CAPE OPEN Annual Meeting
Ghent, October 30th, 2025

PR1ME: A SIMULATION FRAMEWORK FOR HYDROPROCESSING

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hydroprocessing

heavy petroleum fractions (~ 350 °C – 550 °C) are converted into valuable lighter products

Vacuum Gas Oil (VGO)

catalytic conversion

products

- naphtha
- jet fuel
- diesel
- lube oils

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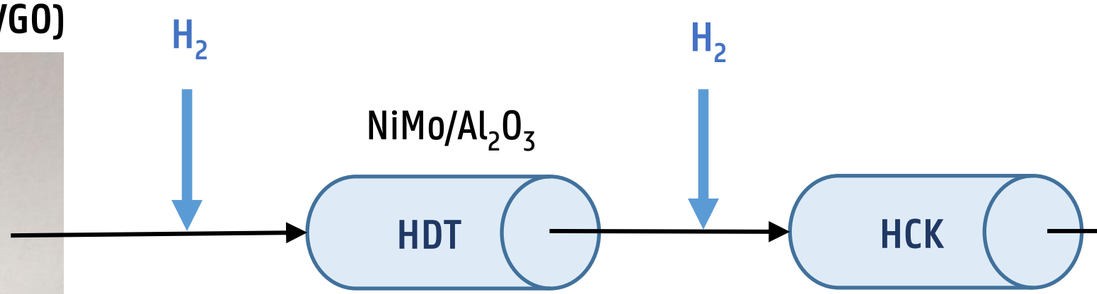
hydroprocessing

one or two-stage process: hydrotreating (HDT) and hydrocracking (HCK)

Vacuum Gas Oil (VGO)



Zeolite based
(metal-acid)
bi-functional

products

- naphtha
- jet fuel
- diesel
- lube oils

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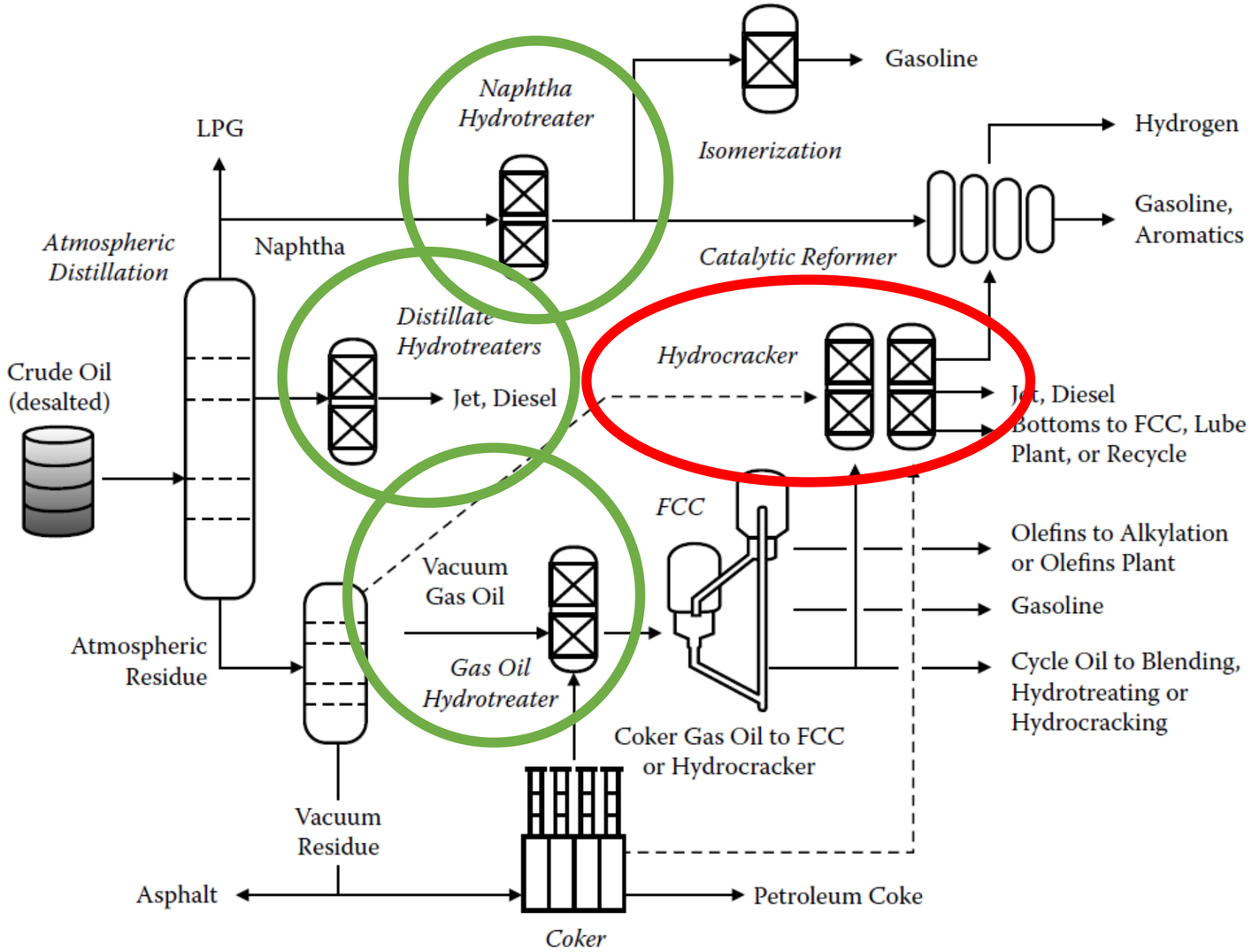
hydroprocessing in a refinery

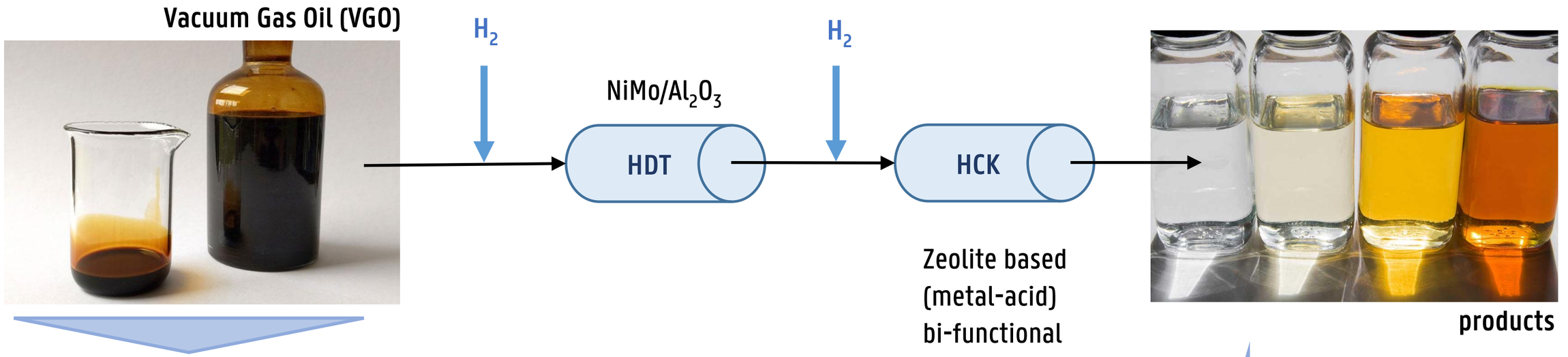
- almost all streams in a refinery are hydroprocessed at some stage
- **HDT**: upgrading
- **HCK**: conversion

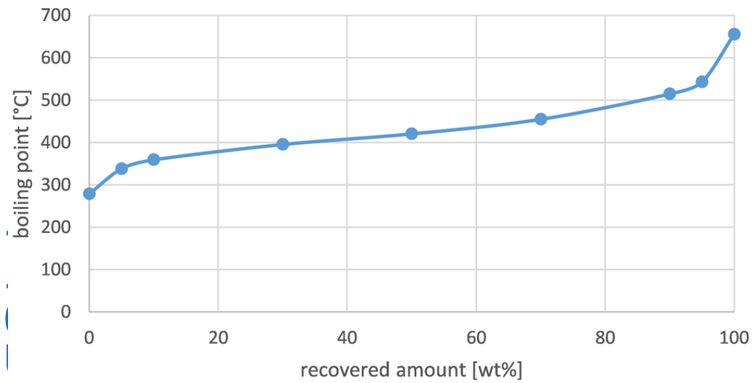


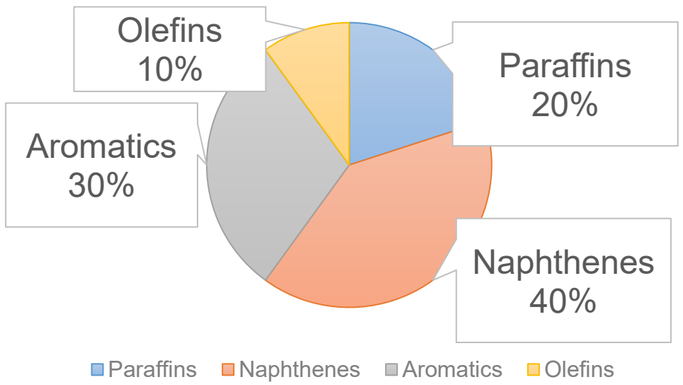
Juárez & Speight, Hydroprocessing of Heavy Oils and Residua, 2020.

VGO hydroprocessing

- at industrial scale feed and product streams are characterized in terms of bulk properties
- True Boiling Point (TBP) curve, P(I)ONA, etc.







- naphtha
- jet fuel
- diesel
- lube oils

outline

- Bulk properties and the Petroleum Fractions Interface
- PR1ME: from bulk properties to fundamental kinetics
- integration with PME through Petro Fractions: proof of concept
- future plans

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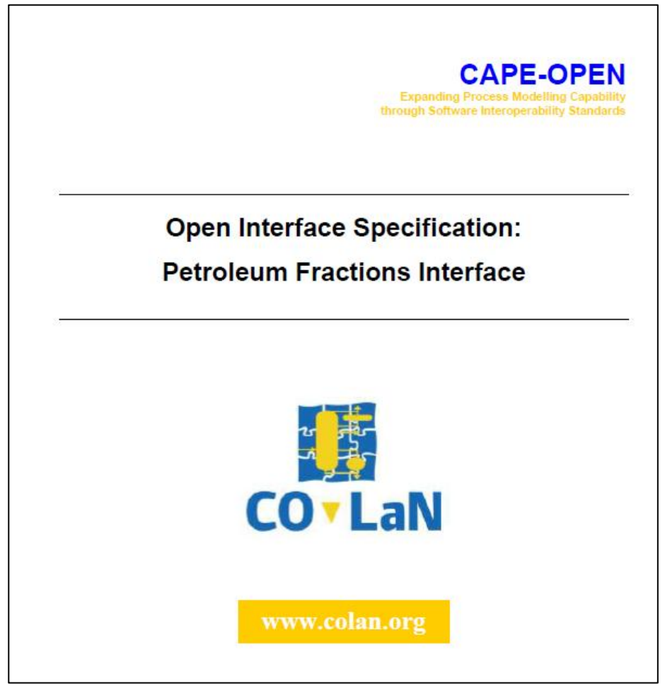
bulk properties and the Petroleum Fractions Interface

`ICapeThermoPetroleumFractions`

- Handles petroleum mixtures within a Material Object.
- Enables UO to read and modify petroleum-specific properties:
  - Dist. curves, PNA, cloud point, … (bulk properties)
- Enables run-time re-characterization of fraction properties:
  - (NBP, MW, SG, .. etc.).
- Currently supported by AVEVA™ PRO/II™



First release - 2003

Second release - 2023

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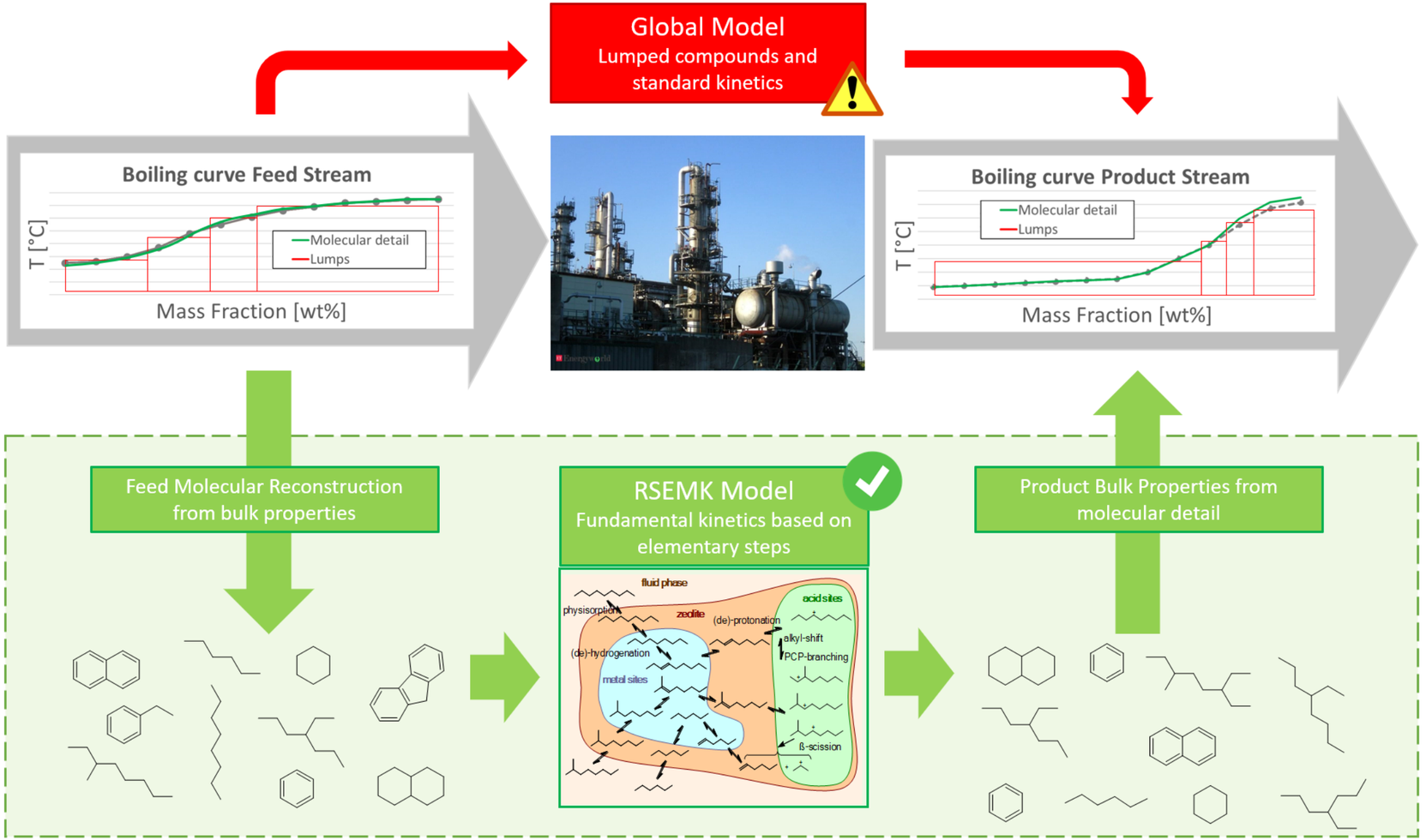
PR1ME: from bulk properties to fundamental kinetics

PR1ME integrates a Single-Event MicroKinetic model with a molecular reconstruction engine



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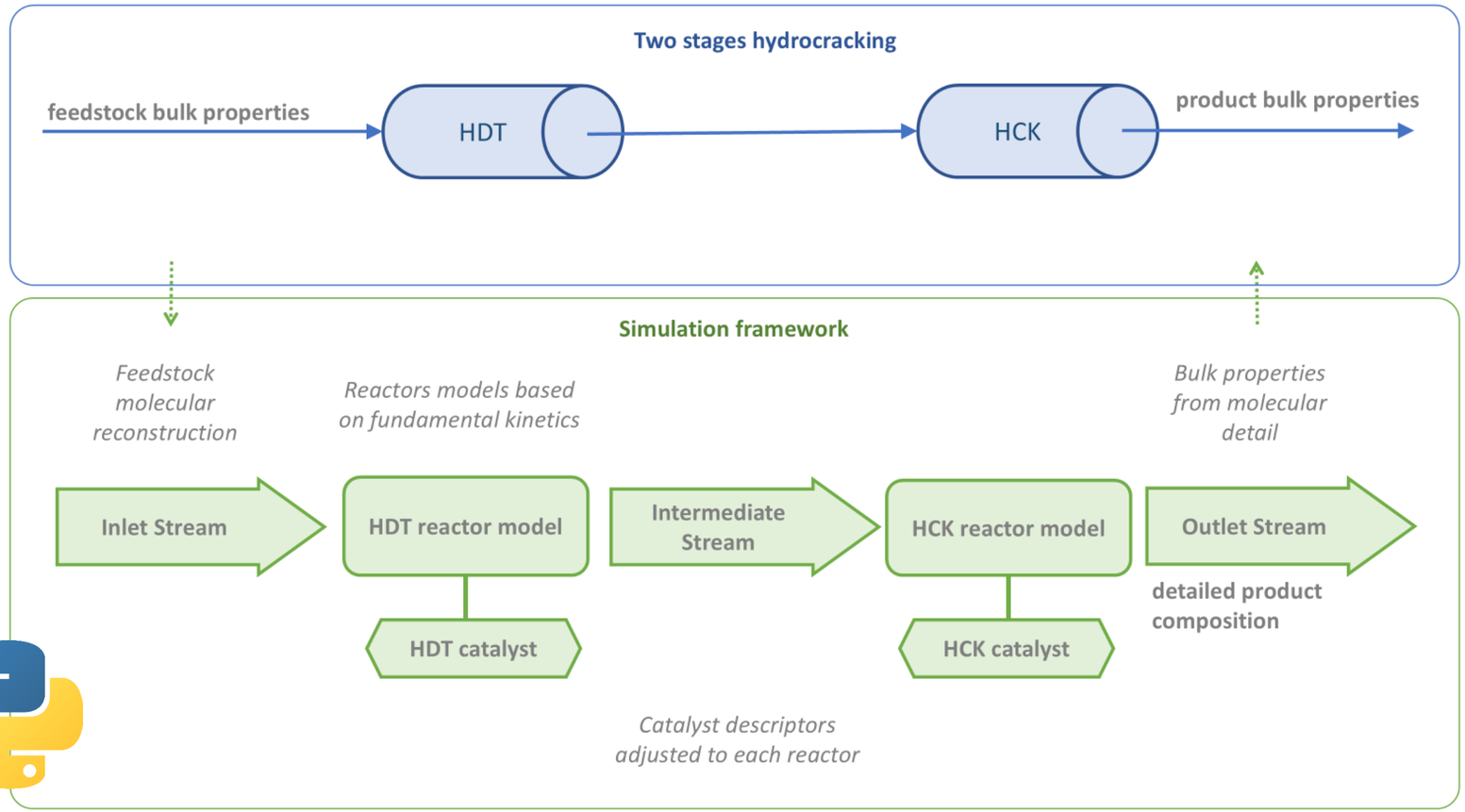
Pernalete et al. *Industrial & Engineering Chemistry Research* **2024**, *63*, 50, 21841.
DOI: 10.1021/acs.iecr.4c03637

PR1ME is a python framework

- Object-oriented architecture allows to create a combined objects flowsheet-wise




```
>>
>> import pr1me
>>
```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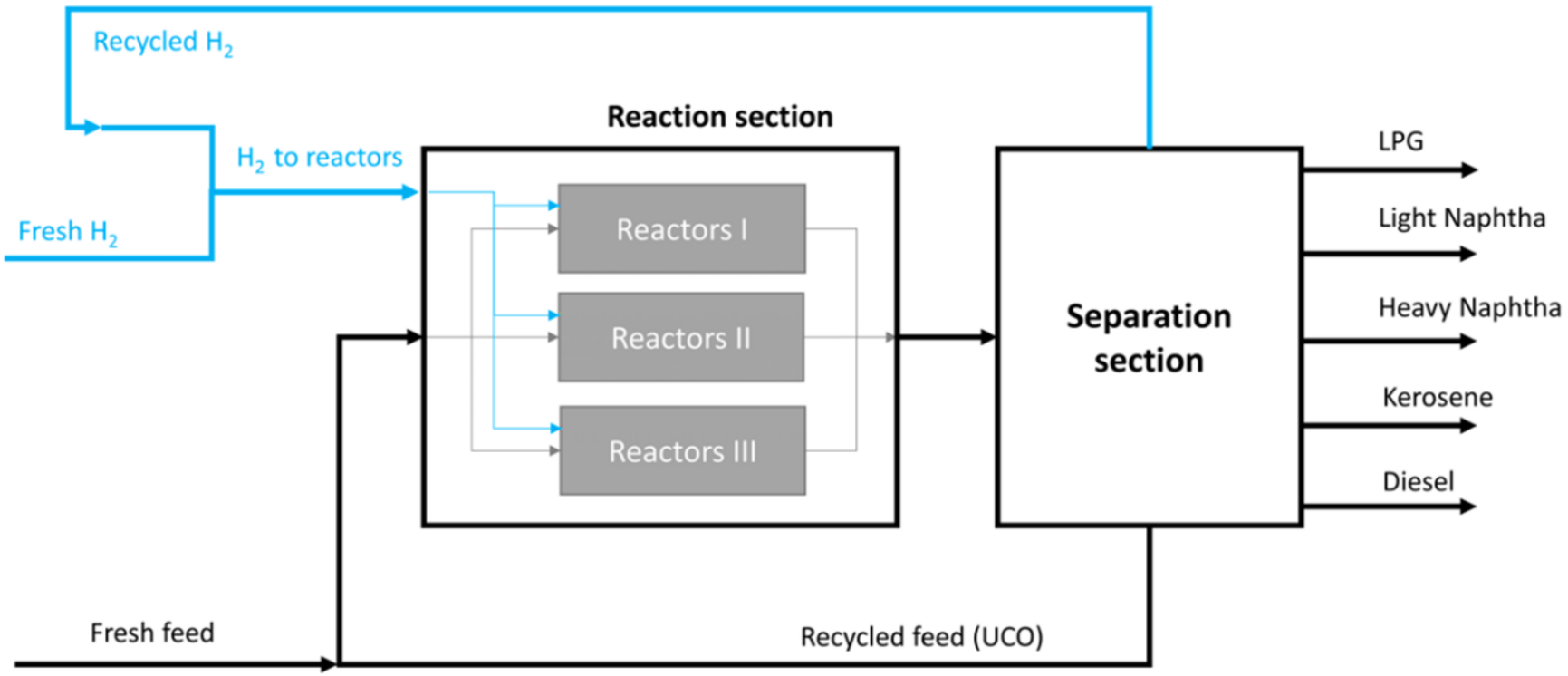
Pernalete et al. *Catalysis Today* **2021**, *378*, 189-201.
DOI: 10.1016/j.cattod.2021.06.010

VGO hydroprocessing at industrial scale

A configuration of three parallel downflow trickle-bed reactors with recycle was simulated



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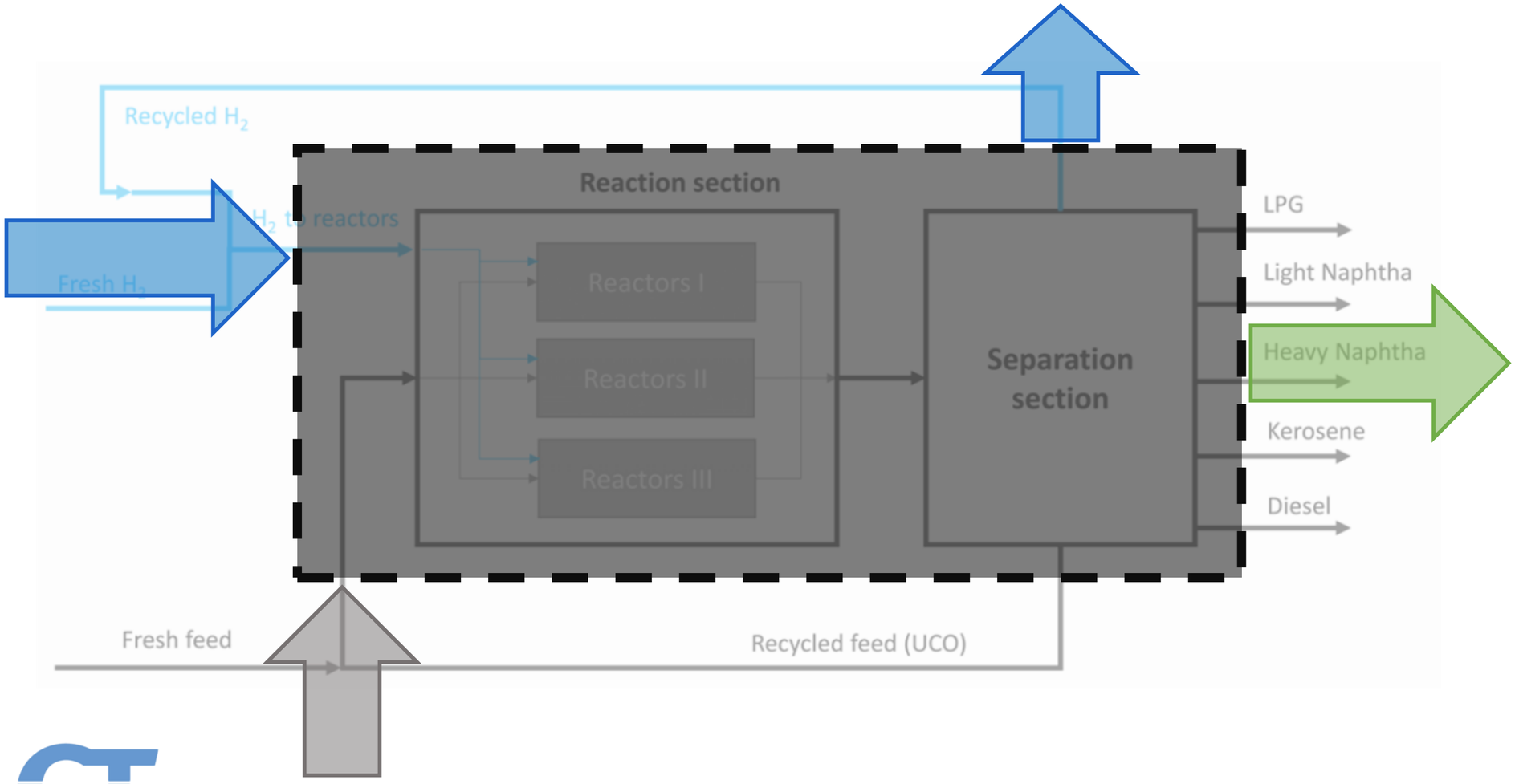
VGO hydroprocessing at industrial scale

A simplified process scheme was selected for a proof-of-concept of the integration with the PME



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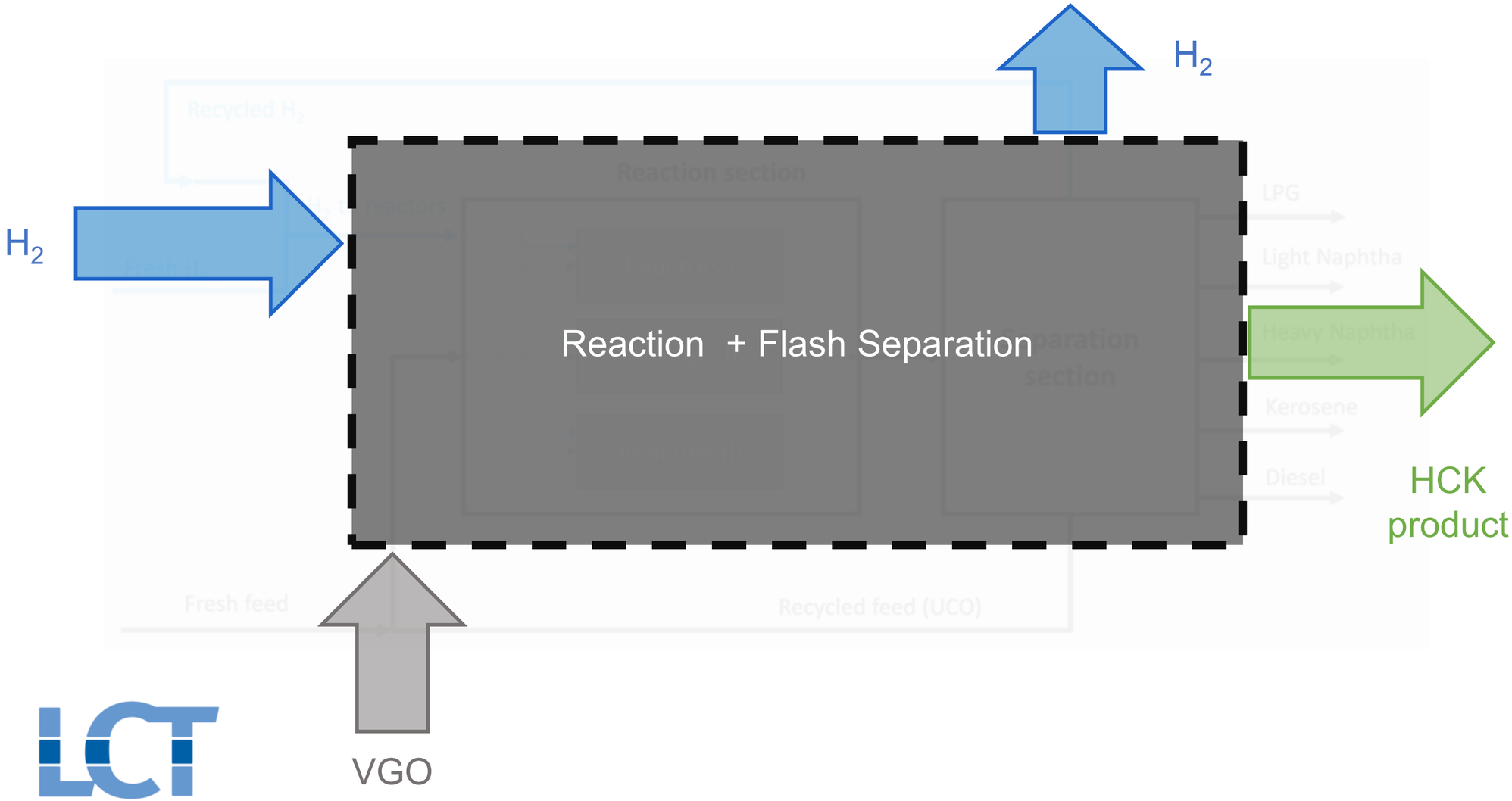
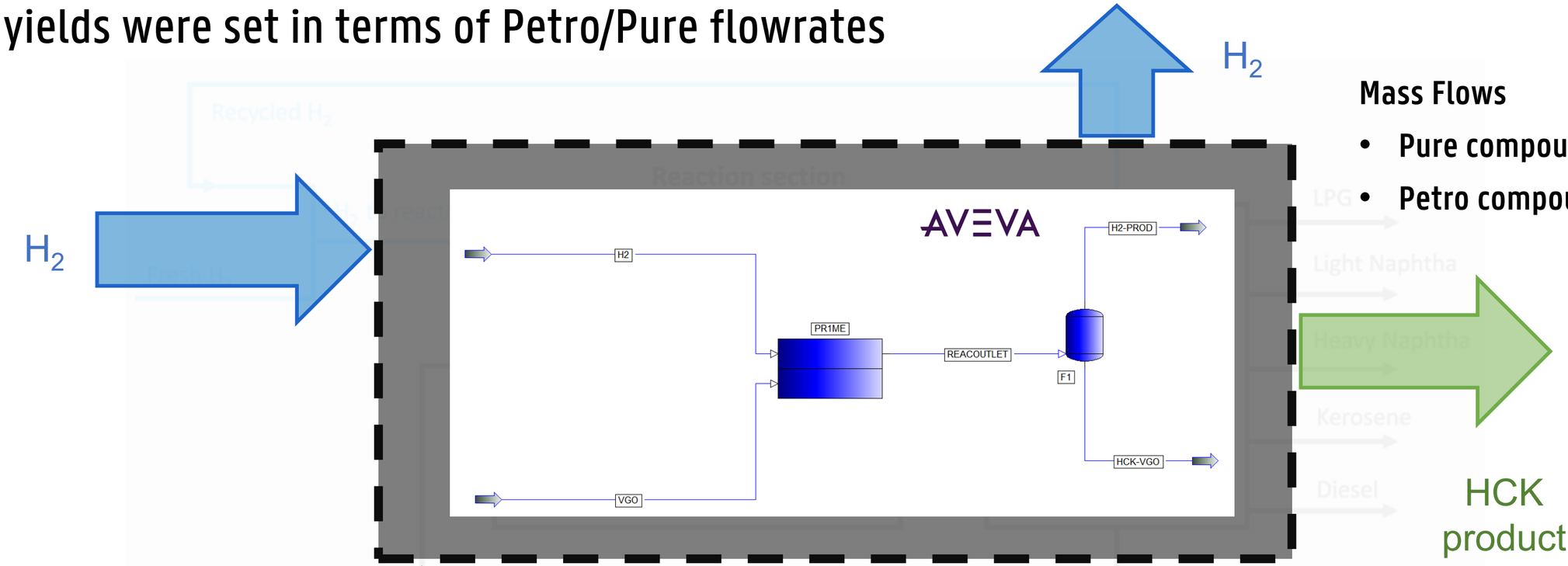


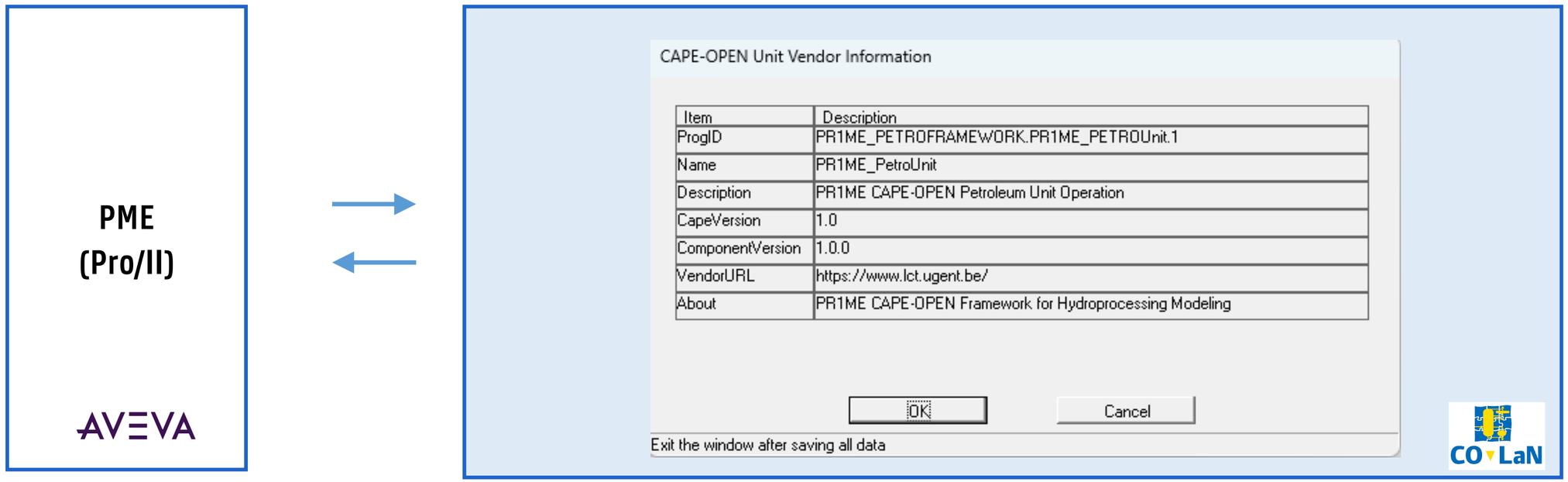
VGO hydroprocessing at industrial scale

- The feed was modeled in terms of bulk properties
- The yields were set in terms of Petro/Pure flowrates



integration with PME through Petro Fractions: POC

- An ATL COM Unit Operation was implemented including `ICapeThermoPetroleumFractions`.



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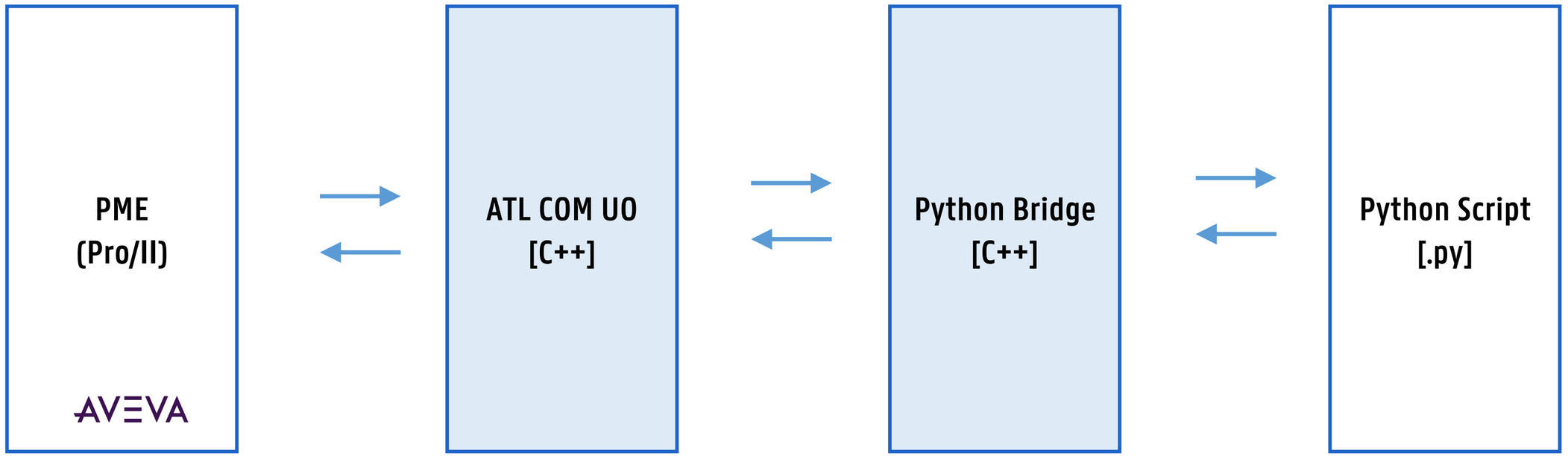
integration with PME through Petro Fractions: POC

- The ATL COM Unit Operation uses `ICapeThermoPetroleumFractions` via `QueryInterface`



`ICapeThermoMaterial`
`ICapeThermoPetroFractionsII`

`ICapeUnit`

`Python C API`

`pr1me.py`

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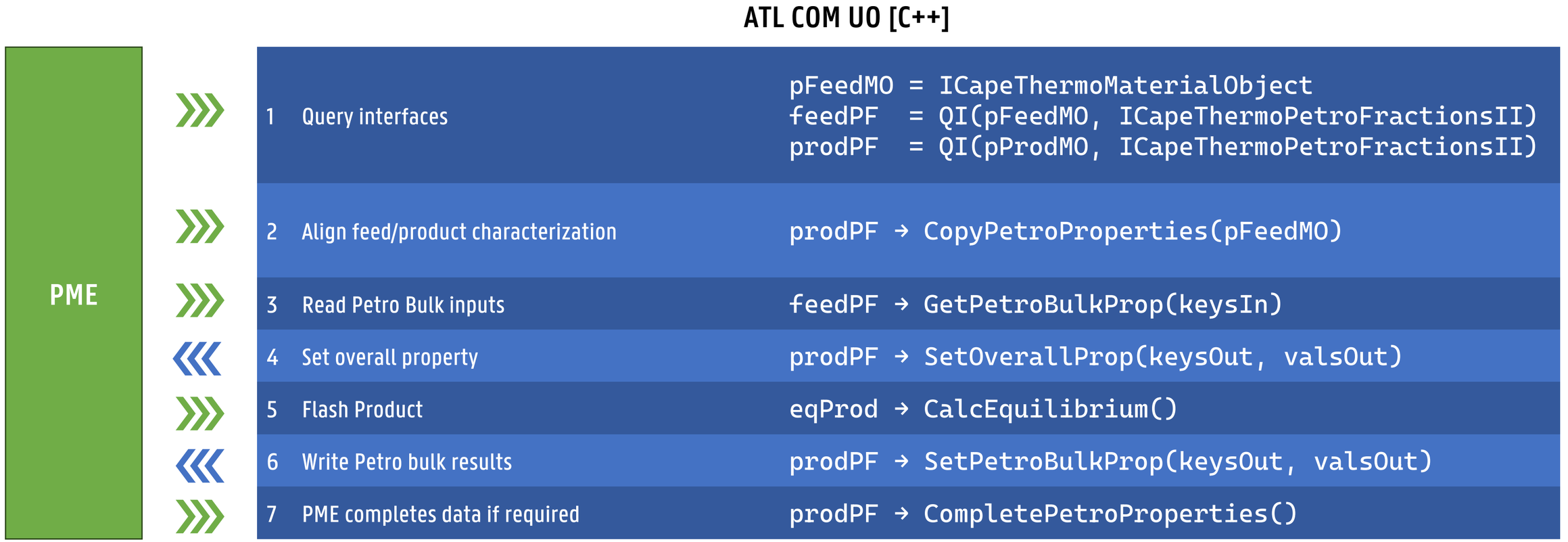
integration with PME through Petro Fractions: POC

- Communication with the PME requires specific protocol



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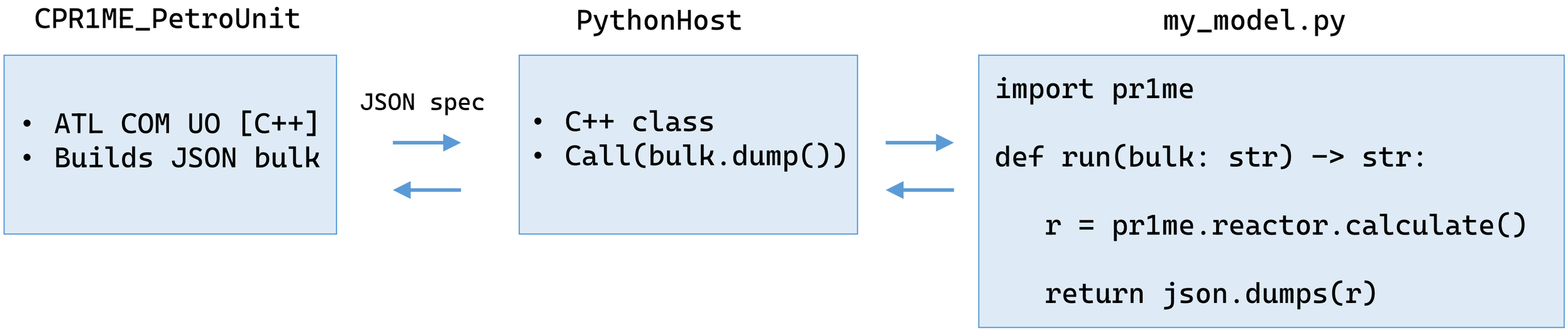
native C++ COM bridge to Python

- The ATL DLL embeds a “bridge” that lets native C++ COM code call Python functions at runtime.
  - Python C API



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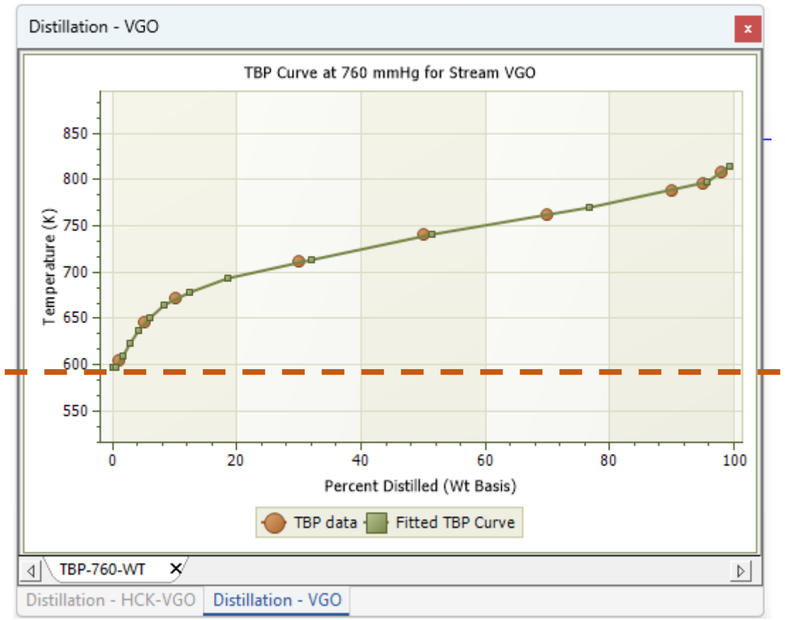
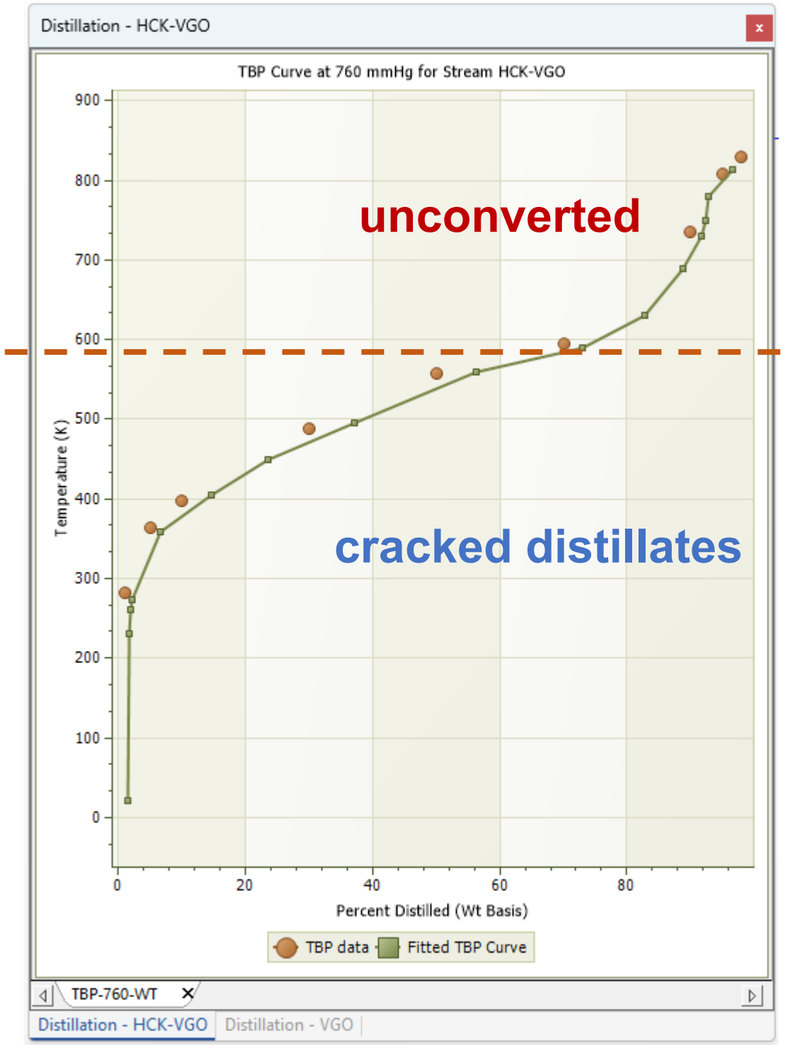
Proof of concept: TBP curve of feed and products

- The integration allows to monitor TBP (bulk prop.) in feed and products
  - ..with the PME





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future plans

- Extend towards additional feed / product bulk properties
    - Detailed PIONA, S, N, Conradson Carbon,…etc
- Test further integration with the PME
    - recycles, sequential beds, quenching
- CAPE OPEN certification

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acknowledgments

Krishna Penukonda (AVEVA)

Jasper van Baten (Amsterchem)

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