Detail representation of molecule flows and chemical sector in TIMES-BE: progress and challenges during PROCURA

ETSAP workshop – Nov 2023

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Agenda

- Model Background
- Progress so far
  - H2 in the model (supply and use)
  - Derived molecules (supply and use)
  - Base molecules and their use (alternatives)
  - CCUS
  - Industrial symbiosis
  - Downstream processes (challenges and approaches/solutions)
- De-fossilization vs decarbonization
- Results, insights and lessons learnt
- Future work

TIMES-BE

Background

- **Modelling horizon:** 2014 – 2050
- **Time-slices:** 120 (10 days & 12 periods)
- **Climate targets:** Net Zero constraint by 2050. CO_2 price by 2050 at €350/tCO_2.
- **Demands:** service demands (i.e., pkm, space heat,) and product output (i.e., ammonia, steel, cement, olefins).

PATHS 2050
The Power of Perspective

Detailed description in (https://perspective2050.energyville.be/paths2050)

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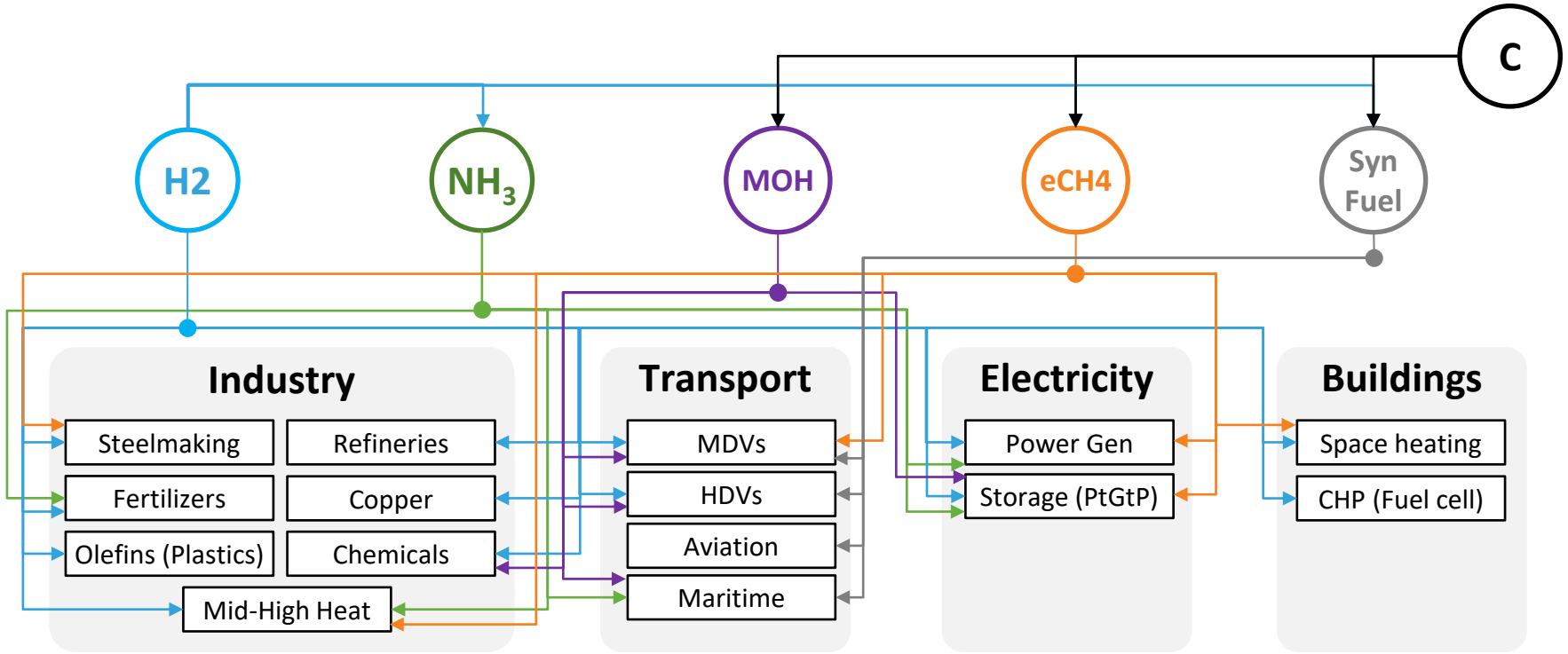
TIMES-BE molecules

The molecules catalogue



Source: VITO/EnergyVille.

Industrial symbiosis

Material exchange is, and will be, important

- Industrial interaction goes beyond energy exchange, as is the case of waste to be burnt.
- Some industrial symbiosis is possible, such as steel sag being used in cement production.
- However, there are more material exchanges happening among industries that are not thoroughly mapped. (i.e., tar as feedstock, ashes as materials, CO_2 use in the food sector)
- New materials interactions include CO_2, as CCU becomes interesting and economically attractive under certain conditions.

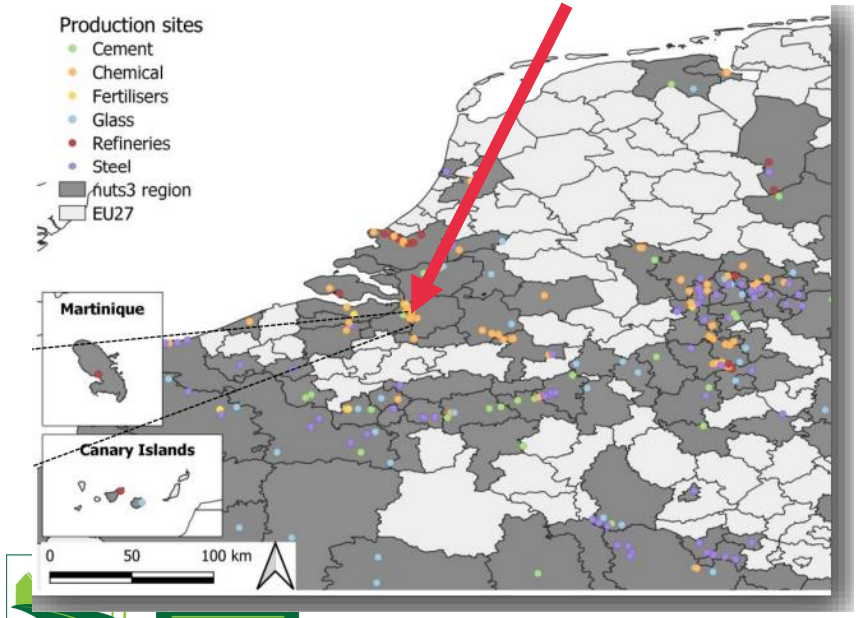
Downstream processes

The chemical sector case: circularity and alternatives

Why?

- Ammonia
- Chlorine
- Other CH

One of the largest petrochemical clusters in EU



Source: AIDRES Project

Today

- Ammonia
- Chlorine
- Ethylene → Ethylene Oxide
- Propylene
- BTX/C4
- Other CH

Tomorrow

- Ammonia → Nitric Acid
- Ammonia → Ammonium Nitrate
- Ammonia → Other derivatives
- Chlorine
- Ethylene → Ethylene Oxide
- Ethylene → Polymers
- Ethylene → Solvents, additives & others
- Propylene → Thermoplastics
- BTX/C4 → Polyamides, thermosets
- Secondary reactants
- Other CH

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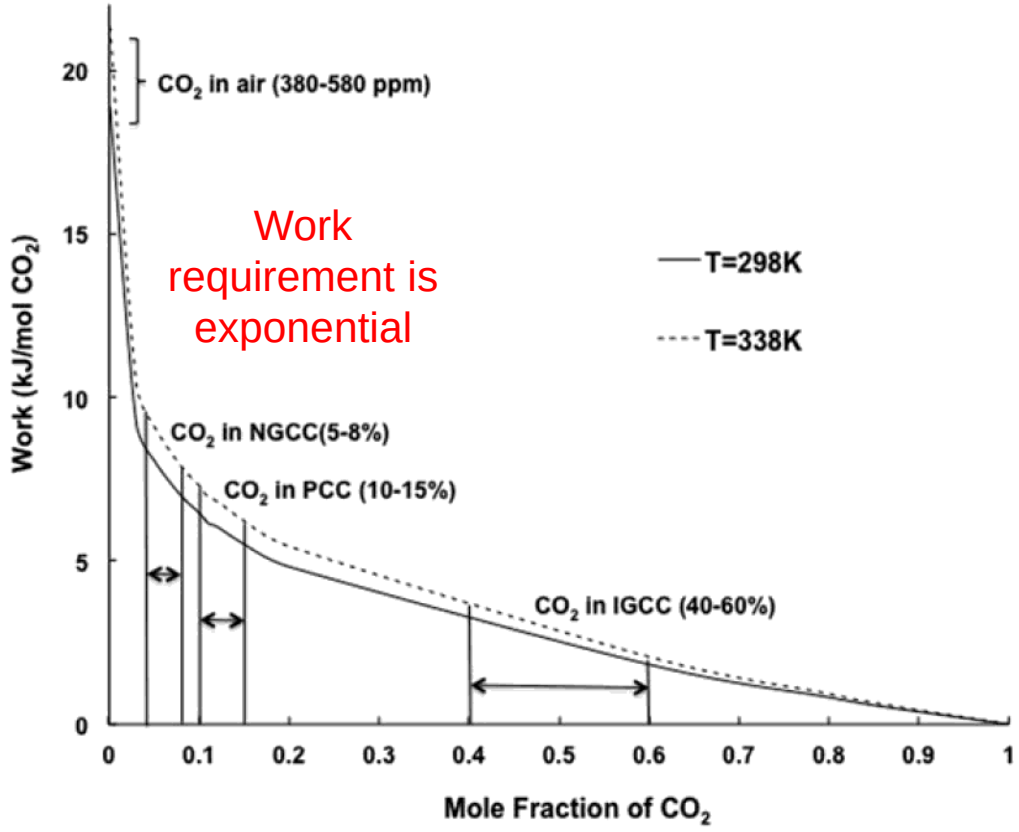
CCUS

Generic parameters don’t represent reality



Source: Wilcox, J., Carbon Capture 2012: Springer.

- **Sector-specific** CO_2 commodities.
- Biogenic CO_2 emissions are included.
- CAPEX, capture efficiency and energy consumption based on sector-specific emissions (flue gases) characteristics.
- Units can be installed independently of other processes (i.e., power plants, furnaces, kilns).
- CO_2 pipeline and export terminal (CAPEX, **energy use**).
- Correlation curves to derive specific techno-economic parameters.

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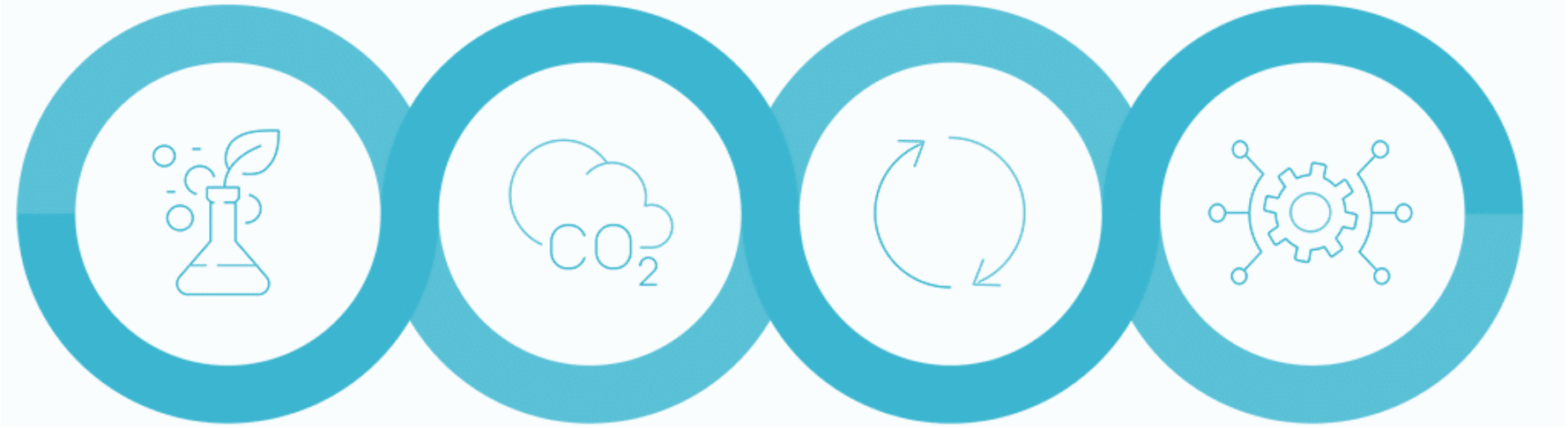
De-fossilization vs Decarbonization

Carbon is, also, a valuable molecule



Chemical Feedstock

- Plastics.
- Solvents.

Other uses

- Greenhouses.
- Food packaging.
- Beverages.
- Synthetic fuels.

Circularity

- Carbon in waste.
- Close loops.

Material

- Concrete.
- Carbonates
- Tarmac.

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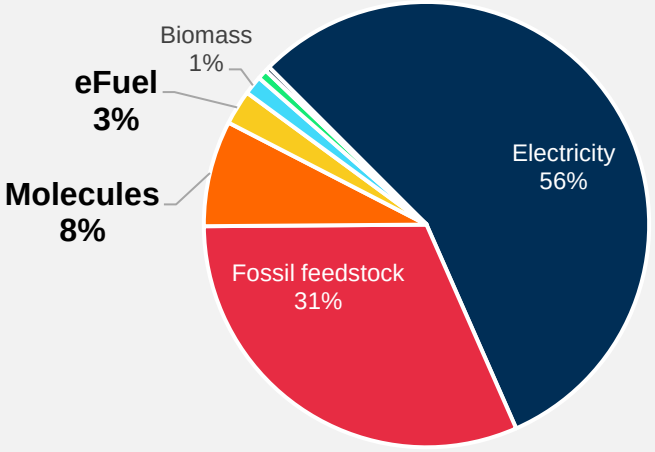
Results

Preliminary Results

Molecules (H_2) demand

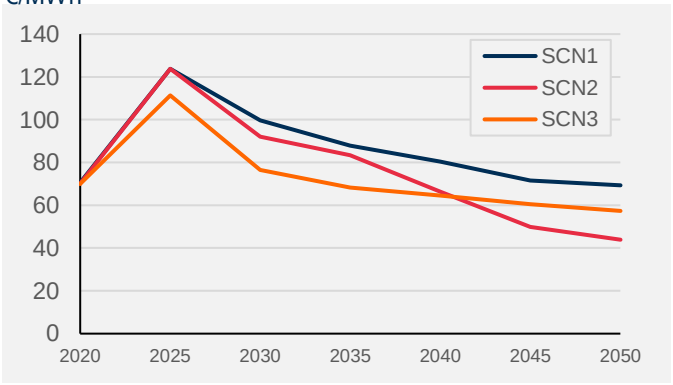
Hydrogen and derivatives account for 11% of final energy demand by 2050



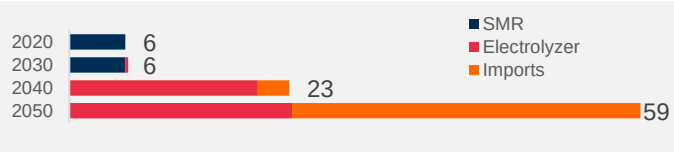
Simultaneously

Molecules will might be cheaper

Hydrogen cost for demand sectors
€/MWh

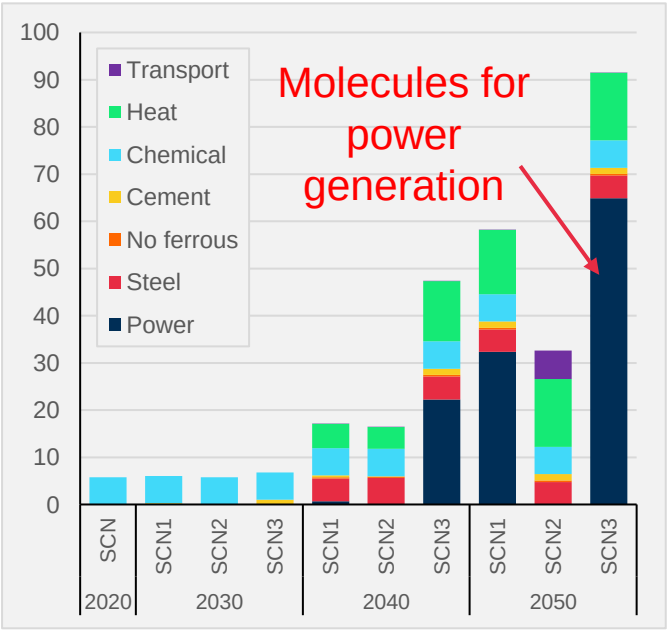


Hydrogen supply, TWh



Molecule demand will vary depending on the context (assumptions)

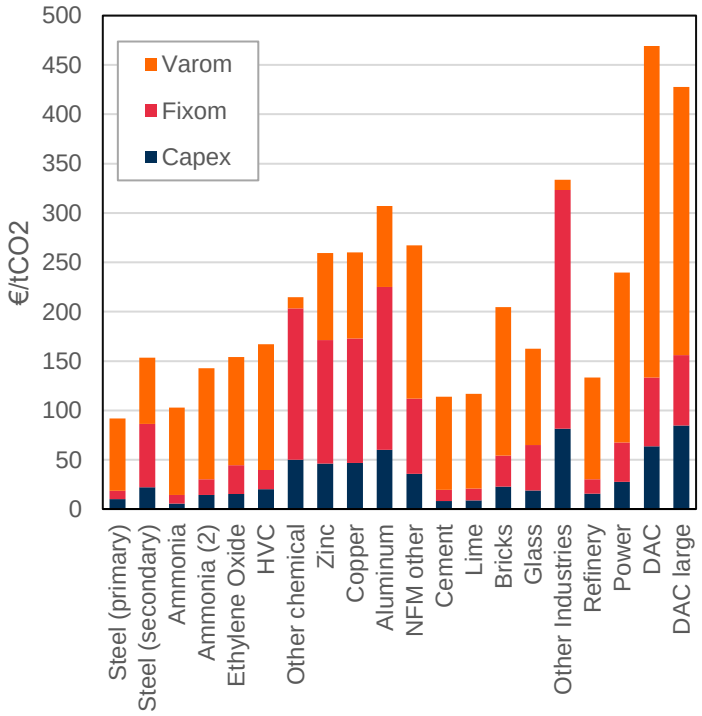
Hydrogen Demand, TWh



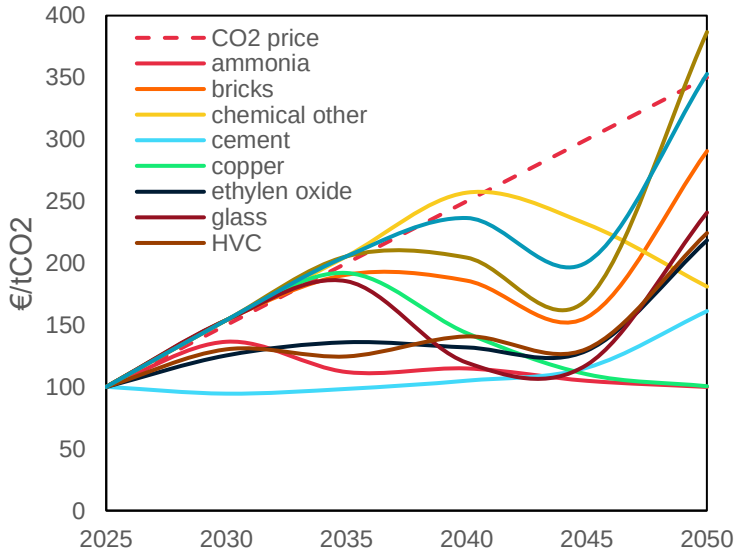
Preliminary Results

CO_2 captured cost and volumes differ by sector

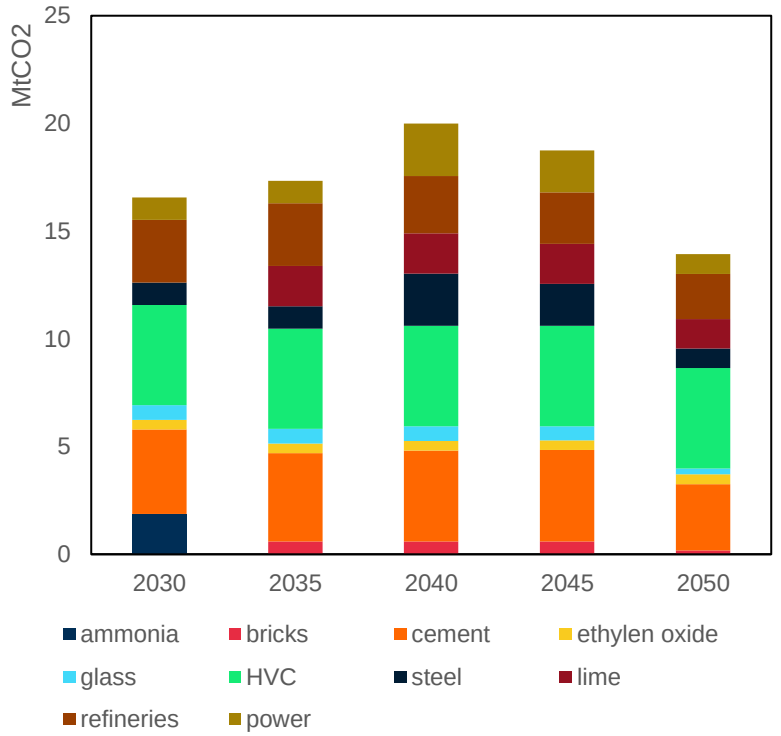
Simulated CO_2 capture cost by industry (correlations methodology)



TIMES-BE perceived capture cost and storage by industry



TIMES-BE Captured CO2 by sector



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Conclusions (by now)

Lessons learnt

- Scarce data on industrial material flows (we are improving our database for Belgium).
- Production capacities and rates are difficult to find for some industrial sectors.
- Without defining limits, hydrogen imports can dominate the molecule market.
- Molecule seasonal storage is not used as imports from RoW are “unlimited”.
- How to tackle the “de-industrialization” dilemma of importing semi-finished products (e.g. ammonia, sponge iron, methanol, ethylene, etc.).
- Chemical components and base-molecules require special attention to mass balances and energy requirements, for example, syngas.

Future work

Models are always evolving and improving

- Modell downstream chemical production first and second tier.
- Improve refineries model to desegregate H_2 consumption, diluted and concentrated CO_2 streams.-> in line with sector plans.
- Include technologies for the chemical sector beyond H_2 and CO_2, such as aromatic production from biomass (easier to produce aromatics from sugars/glucose).
- Validate the link with transport sector demand for synthetic, no-emissions fuels in the transport sector.

Thanks!

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