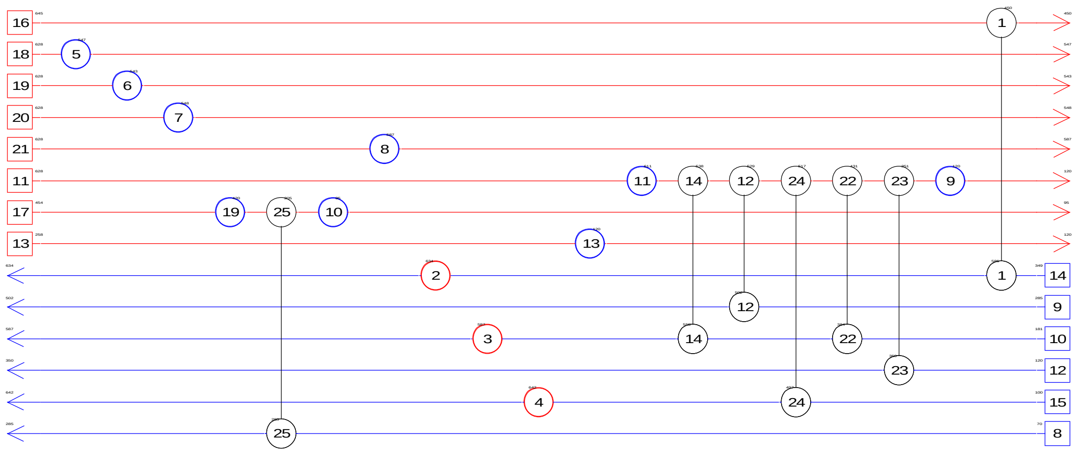
Pinch Analysis – HEN and Utilities

- Composite Curves – Pinch Point, Energy Targets
- Grand Composite Curves – Utility Placement
- Grid Diagram – Network Design

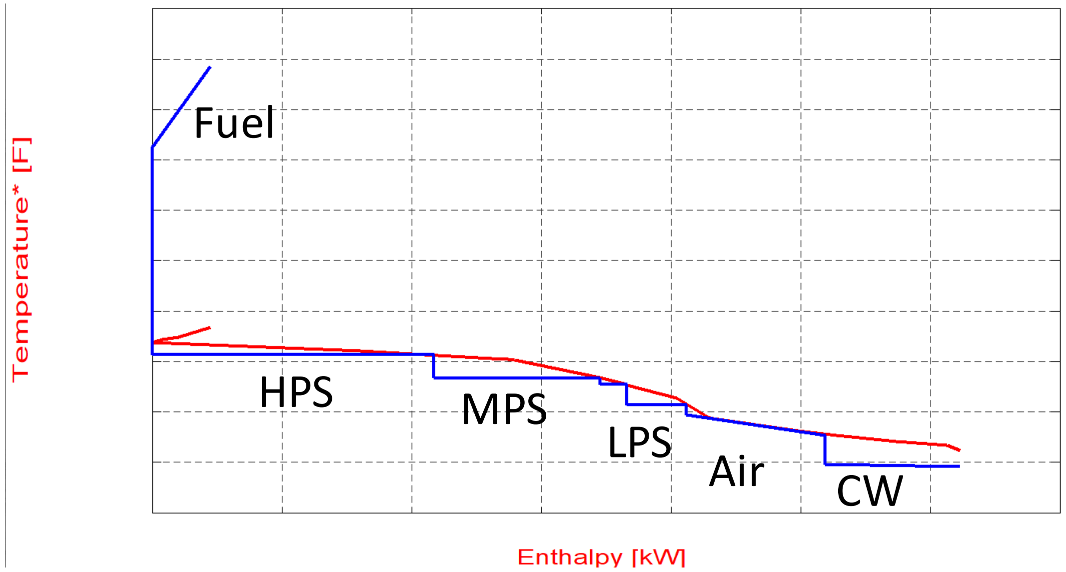
Composite Curve



Grid Diagram



Grand Composite Curve



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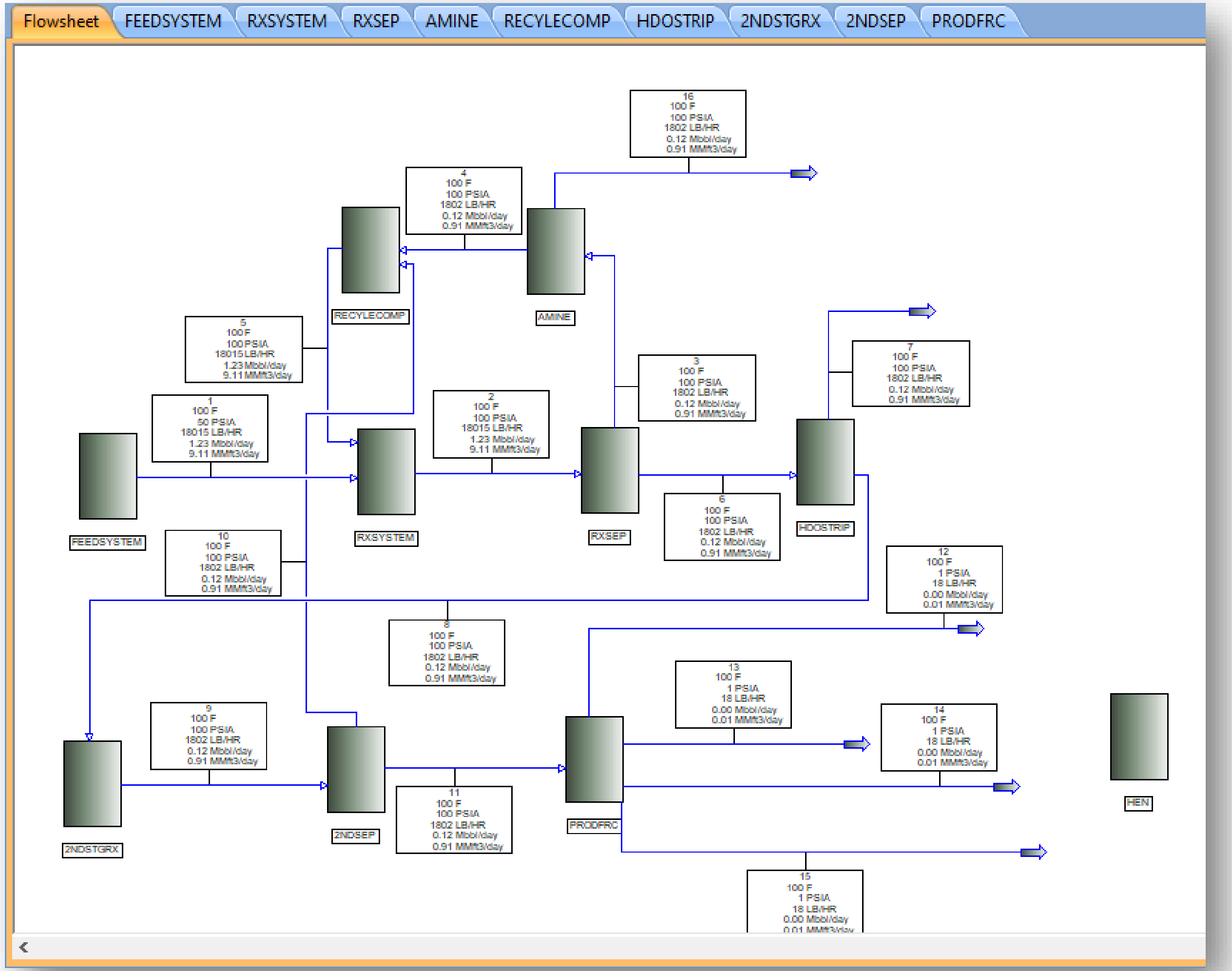
Putting it All together

- Use Block Diagrams to segregate systems
  - Block Diagrams can represent actual PFD
  - Enables testing each system separately
- Minimize mass recycles
- Avoid heat recycles in the main simulation
- Simulate the heat exchanger network separately using reference streams



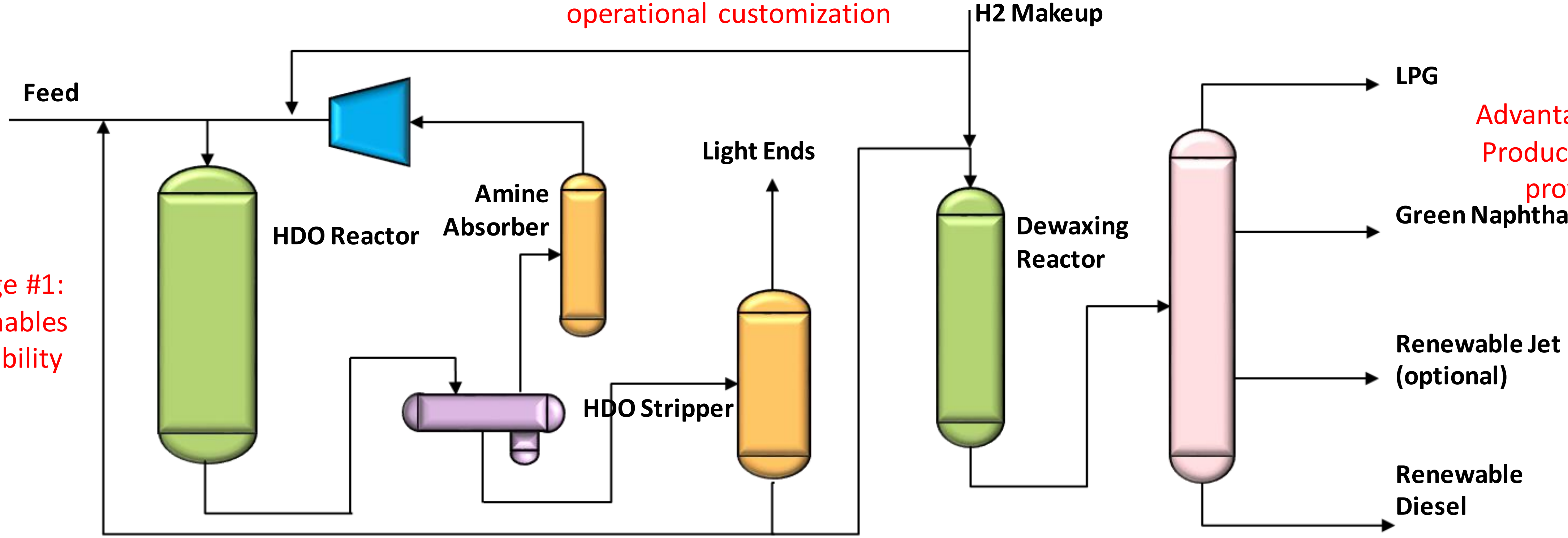
ExxonMobil Renewable Diesel (EMRD™) process

ExxonMobil is an **industry leader** in design and operation of hydroprocessing units and **advantaged dewaxing technology**, and is utilizing this expertise to be a **single provider** of renewable fuels

Advantage #2: Two stages allows operational customization

Advantage #1: Design enables feed flexibility

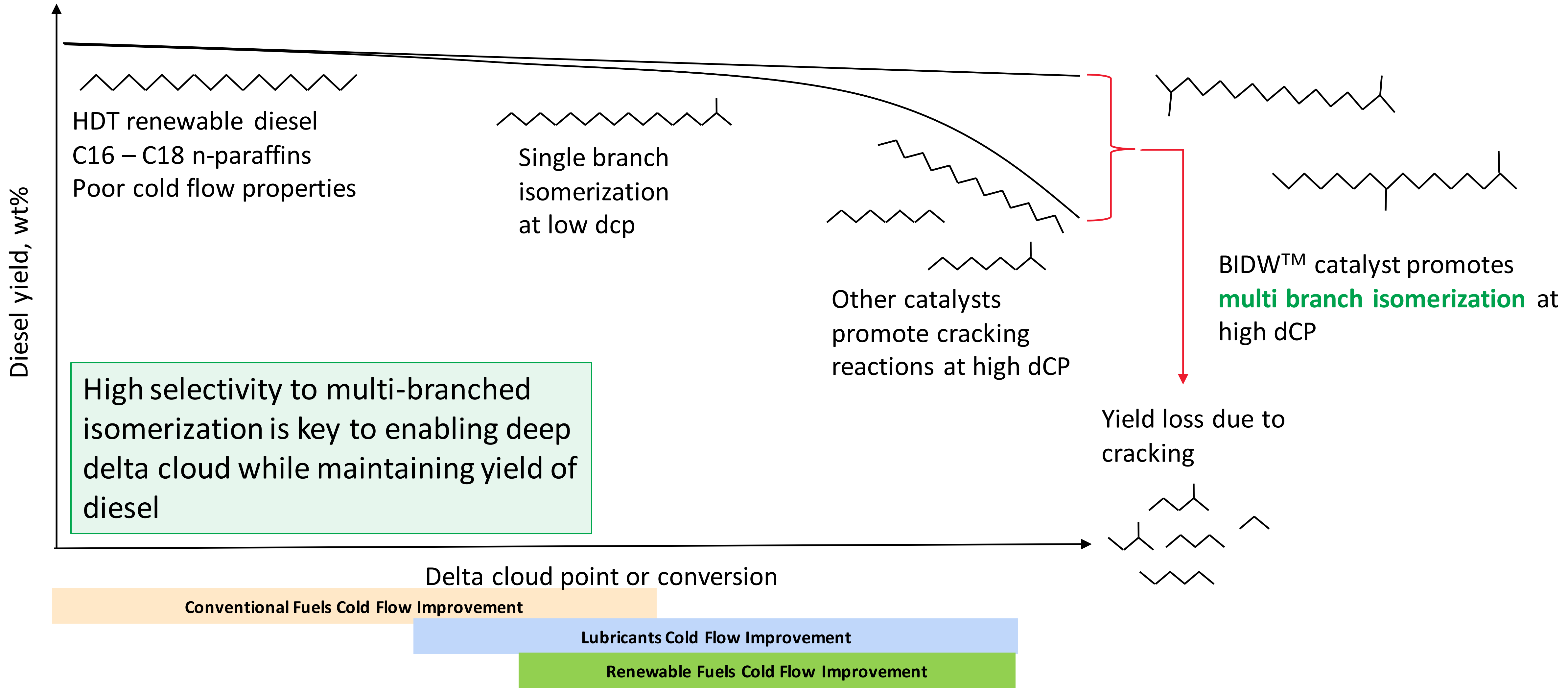
Advantage #3: Product yield profile



*Simplified flow diagram

Source: Green, S and Trivedi, K., "How to enable high yields from bio-feedstocks with ExxonMobil Renewable Diesel (EMRD™) Process Technology, AIChE Spring Meeting, April , 2022

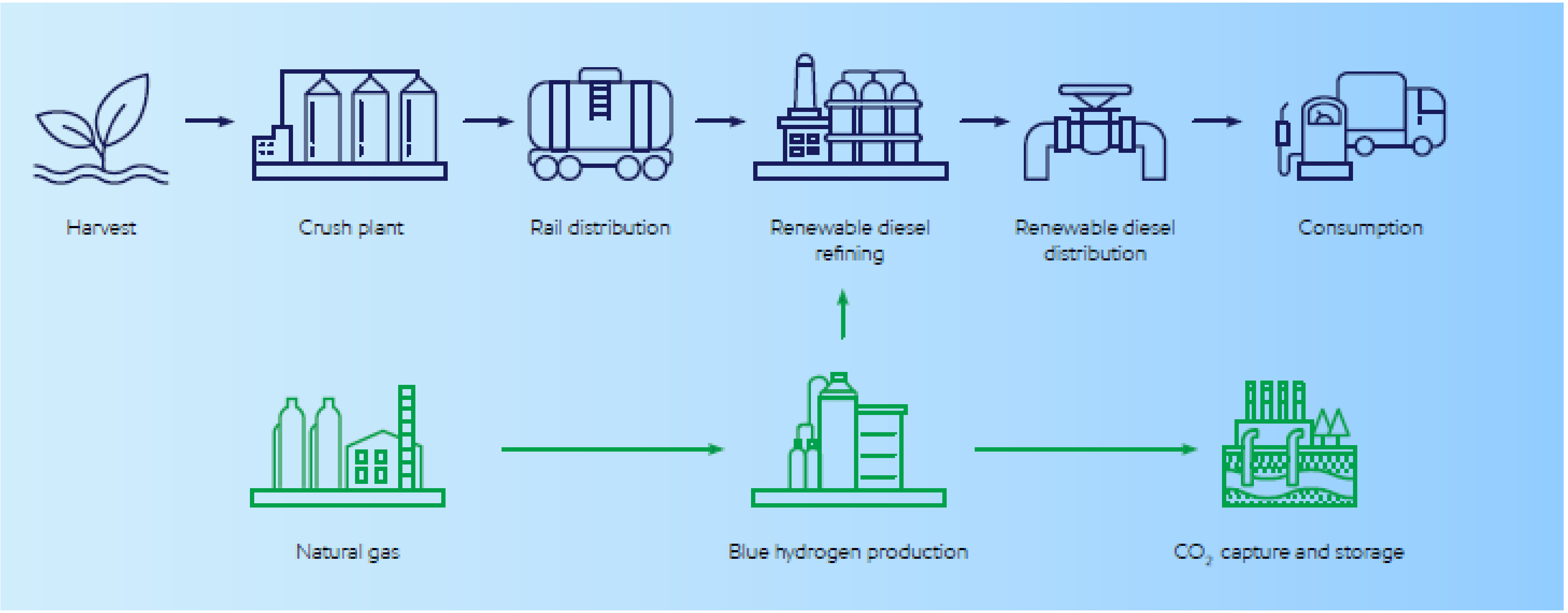
Maintaining high diesel yield at deep delta cloud



Source: Green, S and Trivedi, K., "How to enable high yields from bio-feedstocks with ExxonMobil Renewable Diesel (EMRDTM) Process Technology, AIChE Spring Meeting, April , 2022

Strathcona renewable diesel

Leveraging existing refinery assets, fuels marketing access, and project execution capabilities



SCOPE

- 20 Kbd renewable diesel

DRIVERS

- Canada clean fuel regulations
- Locally sourced bio feedstock
- Advantaged blue hydrogen supply and CO2 CCS infrastructure
- Deploying proprietary technology with yield advantage versus competitive offers

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Source: 2022 ExxonMobil Investor Day Presentation.

Source: Advancing Climate Solutions 2022 Progress Report July 2022 Update.

PRO/II Advantages and Improvements

Advantages

- Block Diagrams help simplify simulation
- Intuitive Graphical User Interface
- Good customization features
- Able to add component properties

Improvements

- New ASTM correlations
- Update literature property prediction methods
- Add heavy hydrocarbon molecule properties
- Column optimization tools
- Integration with reaction modelling tools
- Develop similar capabilities in AVEVA Process Simulation (APS)

Positioning for a lower carbon energy future

ExxonMobil is advancing sustainable, effective solutions that help address the world's growing demand for energy and the risks of climate change through...

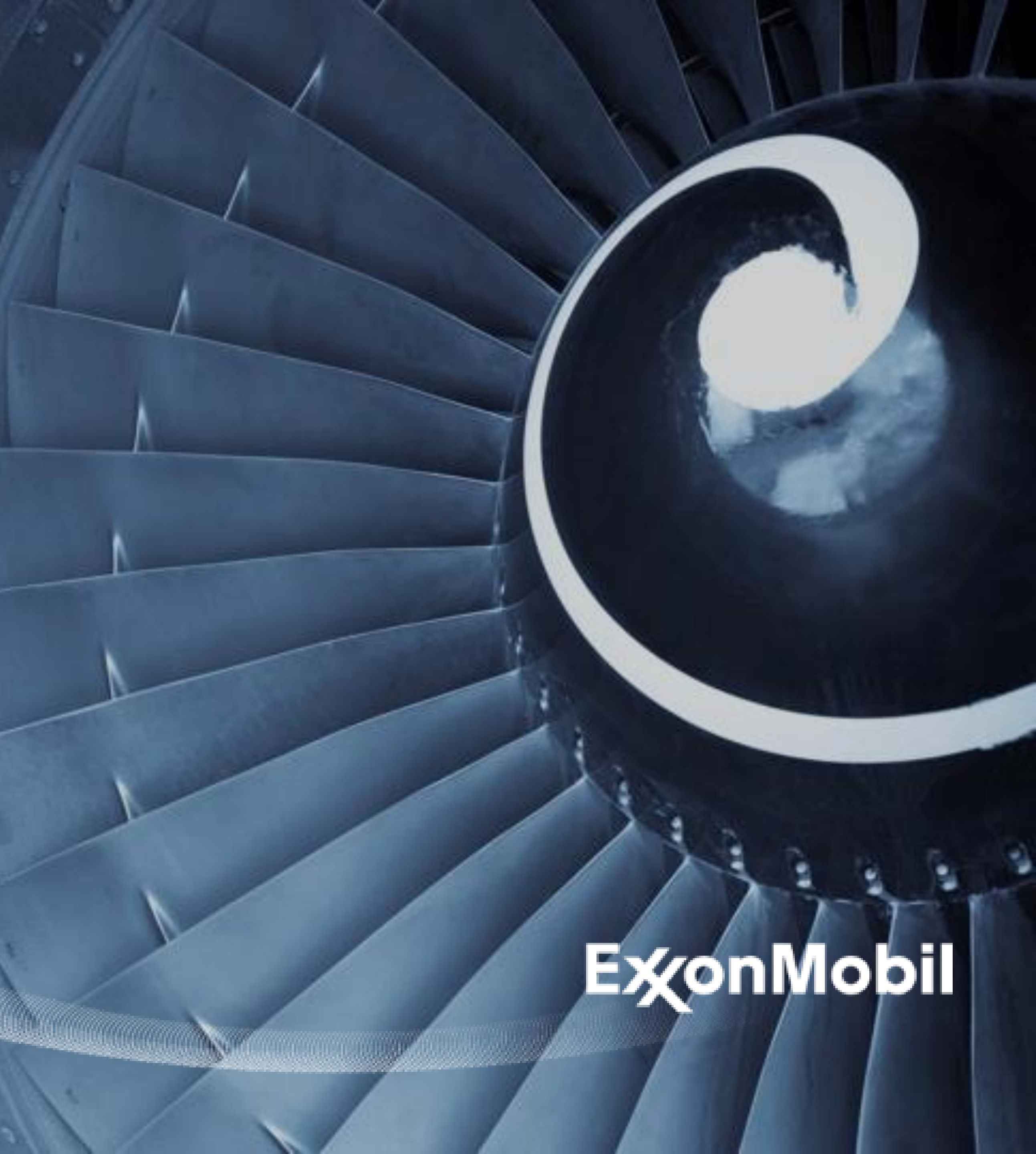
EMRD™ process technology

BIDW™ catalyst solutions

Our approach includes:

PROVIDING PRODUCTS TO HELP CUSTOMERS REDUCE THEIR EMISSIONS

DEVELOPING AND DEPLOYING SCALABLE TECHNOLOGY SOLUTIONS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Questions?

Please wait for the microphone.

State your name and company.

Please remember to...

Navigate to this session in the mobile app to complete the survey.

Thank you!

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ABOUT AVEVA

AVEVA is a global leader in industrial software, sparking ingenuity to drive responsible use of the world's resources. The company's secure industrial cloud platform and applications enable businesses to harness the power of their information and improve collaboration with customers, suppliers and partners.

Over 20,000 enterprises in over 100 countries rely on AVEVA to help them deliver life's essentials: safe and reliable energy, food, medicines, infrastructure and more. By connecting people with trusted information and AI-enriched insights, AVEVA enables teams to engineer efficiently and optimize operations, driving growth and sustainability.

Named as one of the world's most innovative companies, AVEVA supports customers with open solutions and the expertise of more than 6,400 employees, 5,000 partners and 5,700 certified developers. With operations around the globe, we are headquartered in Cambridge, UK and listed on the London Stock Exchange's FTSE 100.

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