



UNIVERSITY OF  
CHEMISTRY AND TECHNOLOGY  
PRAGUE



# Green Chemistry: Obnovitelné suroviny pro chemický průmysl

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**Chemické fórum Ústeckého kraje 2021**

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<http://greencats.vscht.cz>



**“...design of chemical products and processes to reduce or eliminate the use and generation of hazardous substances.”**

**“Sustainability requires objectives at the molecular, product, process, and system levels.”**

*Chem. Soc. Rev.*, **2010**, 39, 301–312,  
*Env. Sci. Tech.* **2003**, 37(5), 94A-101A

- 1962: Rachel Carson, "Silent Spring", a book outlining the devastation that certain chemicals had on local ecosystems → inspired modern environmental movement.
- 1969: US National Environmental Policy Act
- 1970: U.S. Environmental Protection Agency (EPA)
  - banned the use of DDT and other chemical pesticides.
- 1980s: the chemical industry and the EPA were focused **mainly on pollution clean-up** and obvious toxins
- 1990: The Pollution Prevention Act - regulatory policy change **from pollution control to pollution prevention** as the most effective strategy for these environmental issues.
- 1993: EC Chemistry Council, ***Chemistry for a Clean World***.
- 1998: Paul Anastas and John C. Warner, ***Green Chemistry: Theory and Practice***

<https://www.acs.org/content/acs/en/greenchemistry/what-is-green-chemistry/history-of-green-chemistry.html>



|   |   |
|---|---|
| <b>1. Prevention</b>                        | It is better to prevent waste than to treat or clean up waste after it has been created   |
| <b>2. Atom Economy</b>                      | Synthetic methods should be designed to maximize incorporation of all materials used in the process into the final product.   |
| <b>3. Less Hazardous Chemical Synthesis</b> | Wherever practicable, synthetic methods should be designed to use and generate substances that possess little or no toxicity to human health and the environment                          |
| <b>4. Designing Safer Chemicals</b>         | Chemical products should be designed to preserve efficacy of function while reducing toxicity.  |
| <b>5. Safer Solvents and Auxiliaries</b>    | The use of auxiliary substances (e.g., solvents, separation agents, etc.) should be made unnecessary wherever possible and, innocuous when used.  |
| <b>6. Design for Energy Efficiency</b>      | Energy requirements should be recognized for their environmental and economic impacts and should be minimized. Synthetic methods should be conducted at ambient temperature and pressure. |

*Green Chemistry: Theory and Practice, Oxford University Press: New York, 1998, p.30.*





|   |  |
|---|--|
| <b>7. Use of Renewable Feedstocks</b>                         | A raw material or feedstock should be renewable rather than depleting whenever technically and economically practicable.   |
| <b>8. Reduce Derivatives</b>                                  | Unnecessary derivatization (use of blocking groups, protection/deprotection, temporary modification of physical/chemical processes) should be minimized or avoided if possible, because such steps require additional reagents and can generate waste. |
| <b>9. Catalysis</b>   | Catalytic reagents (as selective as possible) are superior to stoichiometric reagents.   |
| <b>10. Design for Degradation</b>                             | Chemical products should be designed so that at the end of their function they break down into innocuous degradation products and do not persist in the environment.   |
| <b>11. Real-time Analysis for Pollution Prevention</b>        | Analytical methodologies need to be further developed to allow for real-time, in-process monitoring and control prior to the formation of hazardous substances.  |
| <b>12. Inherently Safer Chemicals for Accident Prevention</b> | Substances and the form of a substance used in a chemical process should be chosen to minimize the potential for chemical accidents, including releases, explosions, and fire.   |

*Green Chemistry: Theory and Practice, Oxford University Press: New York, 1998, p.30.*



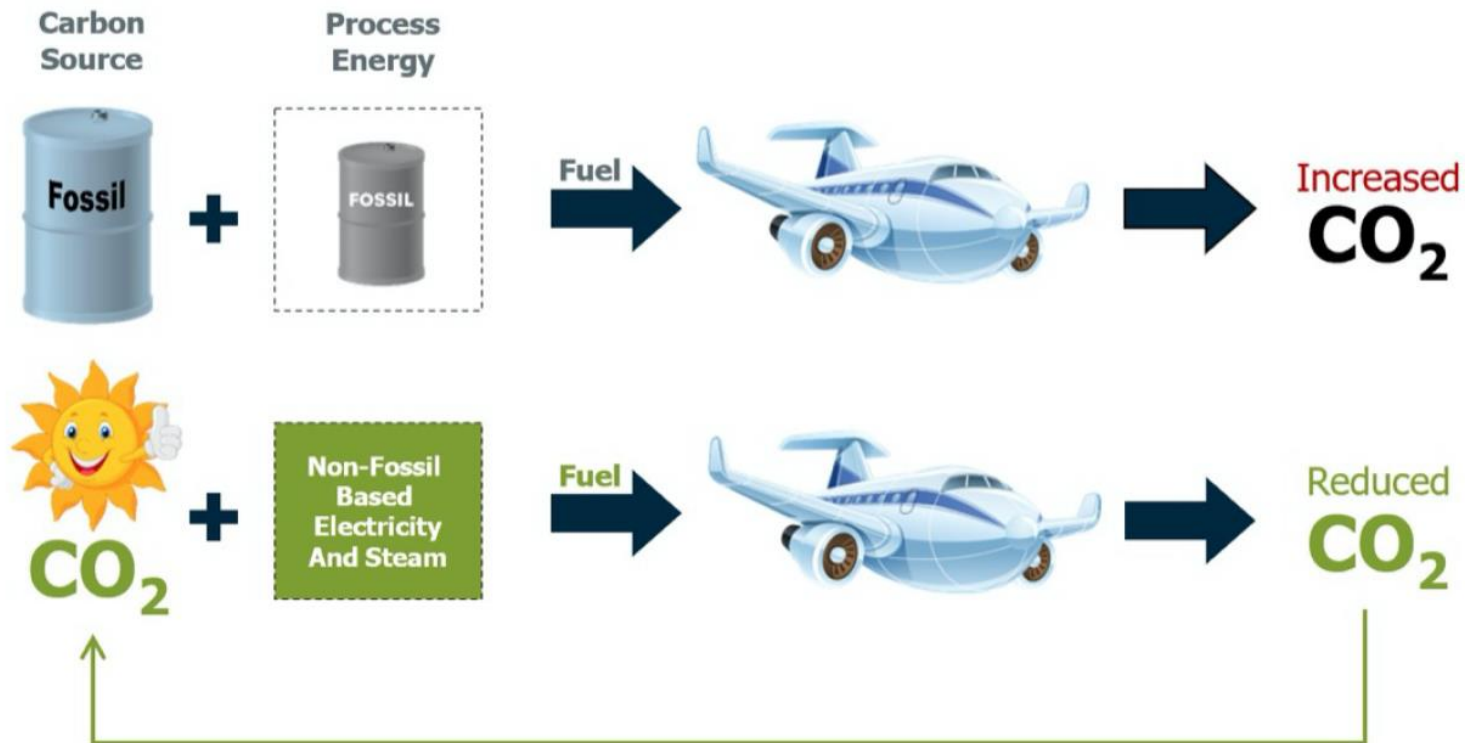


|  |   |
|--|---|
| <b>1. Inherent Rather Than Circumstantial</b>  | Designers need to strive to ensure that all materials and energy inputs and outputs are as inherently nonhazardous as possible.                 |
| <b>2. Prevention Instead of Treatment</b>      | It is better to prevent waste than to treat or clean up waste after it is formed.   |
| <b>3. Design for Separation</b>                | Separation and purification operations should be designed to minimize energy consumption and materials use.                                     |
| <b>4. Maximize Efficiency</b>                  | Products, processes, and systems should be designed to maximize mass, energy, space, and time efficiency.                                       |
| <b>5. Output-Pulled Versus Input-Pushed</b>    | Products, processes, and systems should be "output-pulled" rather than "input-pushed" through the use of energy and materials.                  |
| <b>6. Conserve Complexity</b>                  | <i>Embedded entropy and complexity must be viewed as an investment when making design choices on recycle, reuse, or beneficial disposition.</i> |
| <b>7. Durability Rather Than Immortality</b>   | Targeted durability, not immortality, should be a design goal.  |
| <b>8. Meet Need, Minimize Excess</b>           | Design for unnecessary capacity or capability (e.g., "one size fits all") solutions should be considered a design flaw.                         |
| <b>9. Minimize Material Diversity</b>          | Material diversity in multicomponent products should be minimized to promote disassembly and value retention.                                   |
| <b>10. Integrate Material and Energy Flows</b> | Design of products, processes, and systems must include integration and interconnectivity with available energy and materials flows.            |
| <b>11. Design for Commercial "Afterlife"</b>   | Products, processes, and systems should be designed for performance in a commercial "afterlife."  |
| <b>12. Renewable Rather Than Depleting</b>     | <i>Material and energy inputs should be renewable rather than depleting.</i>  |

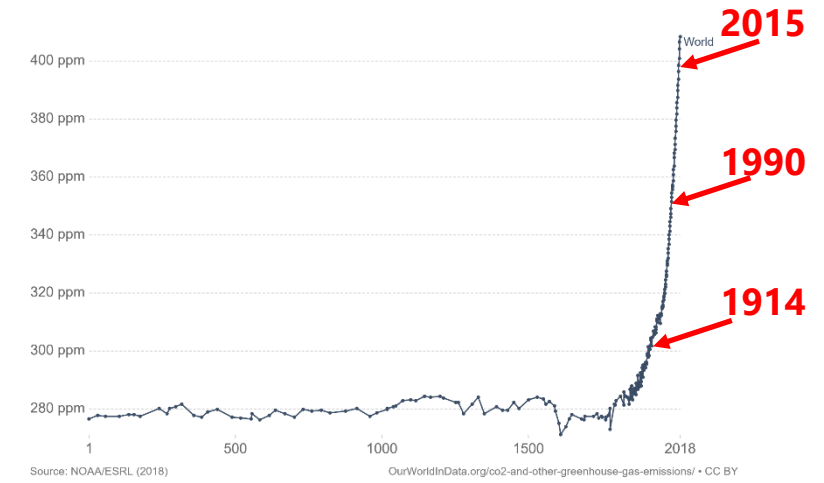
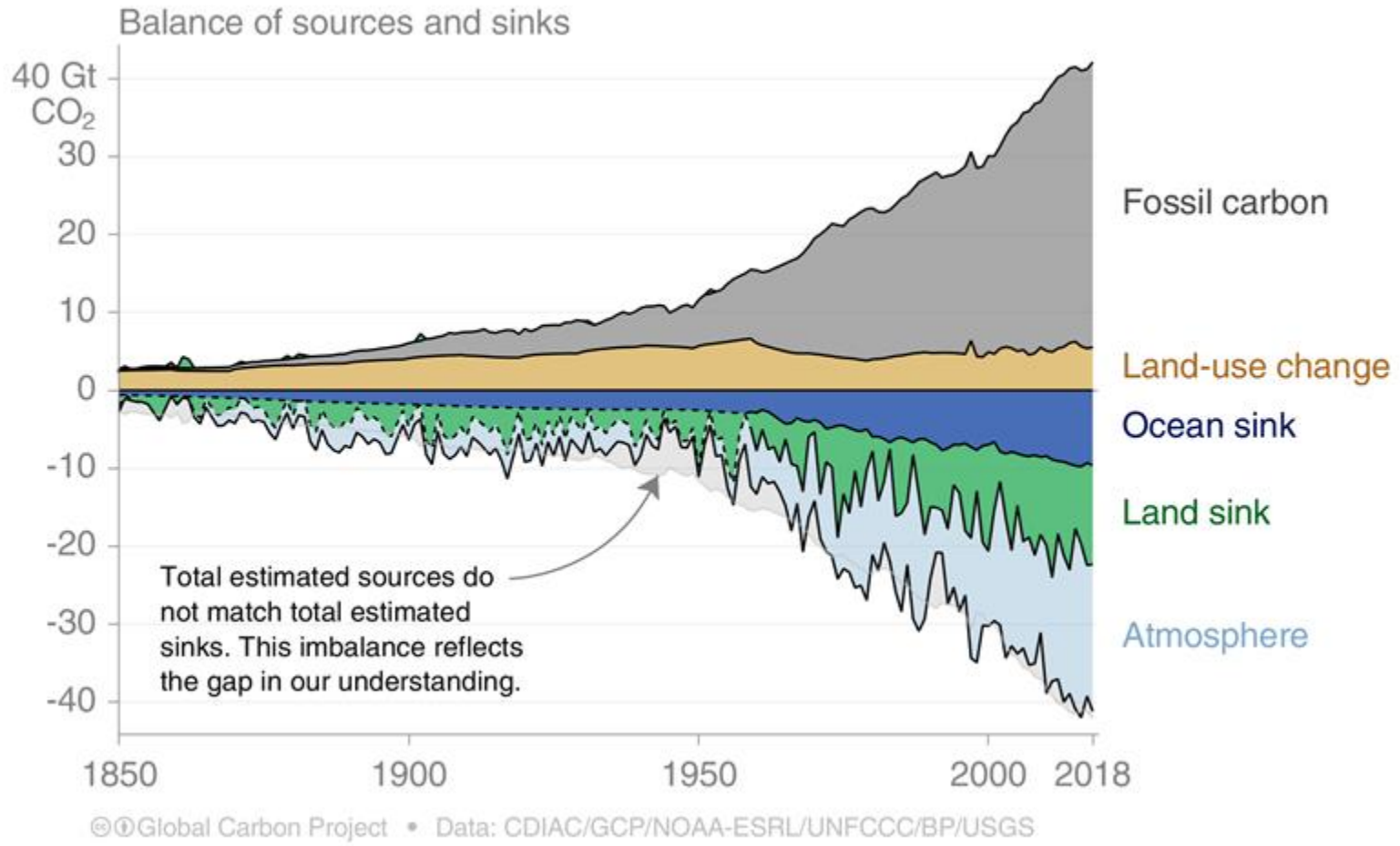




REPLACE THE **CARBON SOURCE** AND **ENERGY SOURCE** TO ELIMINATE GHG'S FROM FUELS

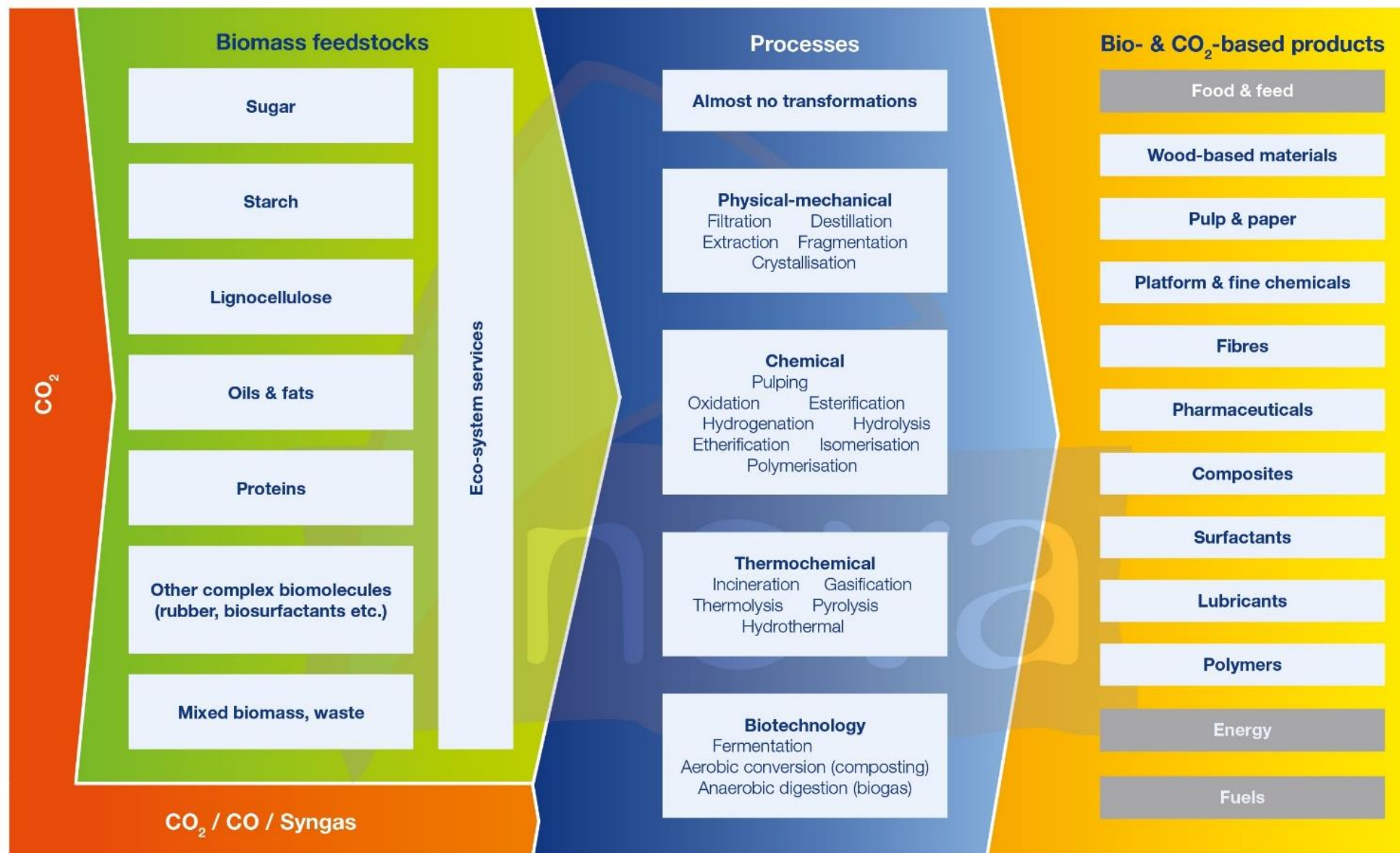


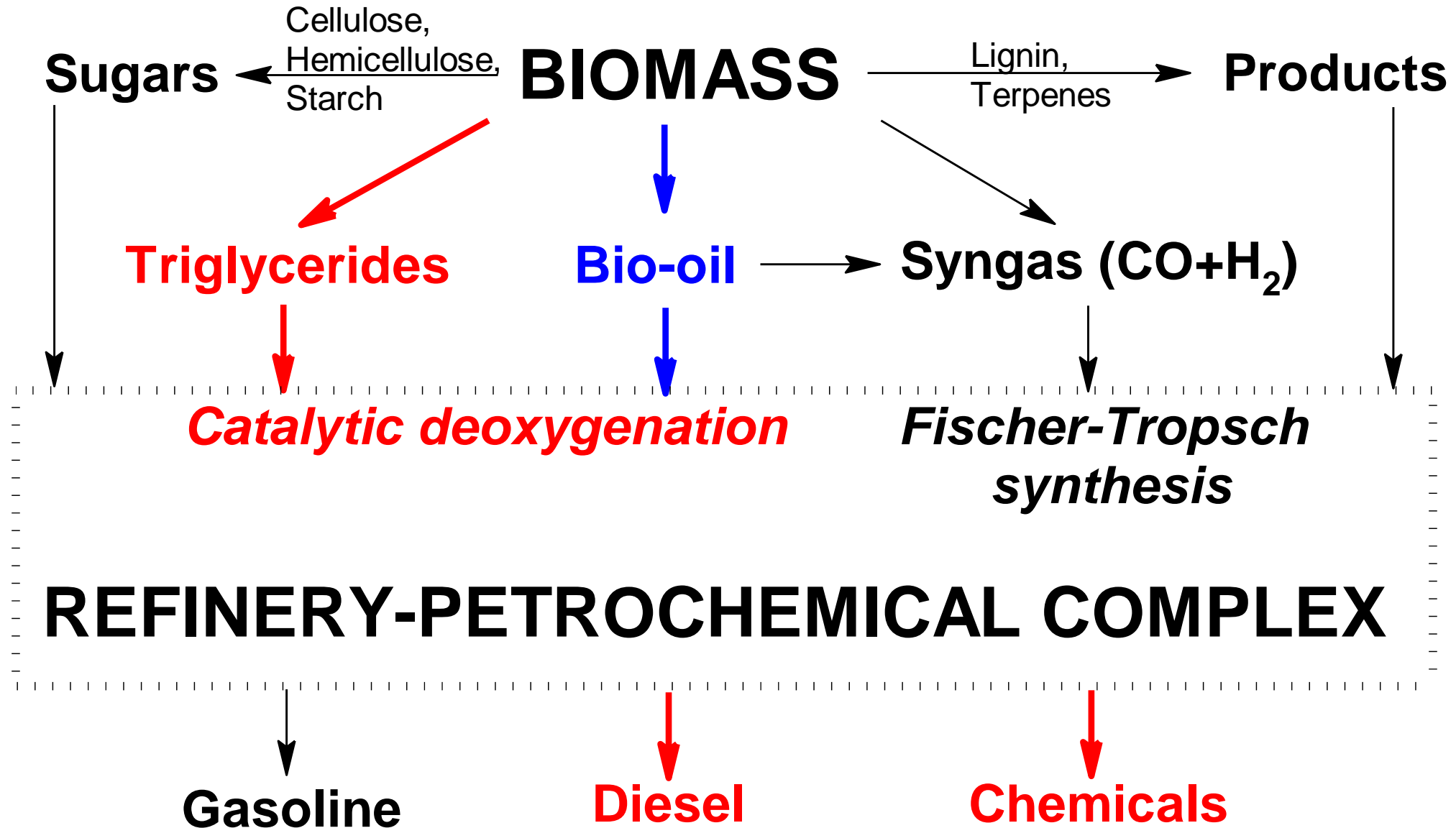
[biofuelsdigest.com/bdigest/2020/05/25/3-things-that-need-to-happen-for-sustainable-aviation-fuel-totake-off/](https://biofuelsdigest.com/bdigest/2020/05/25/3-things-that-need-to-happen-for-sustainable-aviation-fuel-totake-off/)



<https://ourworldindata.org/>

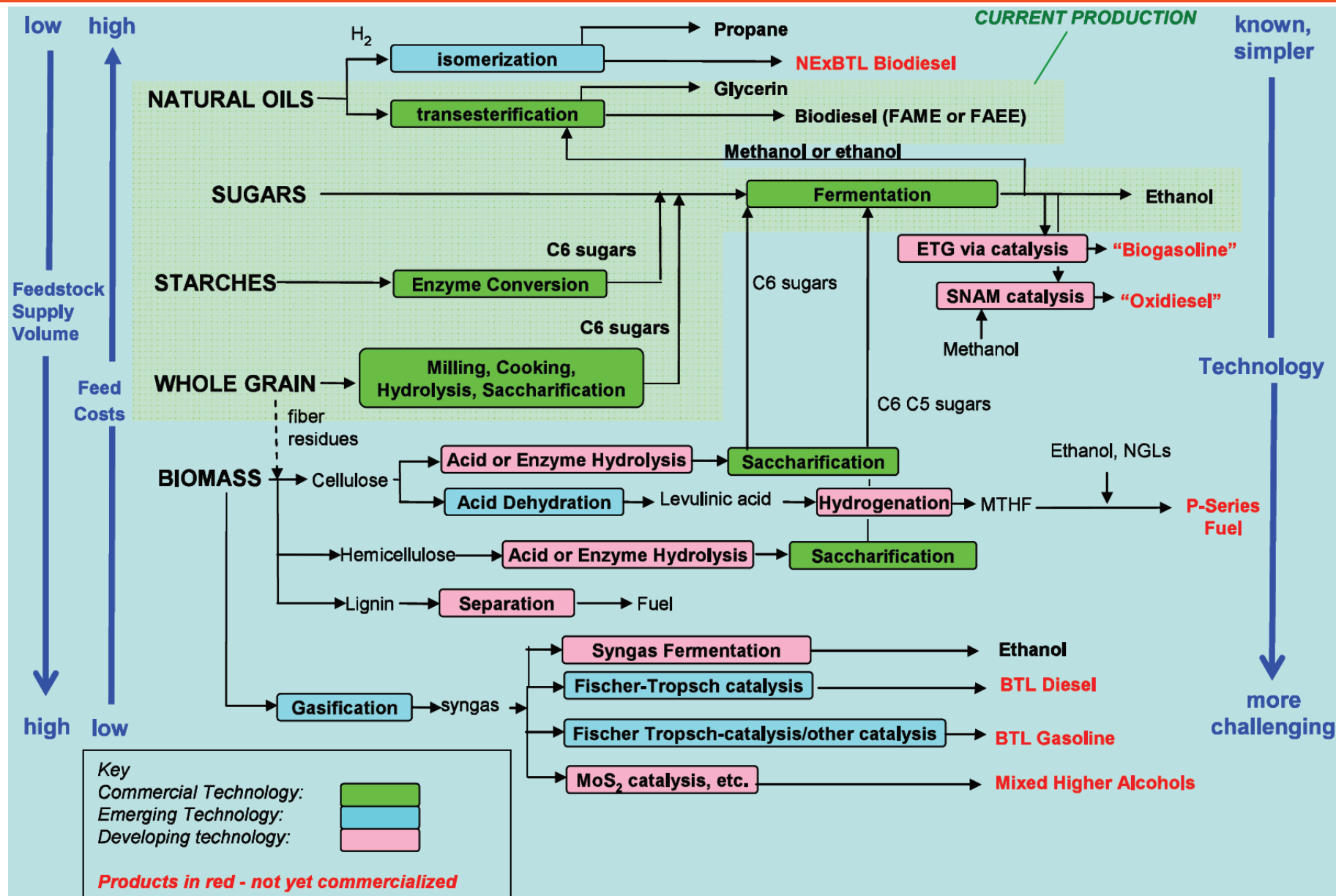








# BIOMASS UPGRADING ALTERNATIVES

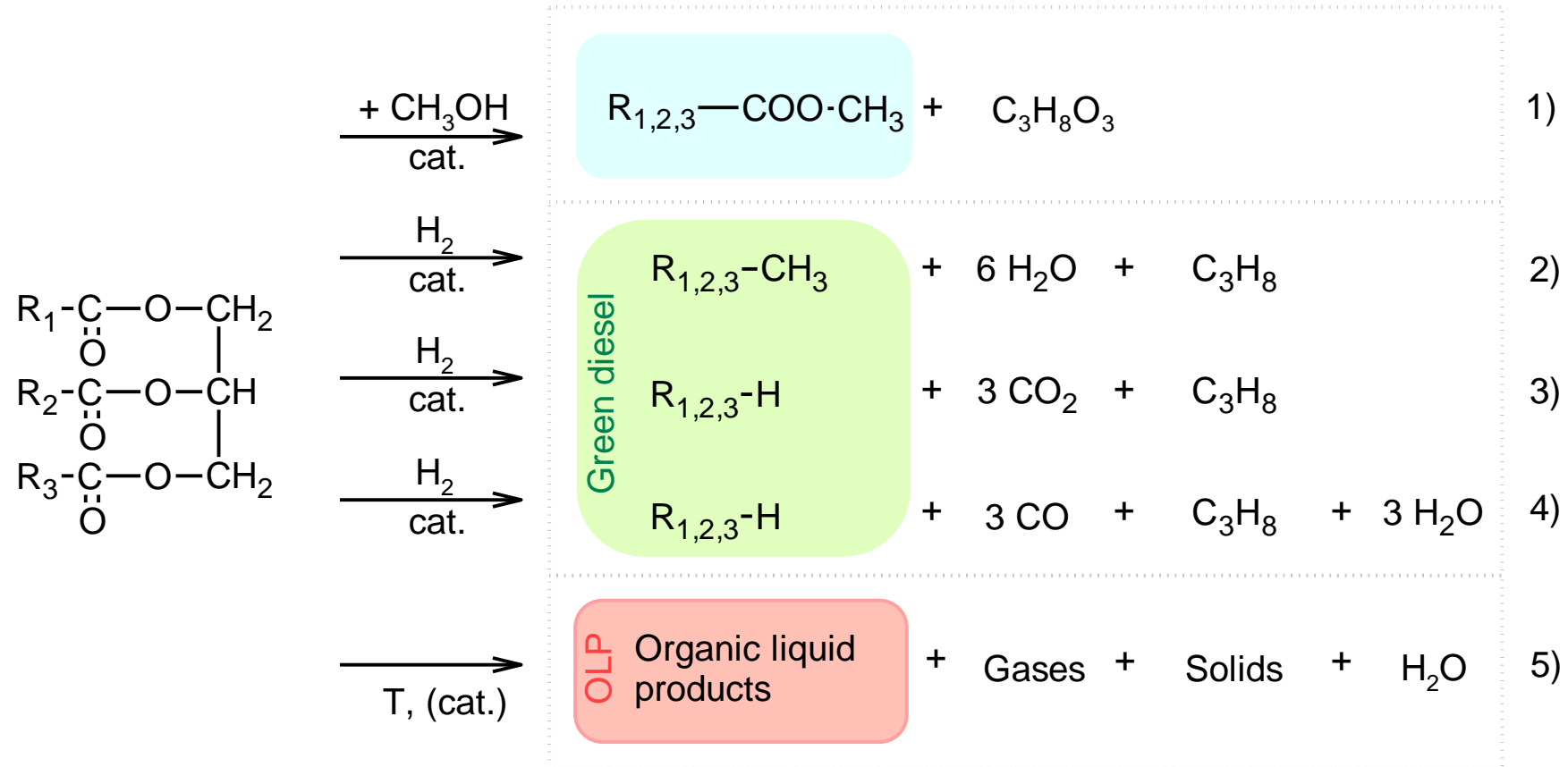


Nexant Chemsystems

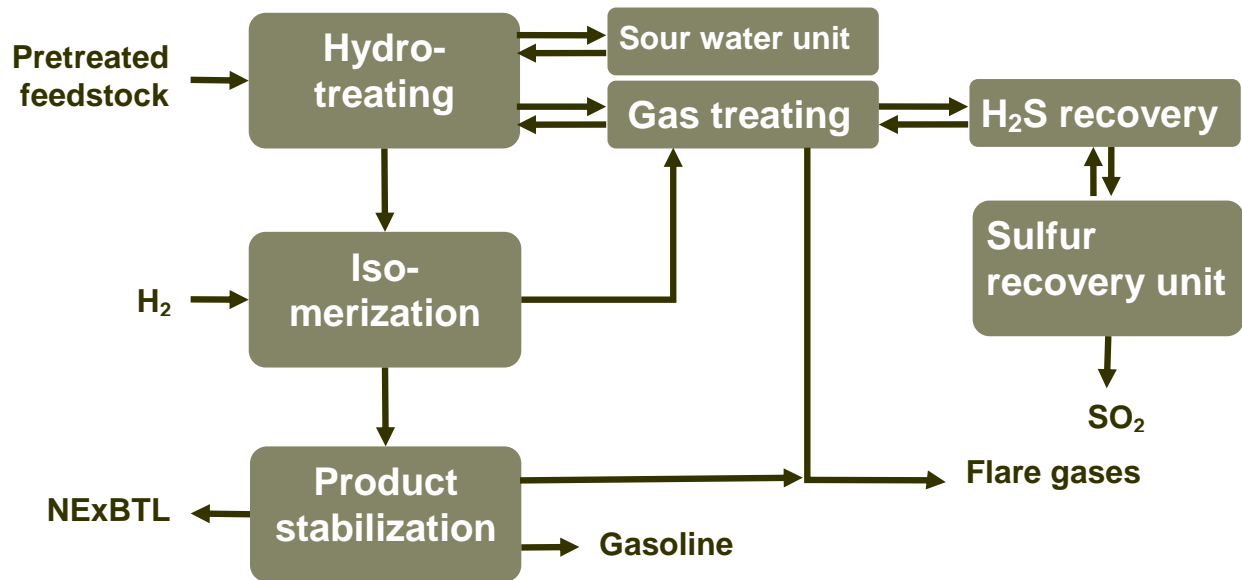




# **RENEWABLES TO FUELS AND CHEMICALS: SOME EXAMPLES**



*Kubičková, I.; Kubička, D. Waste Biomass. Valor. 2010, 1, 293-308.*



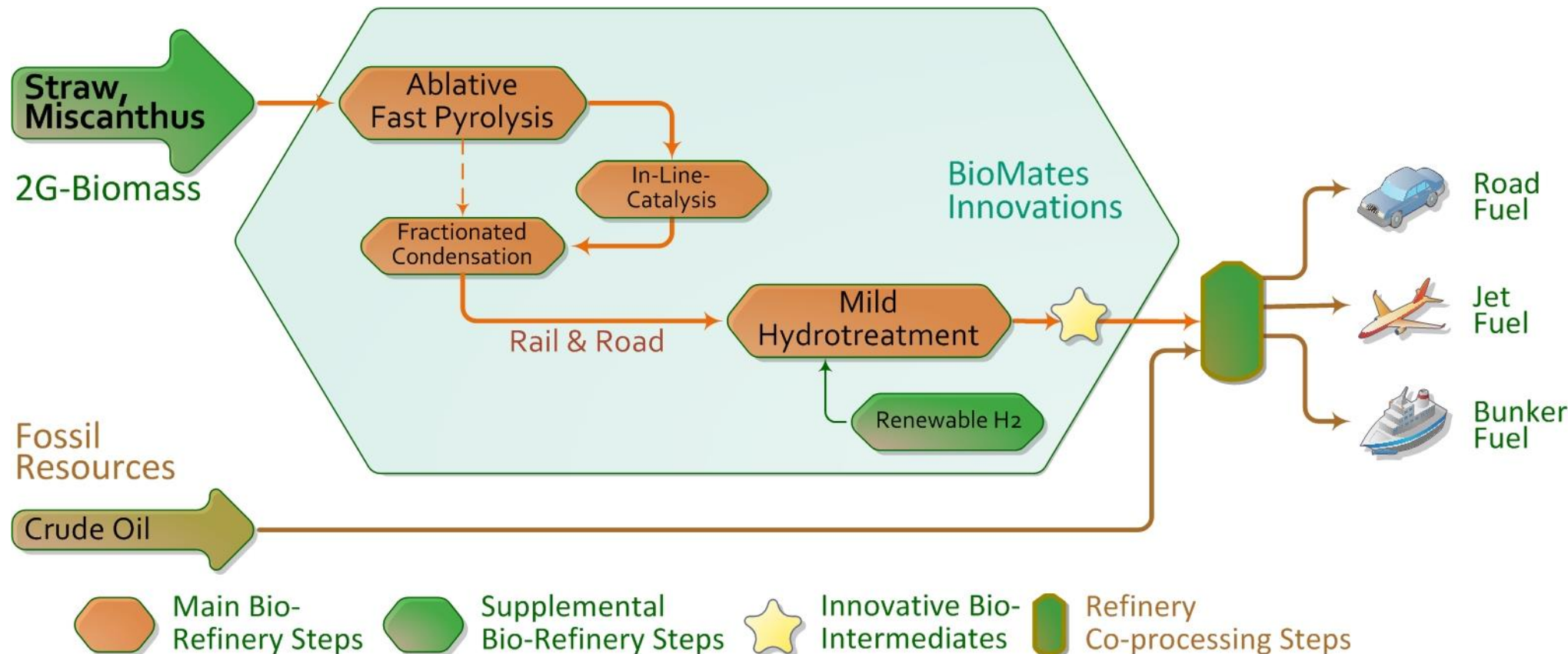
| Technology             | Place                        | Capacity, kt/a   | Start-up                          |
|------------------------|------------------------------|------------------|-----------------------------------|
| NexBTL<br>(NesteOil)   | Finland                      | 210              | 2007                              |
|                        | Finland                      | 210              | 2009                              |
|                        | Singapore<br>Netherlands     | 1000<br>1000     | 2010<br>2011                      |
| Ecofining<br>(UOP/ENI) | USA                          | 500<br>(900)     | 2013<br>(in progress)<br>operated |
|                        | USA                          | 125              |                                   |
|                        | Italy, Venice<br>Italy, Gela | 360 (560)<br>750 | 2014 (2021)<br>2018               |
| Vegan<br>(Axens/IFP)   | La Mede,<br>France           | 500              | 2018                              |
| Bio Verno<br>(UPM)     | Lapeenranta,<br>Finland      | 100              | 2015                              |

*NexBTL process (Hodge, 2006)*



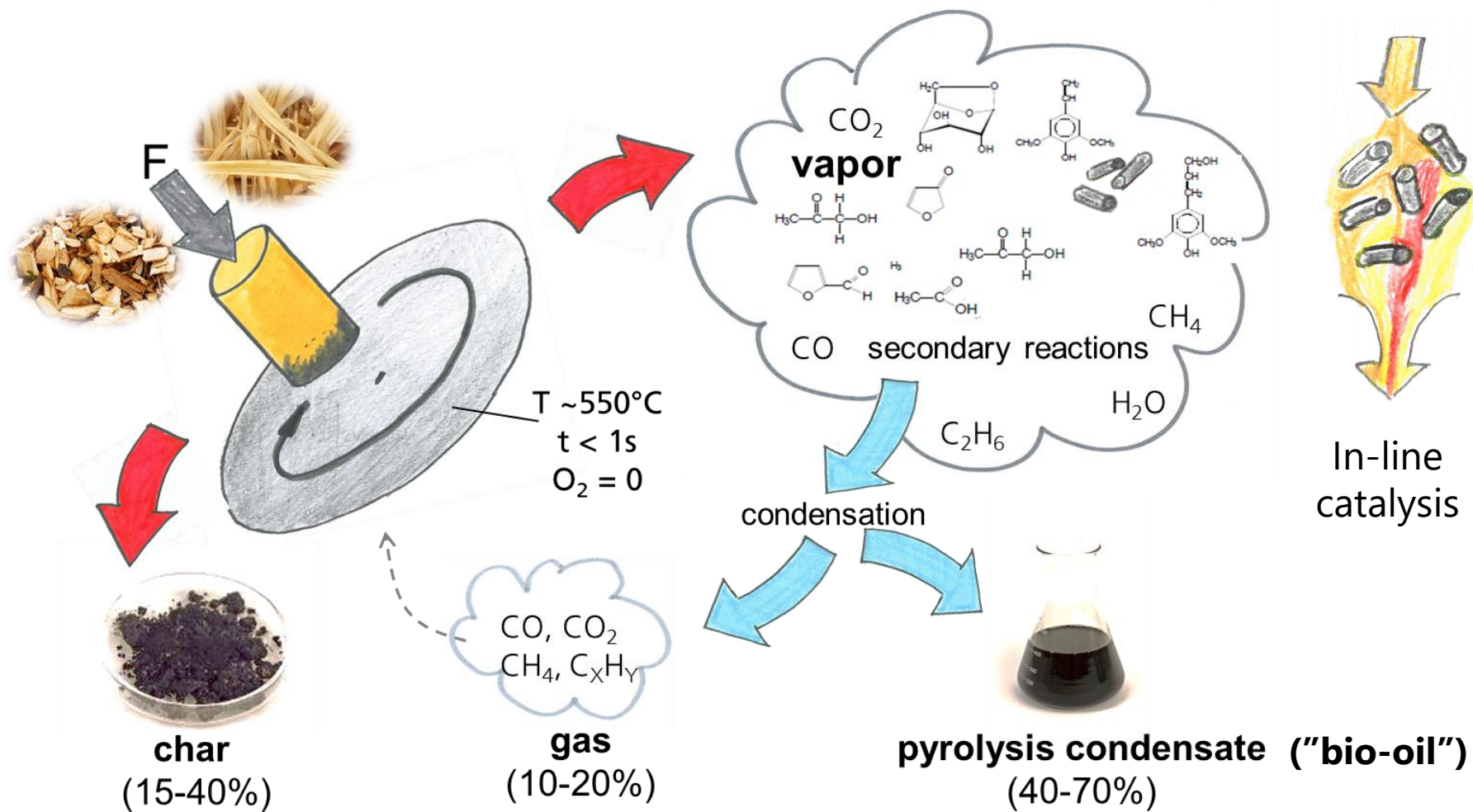


# BIOMASS TO BIOOIL TO BIOFUELS: BIOMATES





# BIOMASS TO BIOOIL TO BIOFUELS: BIOMATES







## THE IH<sup>2</sup> PROCESS – HOW IT WORKS

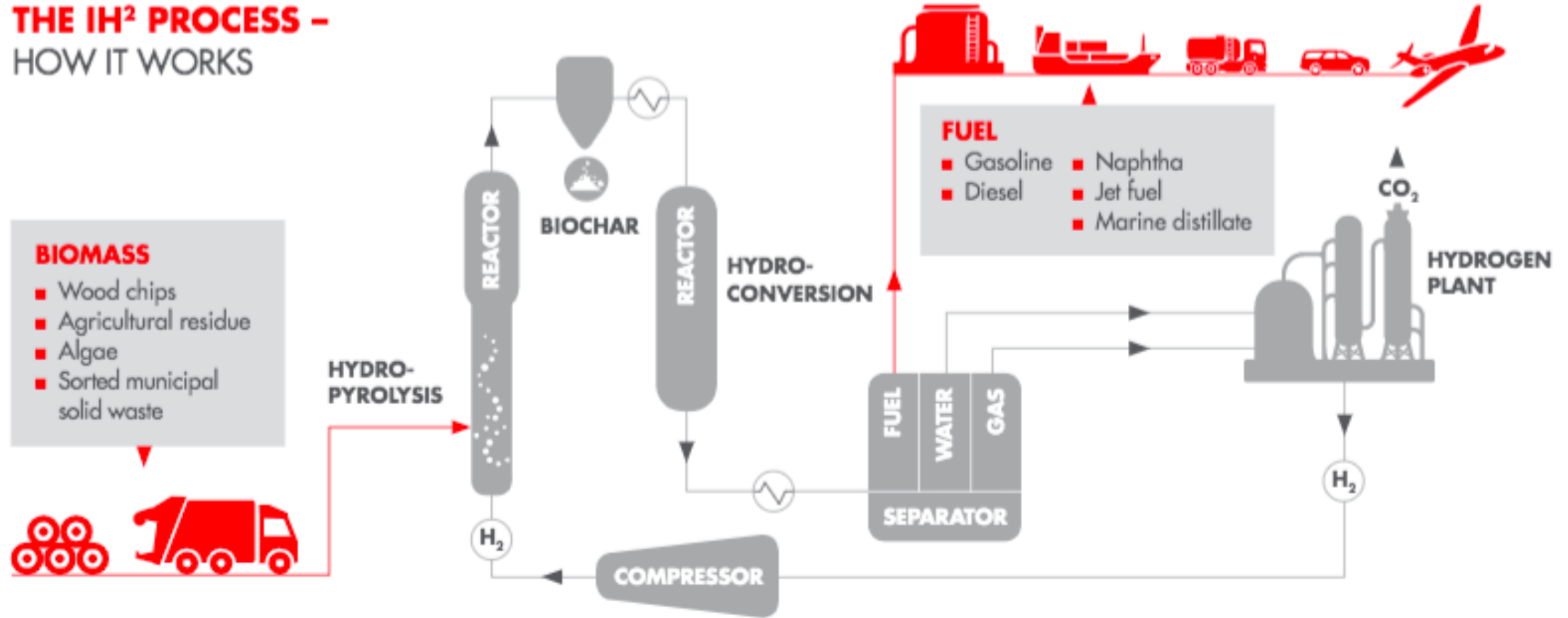
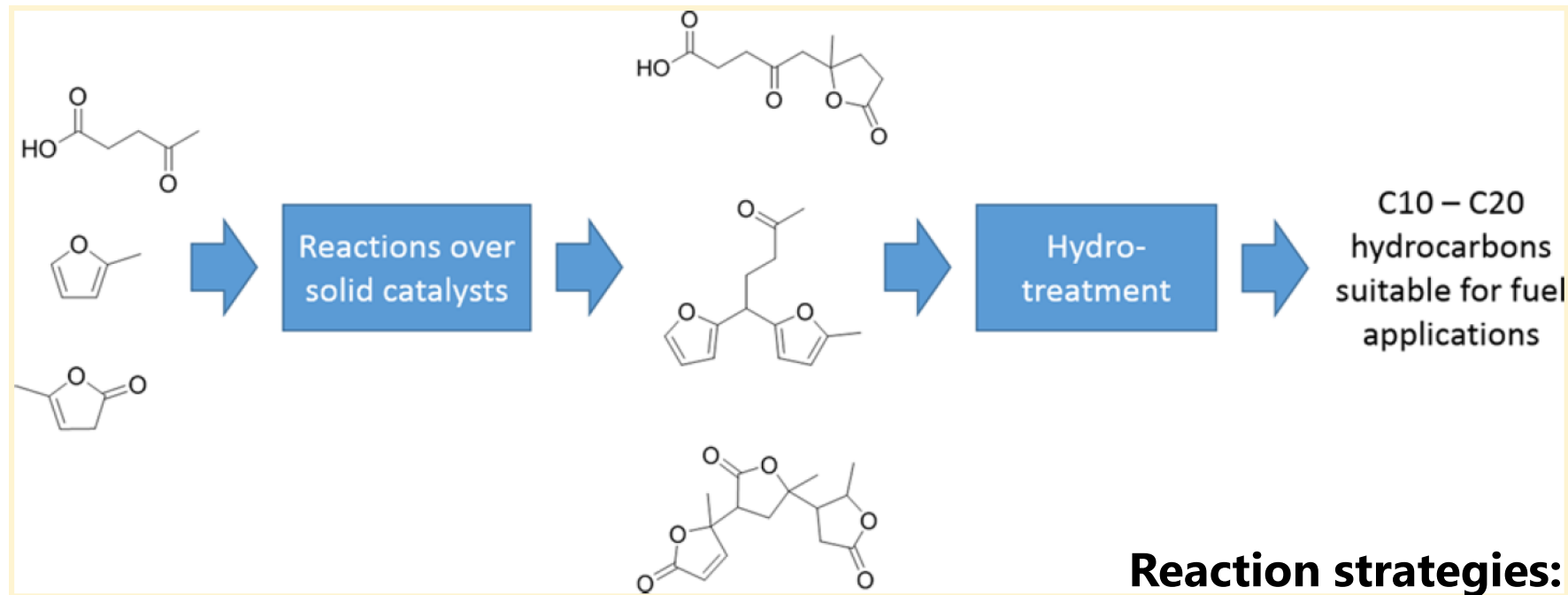


Figure 1: The IH<sup>2</sup> process.

\*IH<sup>2</sup> is a registered trademark of the Gas Technology Institute.

<https://catalysts.shell.com/en/ih2-technology-fact-sheet>

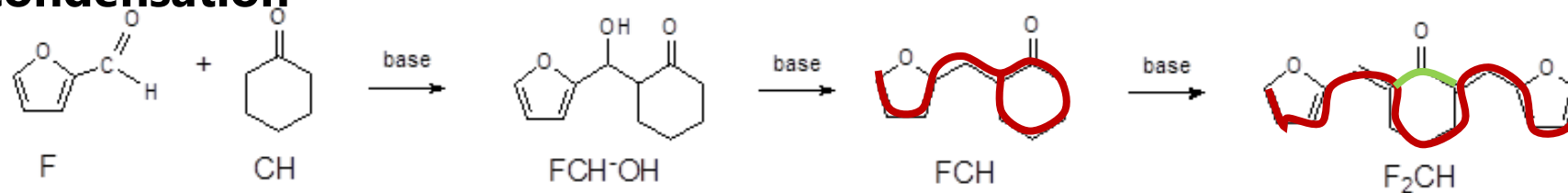


## Reaction strategies:

- Aldol condensation / Condensation
- Guerbet reaction
- Ketonization
- Oligomerization
- Alkylation



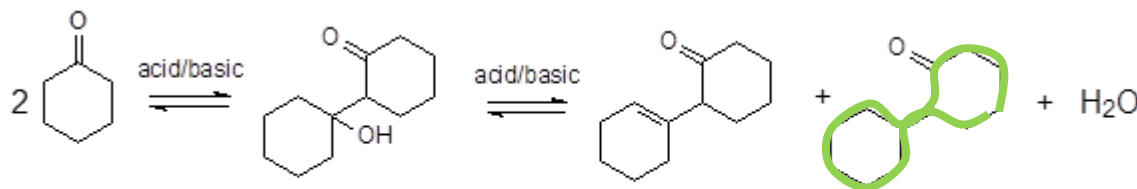
## Aldol condensation



**cyclic-C11**

**cyclic-C16**

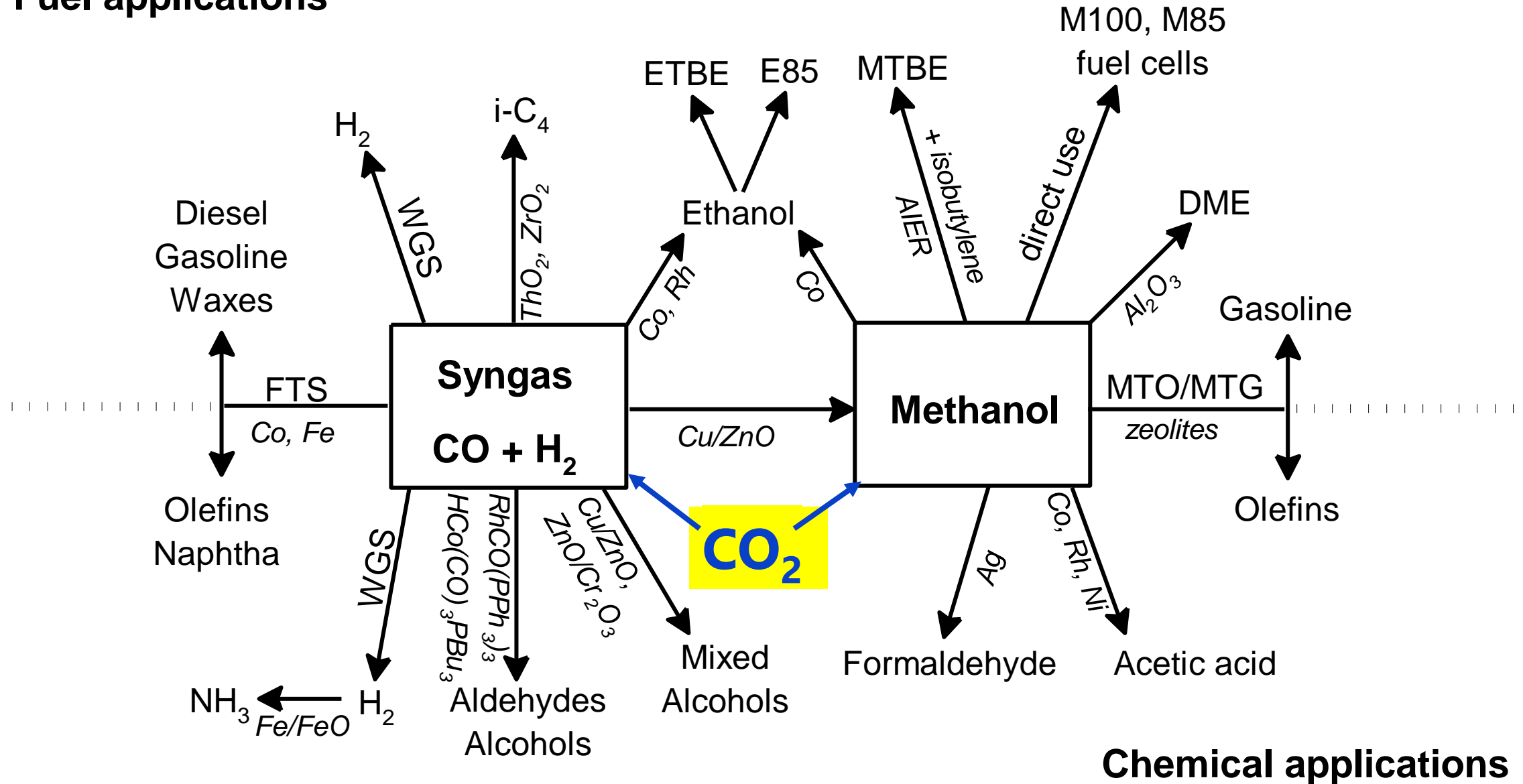
## Self condensation



**cyclic-C12**



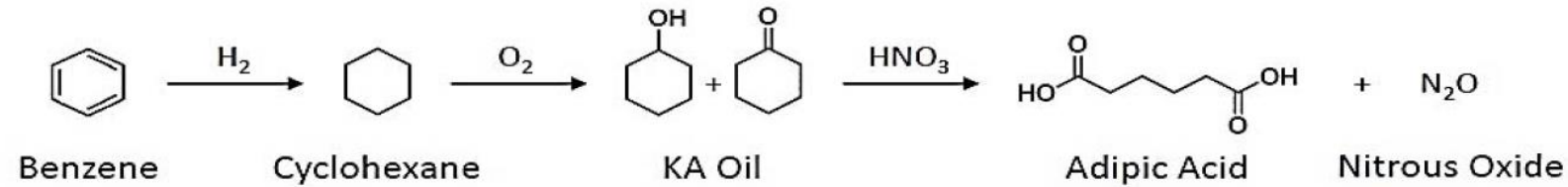
## Fuel applications



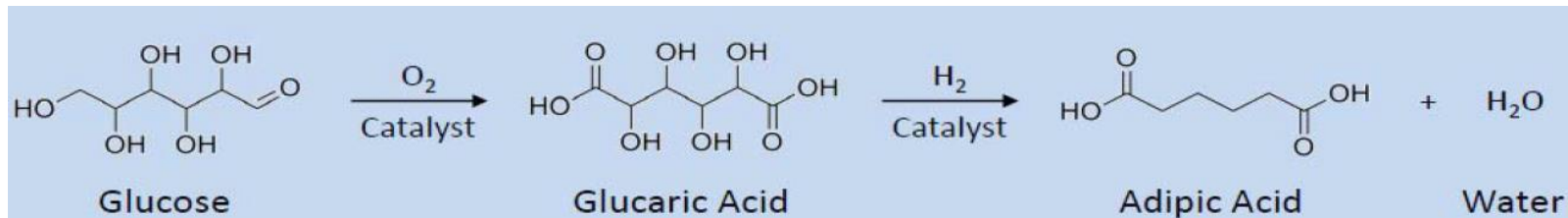
## Chemical applications



## Classical petrochemical route



## Rennovia bio-based route



2 heterogeneous catalyst process steps:

1. Aerobic oxidation of glucose → glucaric acid
2. Hydrodeoxygenation of glucaric acid → adipic acid

Source: Tecnon OrbiChem

- “Bright future” for advanced biofuels
- However, not everything that „looks green is green”
  - No “silver bullet” solutions
  - Catalysis to play a pivotal role
    - “Technology” & “Sustainability” to be addressed simultaneously
    - Thermochemical & biochemical approaches to be combined



- **NCK Chemie pro uhlíkově neutrální ekonomiku**
  - „Obnovitelná chemie“
  - „Cirkulární chemie“

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# EUROPA CAT2023

15<sup>th</sup> European Congress on Catalysis

August 27 – September 1, 2023  
Prague, Czech Republic



**SAVE  
THE DATE**

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