EUROKIN'S 20TH ANNIVERSARY SYMPOSIUM, VAALSBROEK, OCTOBER 16-17 2018

# Large-scale production of fuels and chemicals:

# coping with complex feedstocks and chemistry

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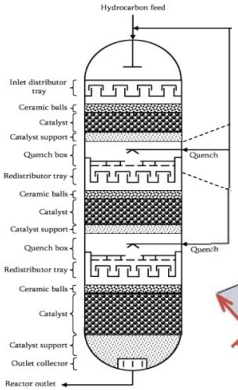
GHENT UNIVERSITY

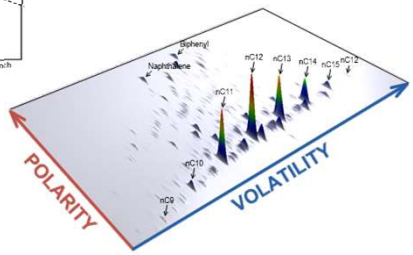
LCT DRIVING CHEMICAL TECHNOLOGY

European Research Institute of Catalysis

# Kinetics: methods and applications

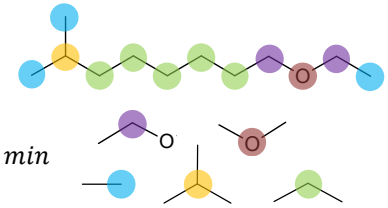



SIMCO



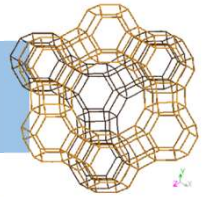

μKE

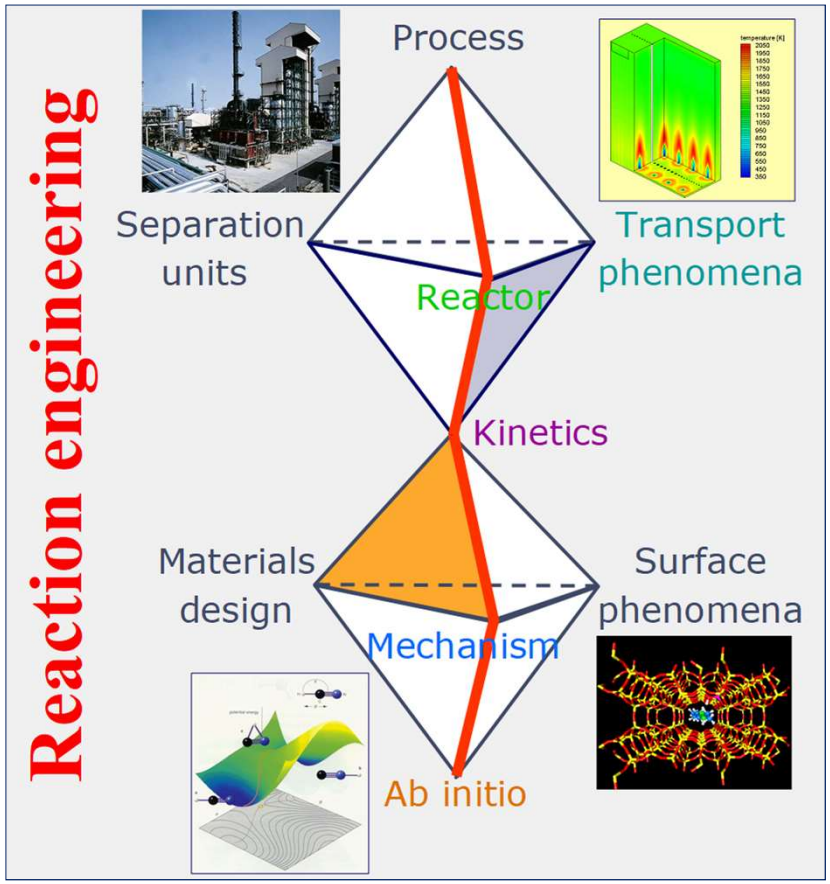
$$\sum_{i=1}^{n_{exp}} \left(F_i - \hat{F}_i\right)^2 \rightarrow min$$

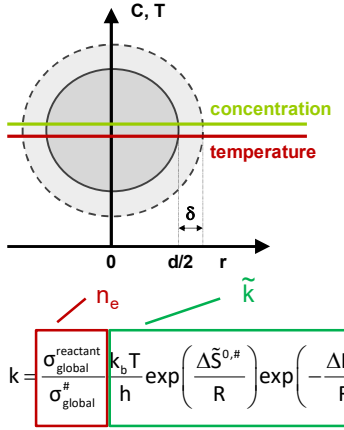


Catalyst descriptors

$K^L$, $\Delta H_{prot}$, $C_{sat}$, $C_{acid}$



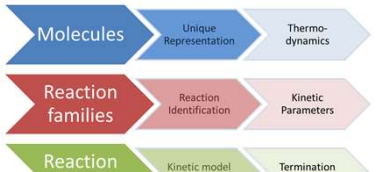


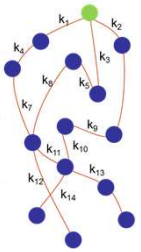



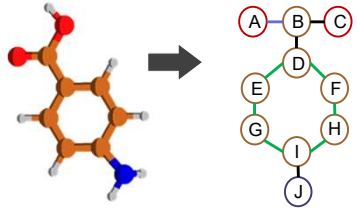

$$k = \frac{\sigma_{global}^{reactant}}{\sigma_{global}^{\#}} \frac{k_b T}{h} \exp\left(\frac{\Delta \tilde{S}^{0,\#}}{R}\right) \exp\left(-\frac{\Delta H^{0,\#}}{RT}\right)$$

($n_e$, $\tilde{k}$)

Genesys, ReNGeP



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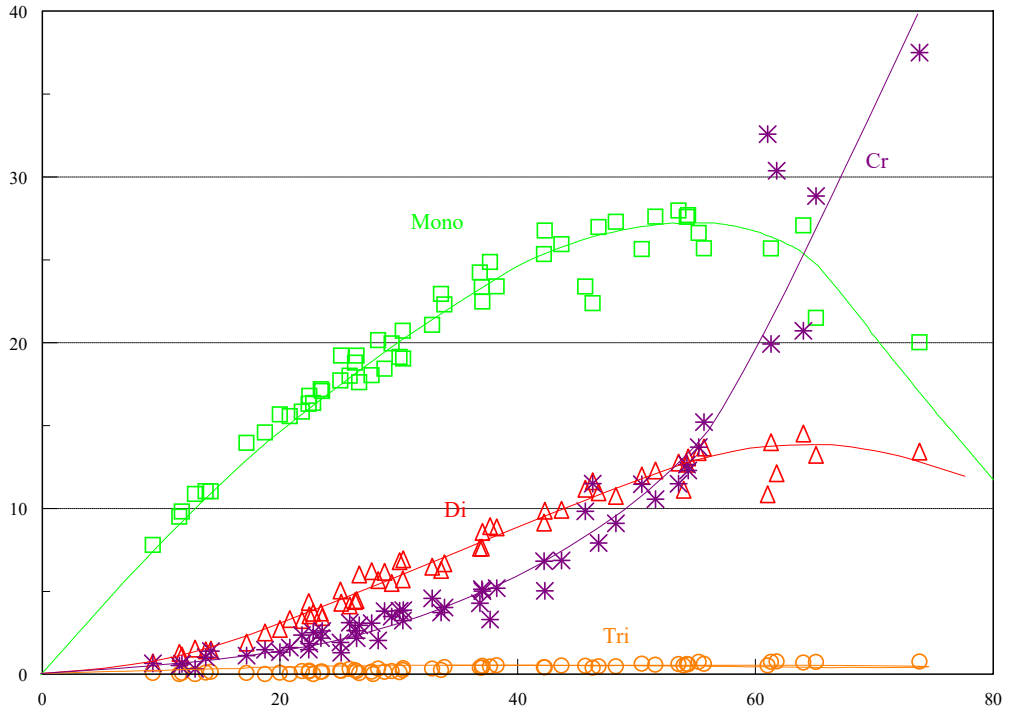
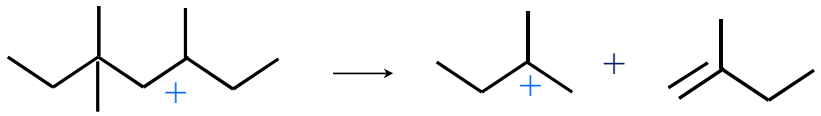
# Outline

- Introduction
- Complex feedstocks: ideal hydroconversion
- Feedstock characterization and reconstruction
- Reaction-network generation
- Complex chemistry: parameter determination
- Reactor design
- Conclusions

# Hydrocracking and isomerization: reaction families

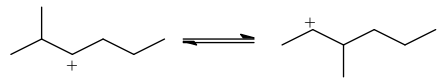
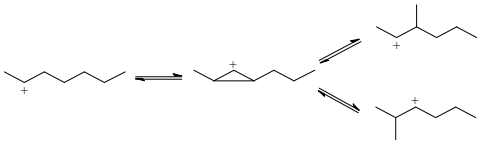
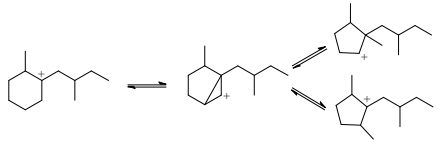
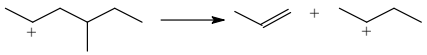
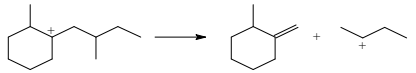
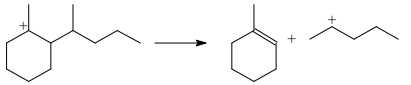
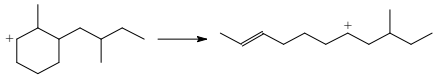


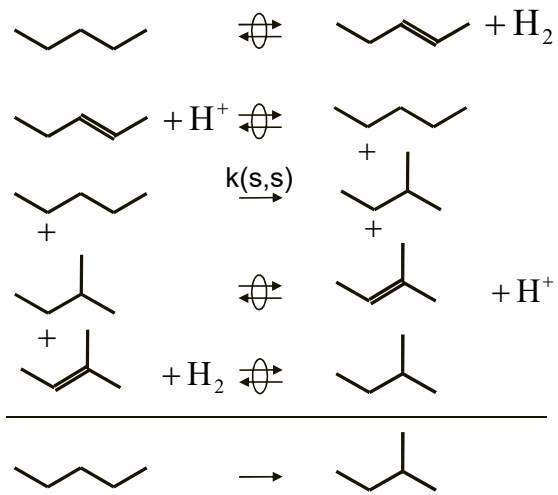
(t;t) β-scission

Thybaut J.W., Marin G.B., Advances in Catalysis, 2016

# Free carbenium ion reaction families: kinetic descriptors

| | Alkanes | Cycloalkanes |
|---|---|---|
| Alkyl shift |  |  |
| PCP branching |  |  |
| Acyclic cracking |  |  |
| Exocyclic cracking | |  |
| Ring opening | |  |

# Kinetic versus Catalyst descriptors




Strength of acid sites

$$\Delta H_{prot}$$

Concentration of acid sites

$$r = \frac{C_{sat}\, C_t\, k\, K_{prot}\, K_{deh}\, K_L\, p_P\, p_{H_2}^{-1}}{1 + K_L p_P}$$

$$k = \frac{\sigma_{gl,r}}{\sigma_{gl,\ddagger}} \frac{k_B T}{h} exp\left(\frac{\Delta \tilde{S}^{0,\ddagger}}{R}\right) exp\left(\frac{\Delta H^{0,\ddagger}}{RT}\right)$$

determined by the reaction network generation code

constant for a reaction family (chain length independent)

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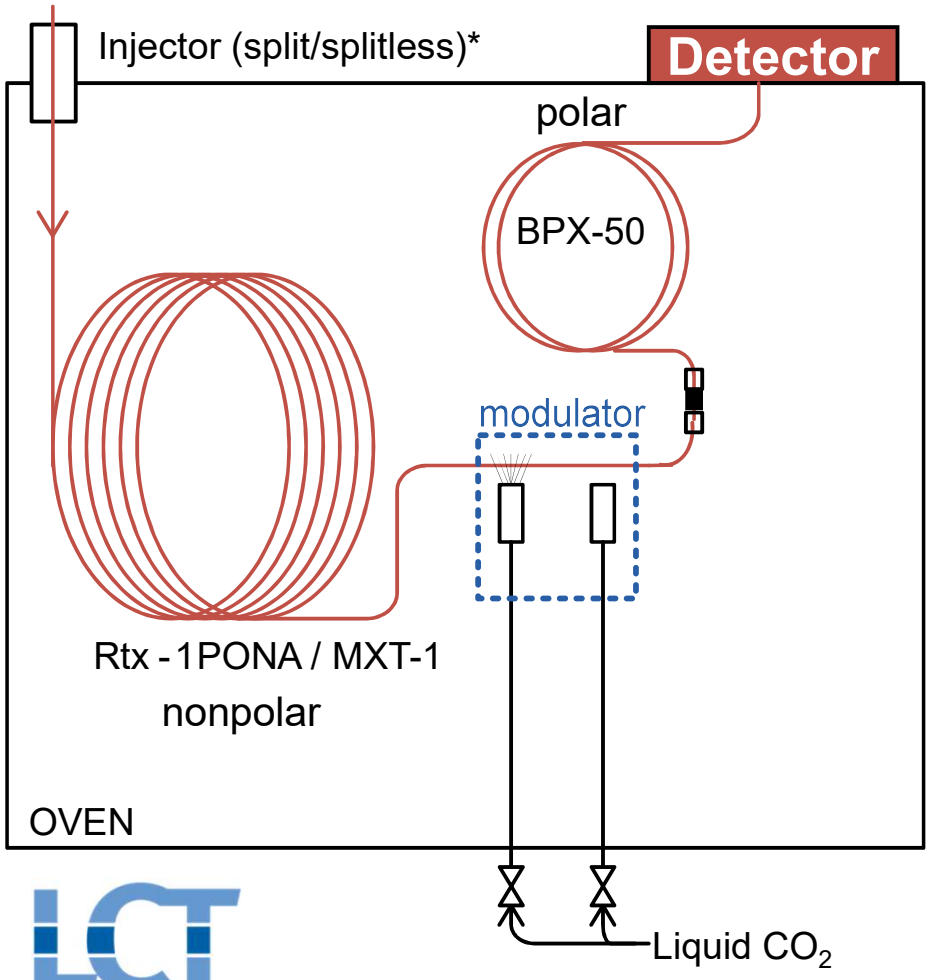
# GC×GC-FID/TOF-MS/NCD/SCD setups

Normal Phase: nonpolar × polar

Reversed Phase: polar × nonpolar




**Detectors:**

250 kEuro

TOF-MS:

- Qualitative analysis

NCD: 25 kEuro

- Quantitative analysis
- Selective to N- compounds

SCD: 25 kEuro

- Quantitative analysis
- Selective to S- compounds

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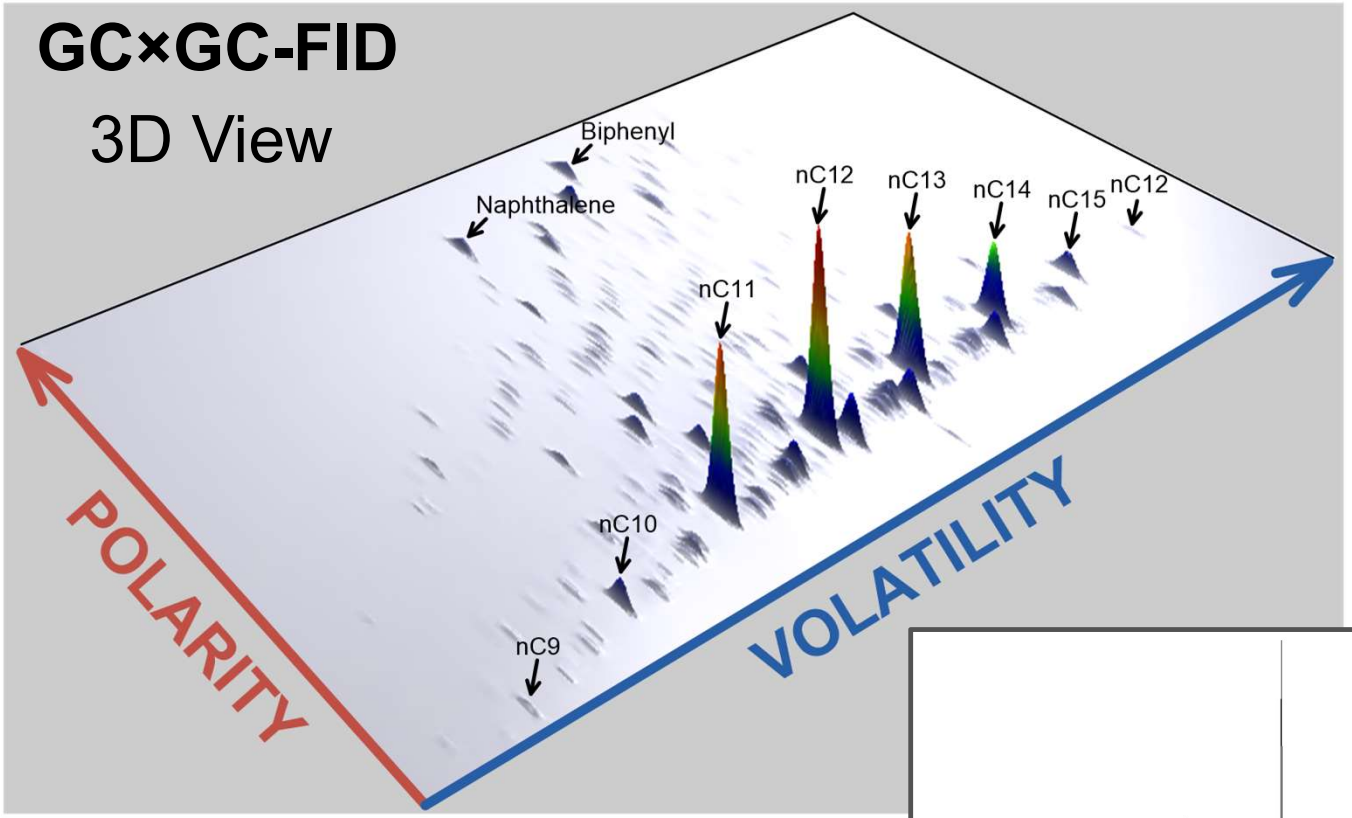
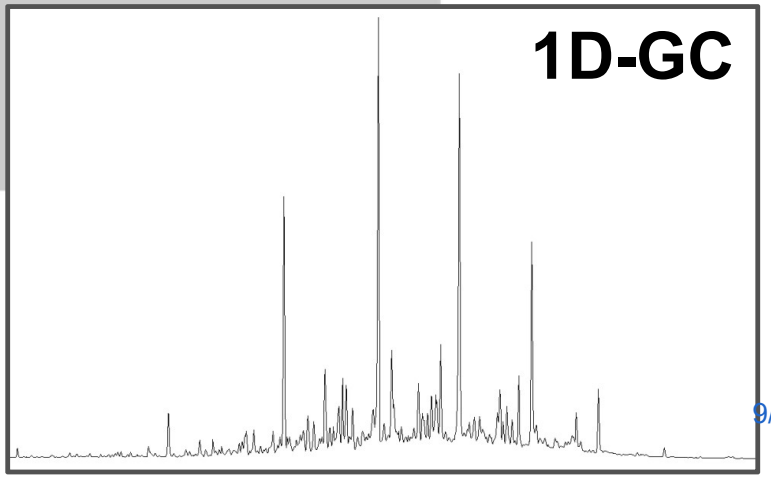
* Injector (PTV) for GCxGC-NCD

# Example: Middle Distillate Analysis




2 independent separation mechanisms
→Enhanced resolution compared to 1D-GC

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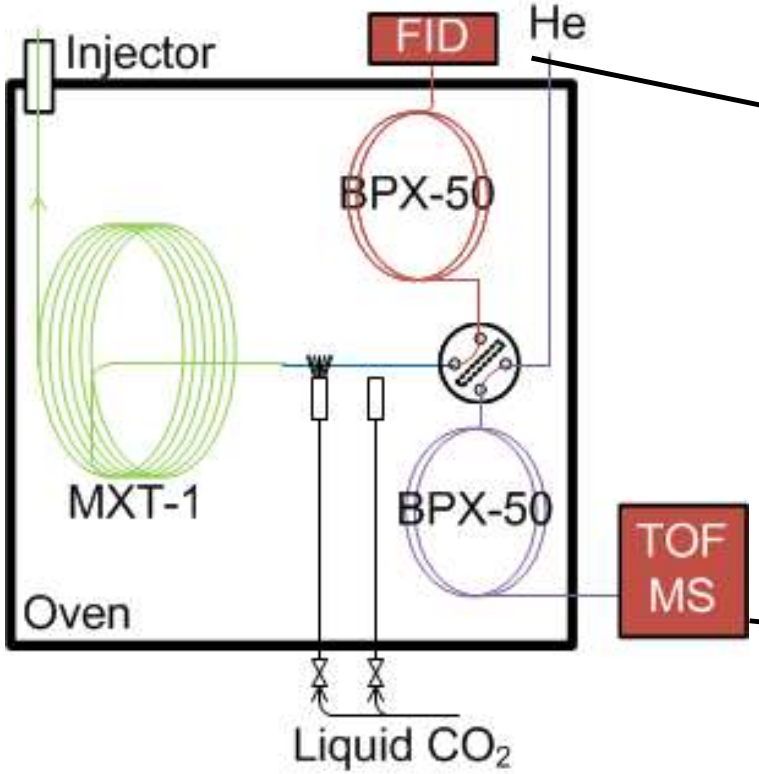
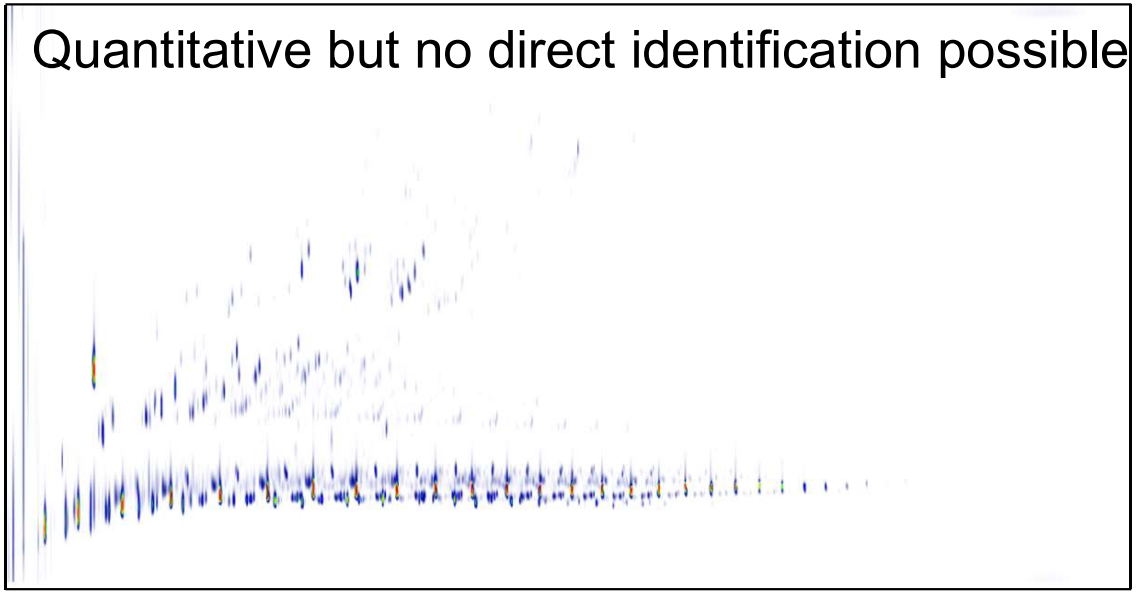
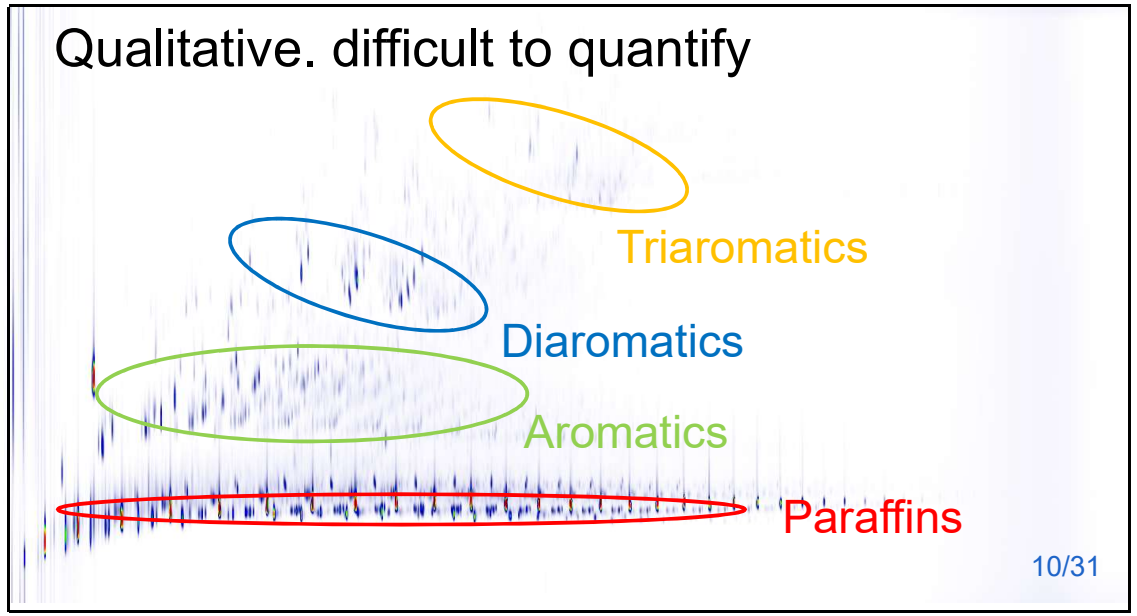
# GC × GC-FID/TOF-MS




Quantitative but no direct identification possible



Qualitative. difficult to quantify

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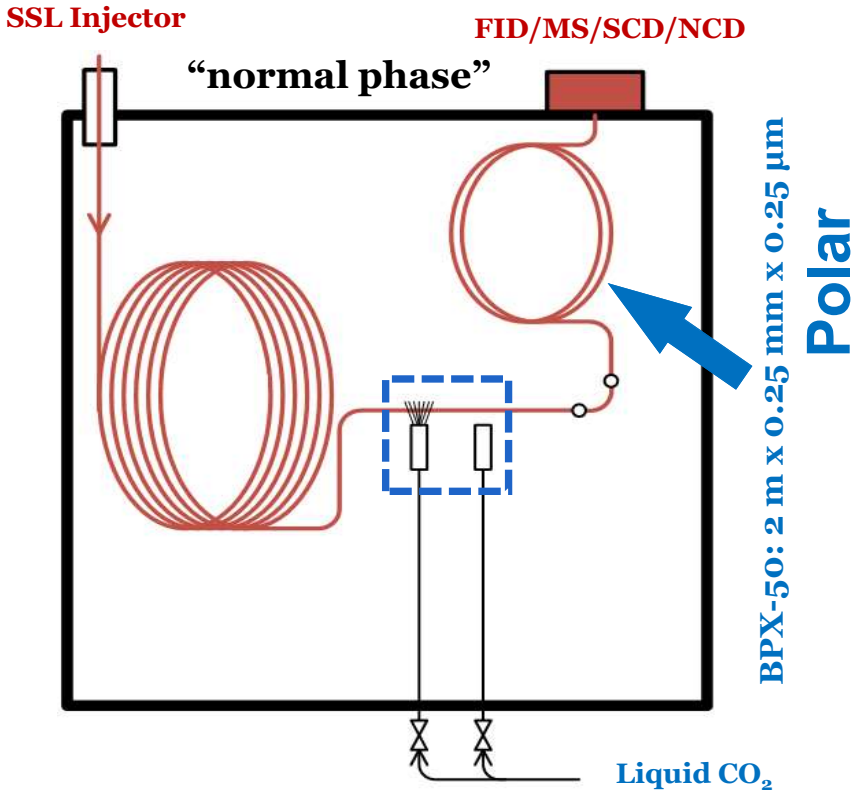
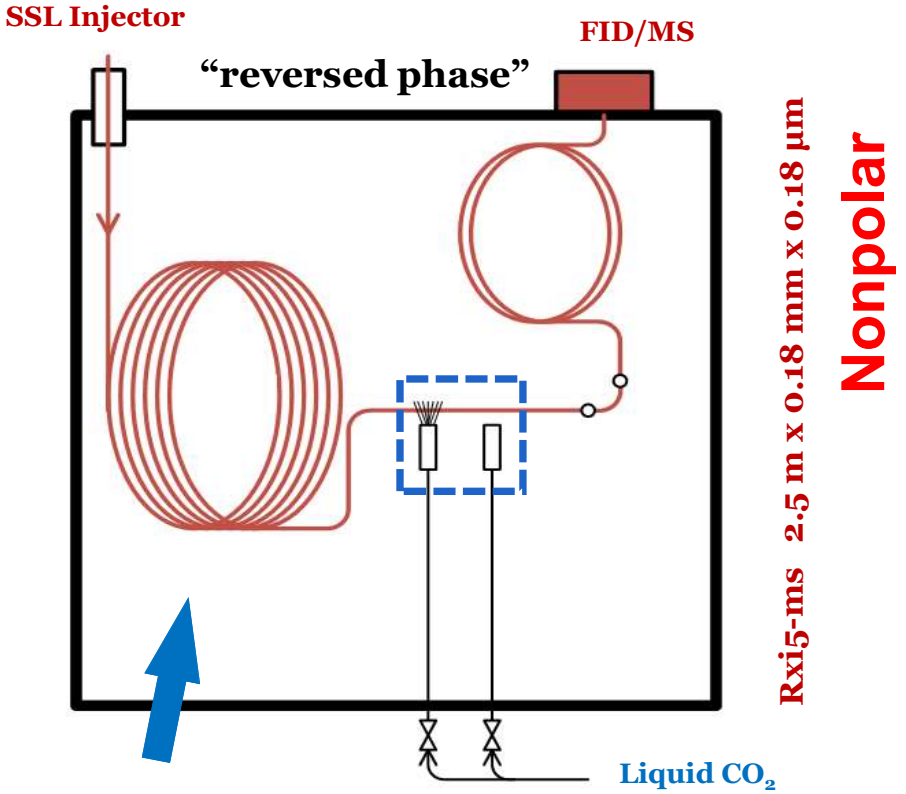
# GC × GC column configuration for Shale Oil Analysis




PONA: 30m x 0.25 mm x 0.25 µm

**Nonpolar**




1. Stabilwax; 60 m x 0.25 mm x 0.25 µm (240 °C)
2. MegaWax: 30 m x 0.25 mm x 0.15 µm (300 °C)

**Polar**

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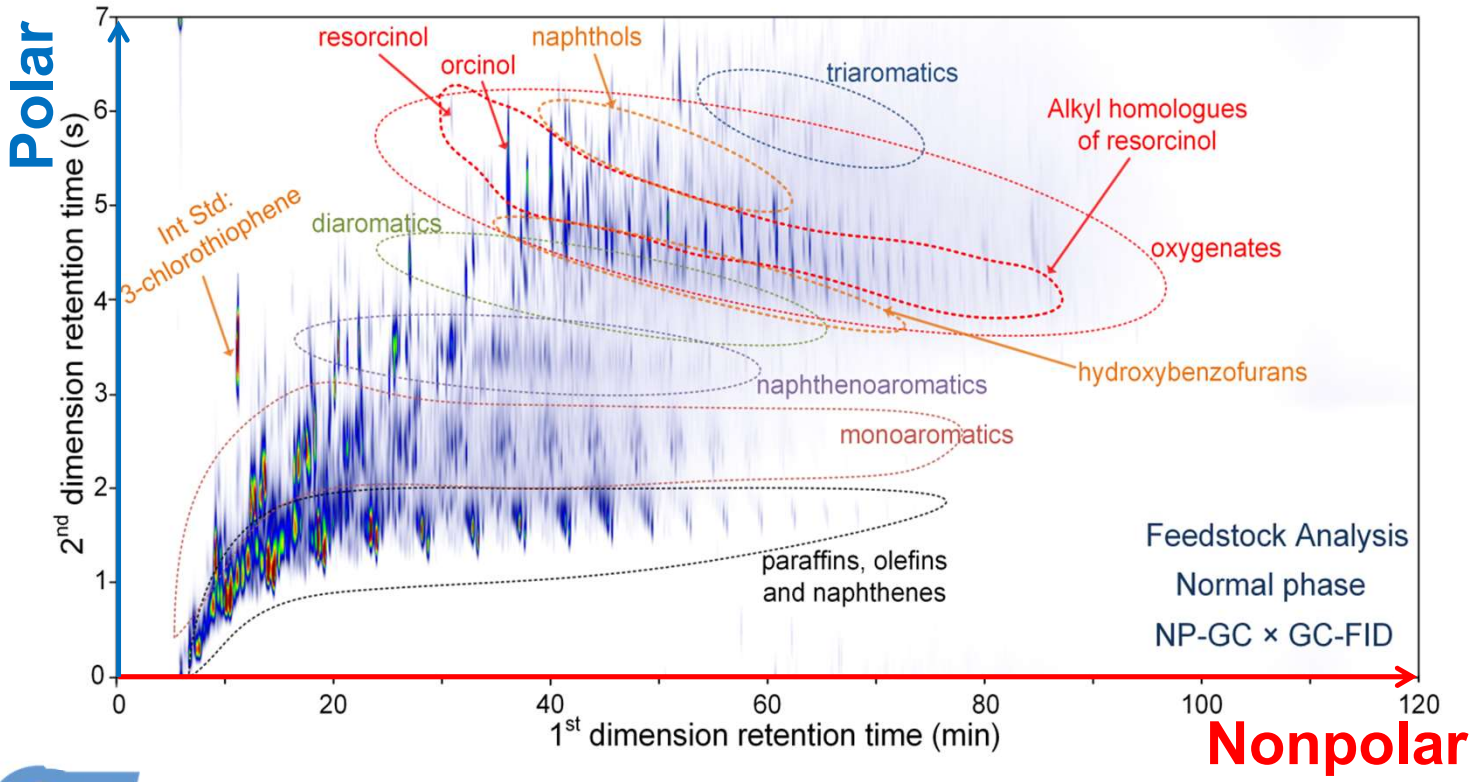
# Shale Oil: NP-GC × GC –FID/TOF-MS

**Estonian Pyrolysis Shale Oil (~ 6 wt% of Oxygen)**

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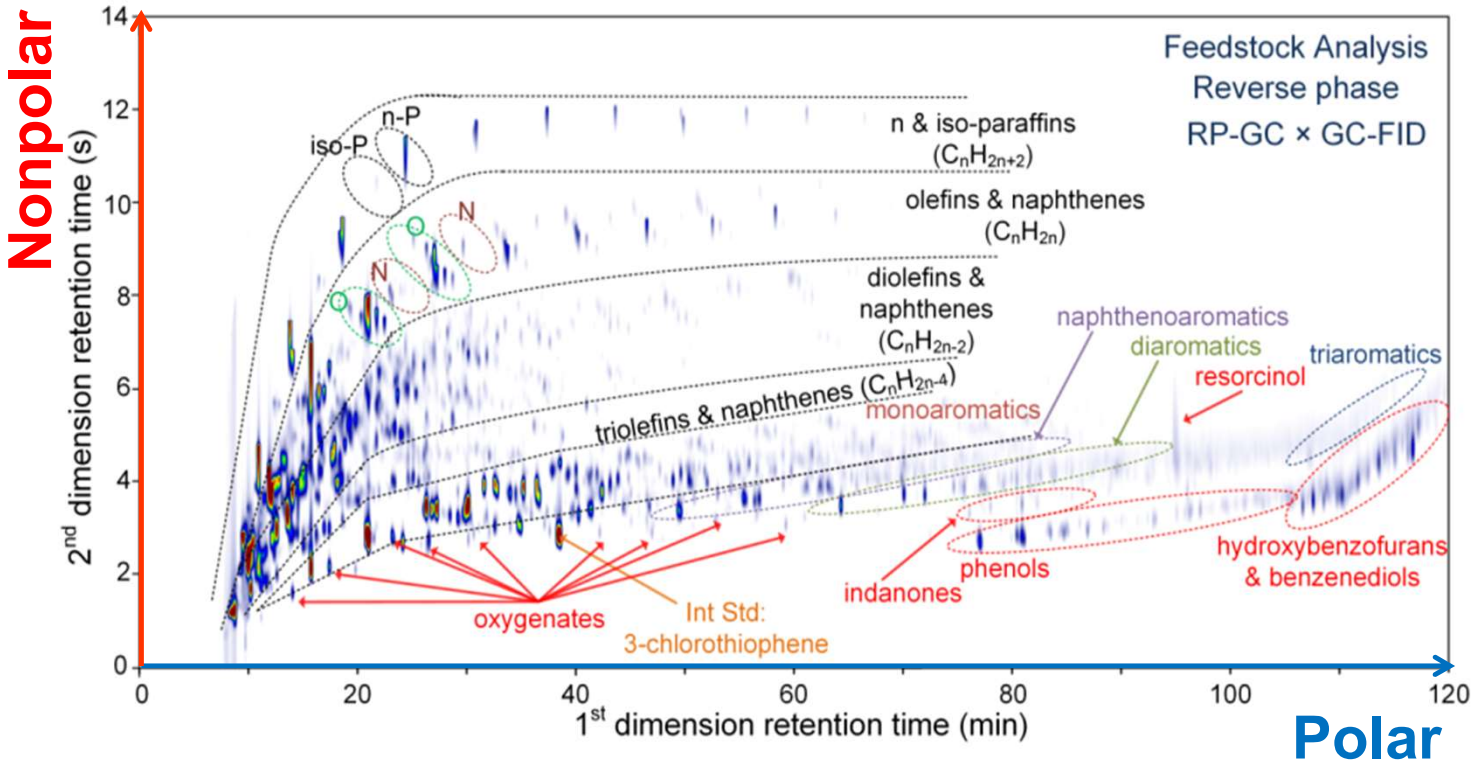
Ristic et al., Fuel Processing Technology, 2017

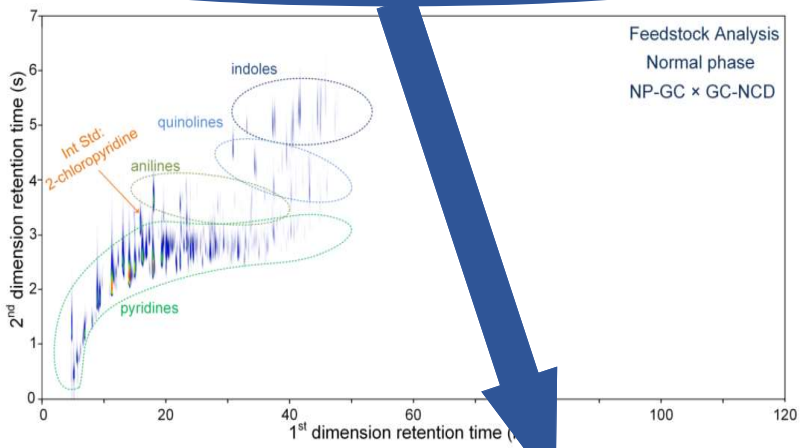
# Shale Oil: RP-GC × GC –FID



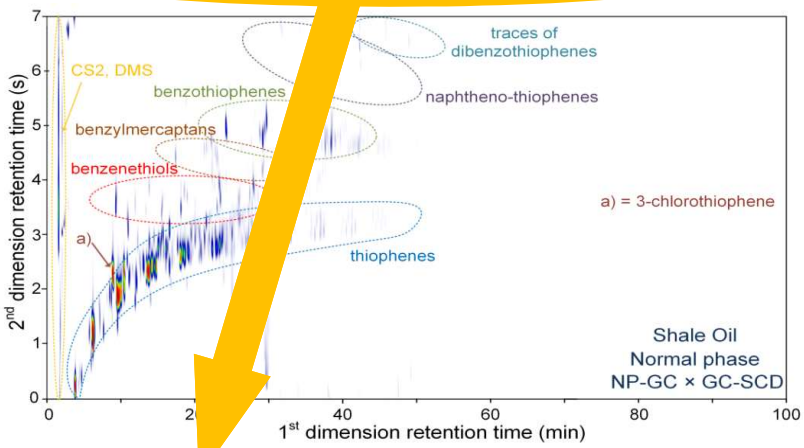

Ristic et al., Fuel Processing Technology, 2017

# Shale Oil: NP-GC × GC –NCD/SCD

**NP-GC × GC –NCD**




**NP-GC × GC –SCD**




| Nitrogen containing chemical classes | Sulfur containing chemical classes |
|---|---|
| Pyridines | Thiols/Sulfides |
| Anilines | Thiophenes |
| Quinolines | Benzenethiols |
| Indoles | Benzylmercaptans |
| | Benzothiophenes |
| | Naphthenobenzothiophenes |
| | Dibenzothiophenes |

Measured **elemental nitrogen** using:
**NP-GC × GC –NCD**
is **0.03 wt.%**
**EA is 0.03 wt.%**

Measured **elemental sulfur** using:
**NP-GC × GC –SCD**
is **0.68 wt.%**
**EA is 0.7 wt.%**

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# Macroscopic Properties

CHNS-O
Elemental Analysis

- ✓ ASTM D5291
- ✓ ASTM D5622
- ✓ Total sulfur using FPD

Distillation

- ✓ ASTM D86
- ✓ ASTM D1160

Density

HPLC

- PIONA
- SARA

Sim Dist

- ✓ ASTM D2887
- ✓ ASTM D7169

Access to: Average MW
$^{1}H$ and $^{13}C$ NMR data …

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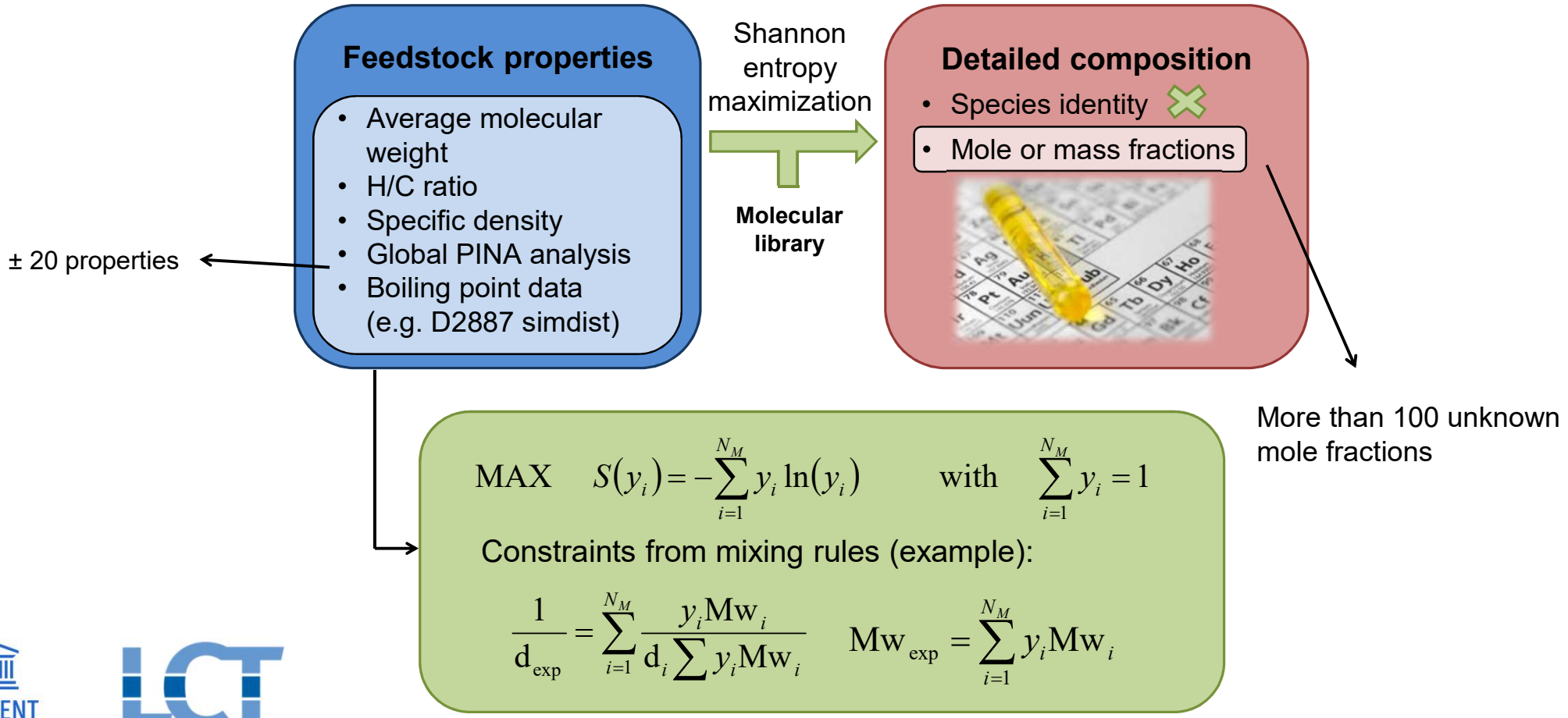
# Shannon entropy maximization

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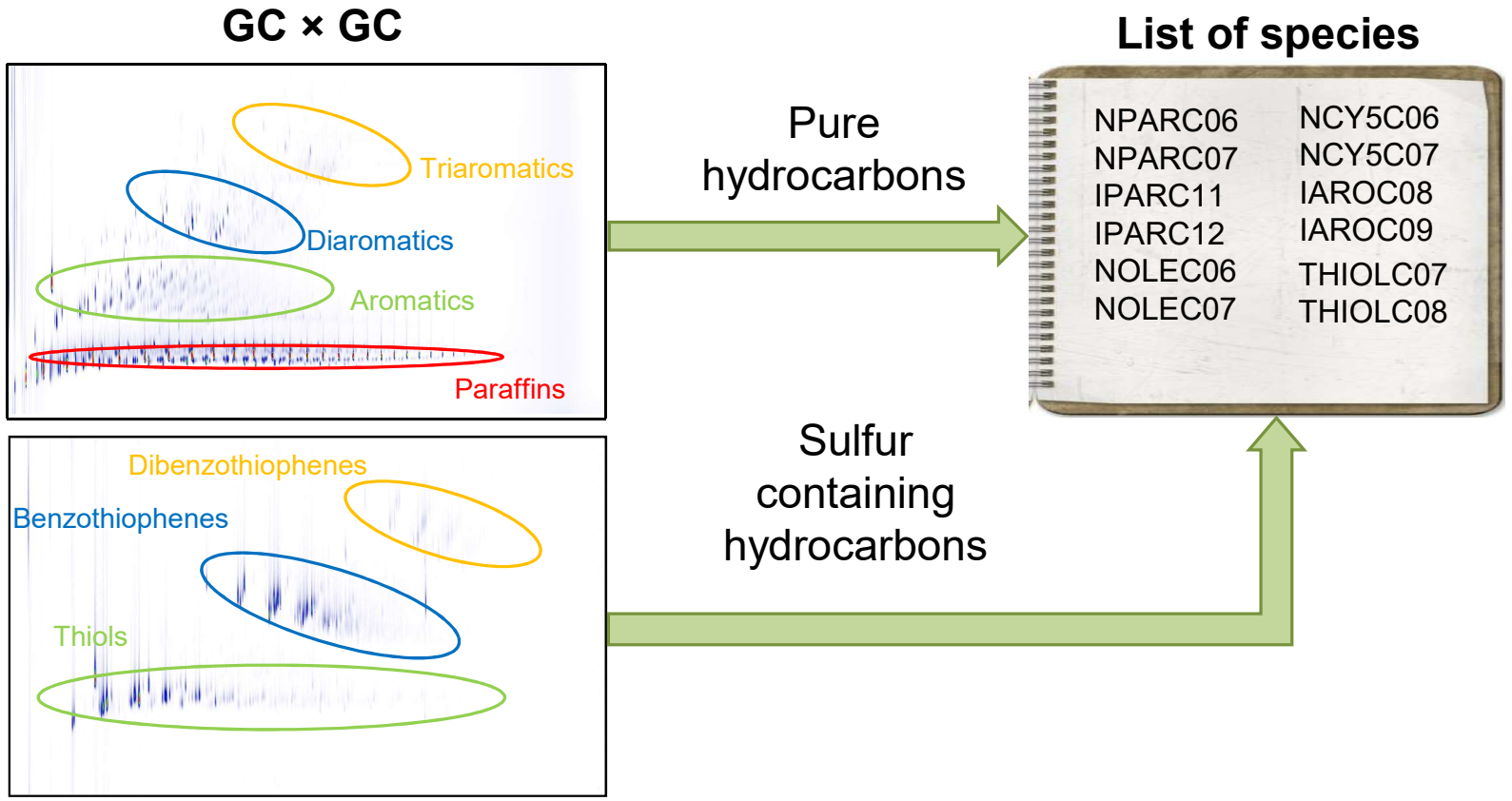
# Molecular library: considered species

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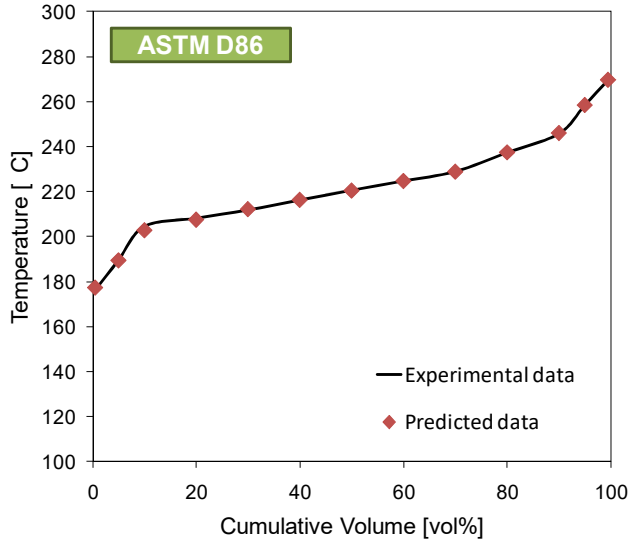
# Example: Middle distillates

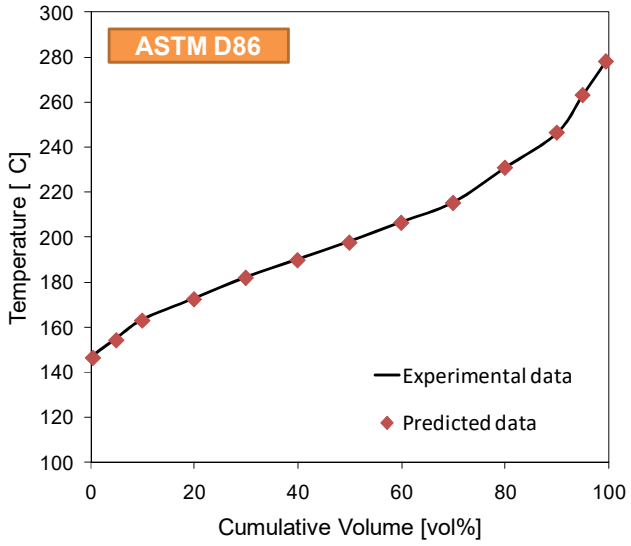
**SAMPLE 1: *Middle East***

| | | INPUT | CALC. |
|---|---|---|---|
| **d** | (g/ml) | 0.7983 | 0.7983 |
| **P** | (wt%) | 23.459 | 23.458 |
| **I** | (wt%) | 25.370 | 25.368 |
| **O** | (wt%) | 0.000 | 0.000 |
| **N** | (wt%) | 34.074 | 34.078 |
| **A** | (wt%) | 17.097 | 17.097 |




**SAMPLE 2: *Brazil***

| | | INPUT | CALC. |
|---|---|---|---|
| **d** | (g/ml) | 0.7987 | 0.7986 |
| **P** | (wt%) | 14.311 | 14.305 |
| **I** | (wt%) | 21.087 | 21.087 |
| **O** | (wt%) | 0.000 | 0.000 |
| **N** | (wt%) | 45.803 | 45.812 |
| **A** | (wt%) | 18.799 | 18.797 |

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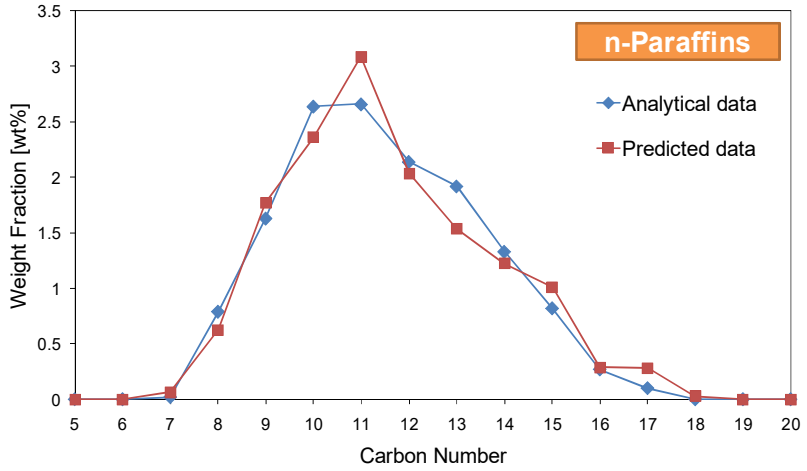
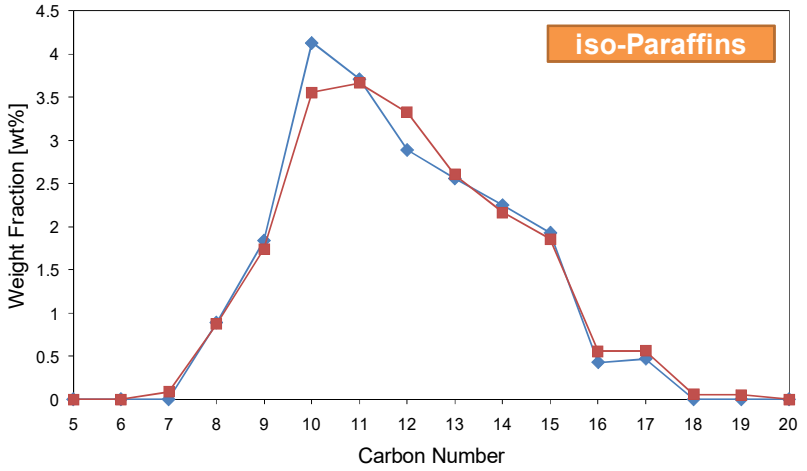
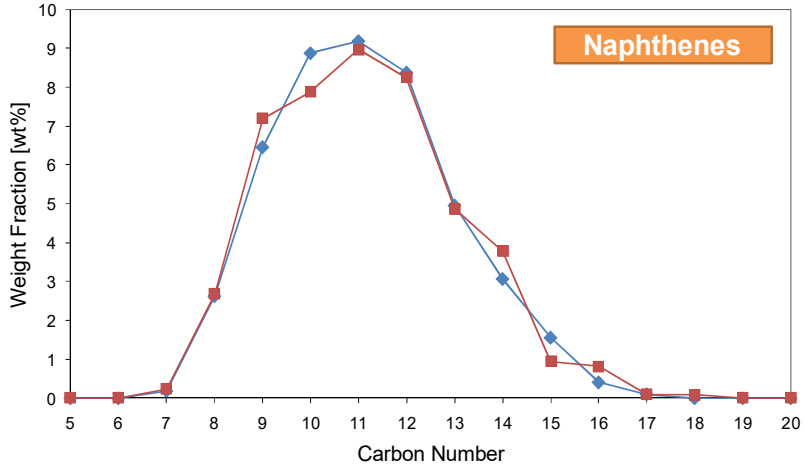
# Example: Middle distillates

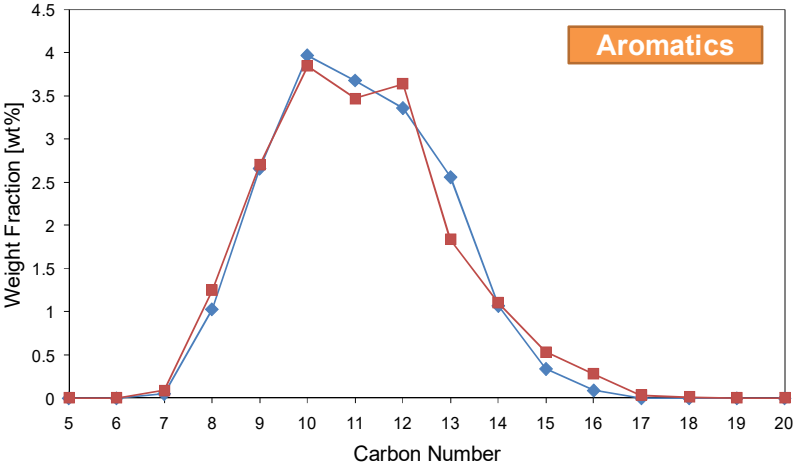
**SAMPLE 2: *Brazil***

**Carbon Number Distribution**

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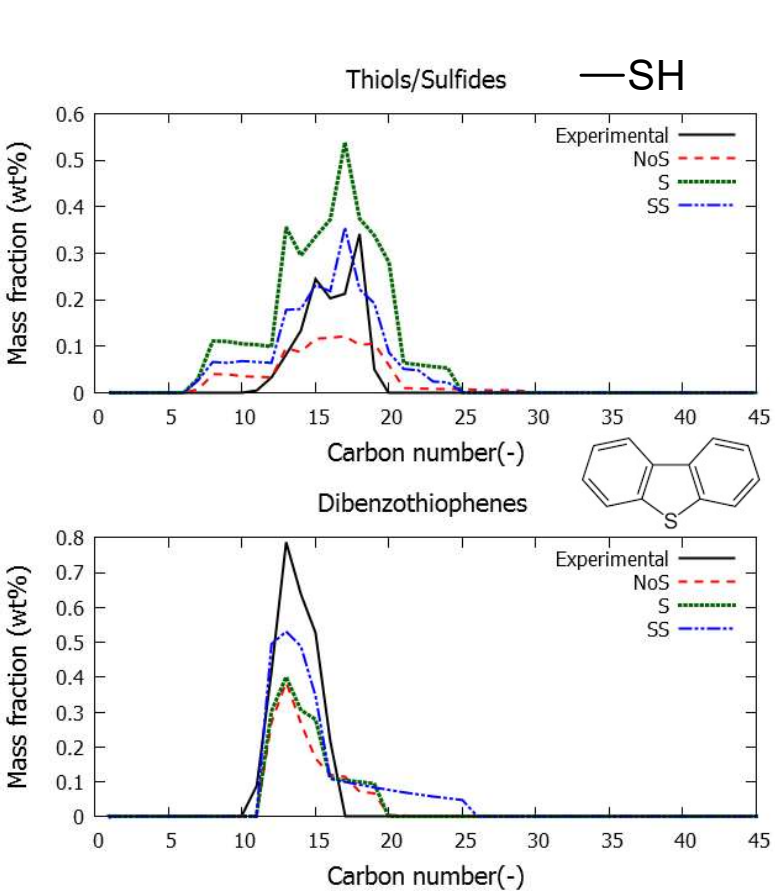
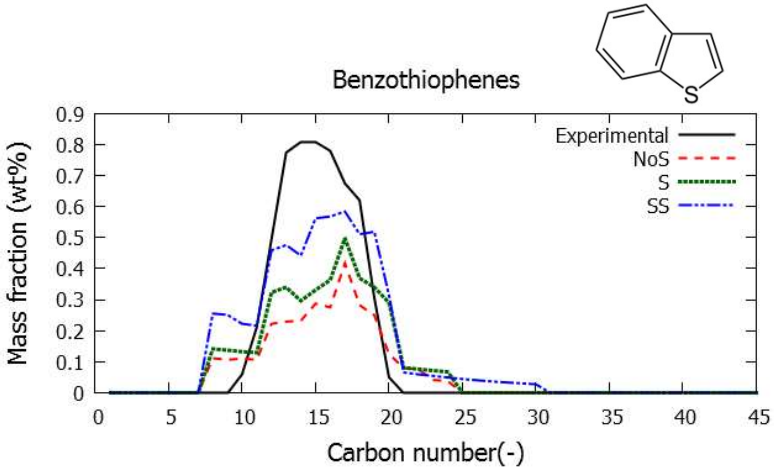
# Example: sulfur containing components

| | Set 1 | Set 2 | Set 3 |
|---|---|---|---|
| **Density** | Yes | Yes | Yes |
| **Total Sulfur** | No | Yes | Yes |
| **Aromatic Sulfur** | No | No | Yes |
| **Group Type analysis** | PINA | | |
| **Boiling point curve** | ASTM-D2887 | | |







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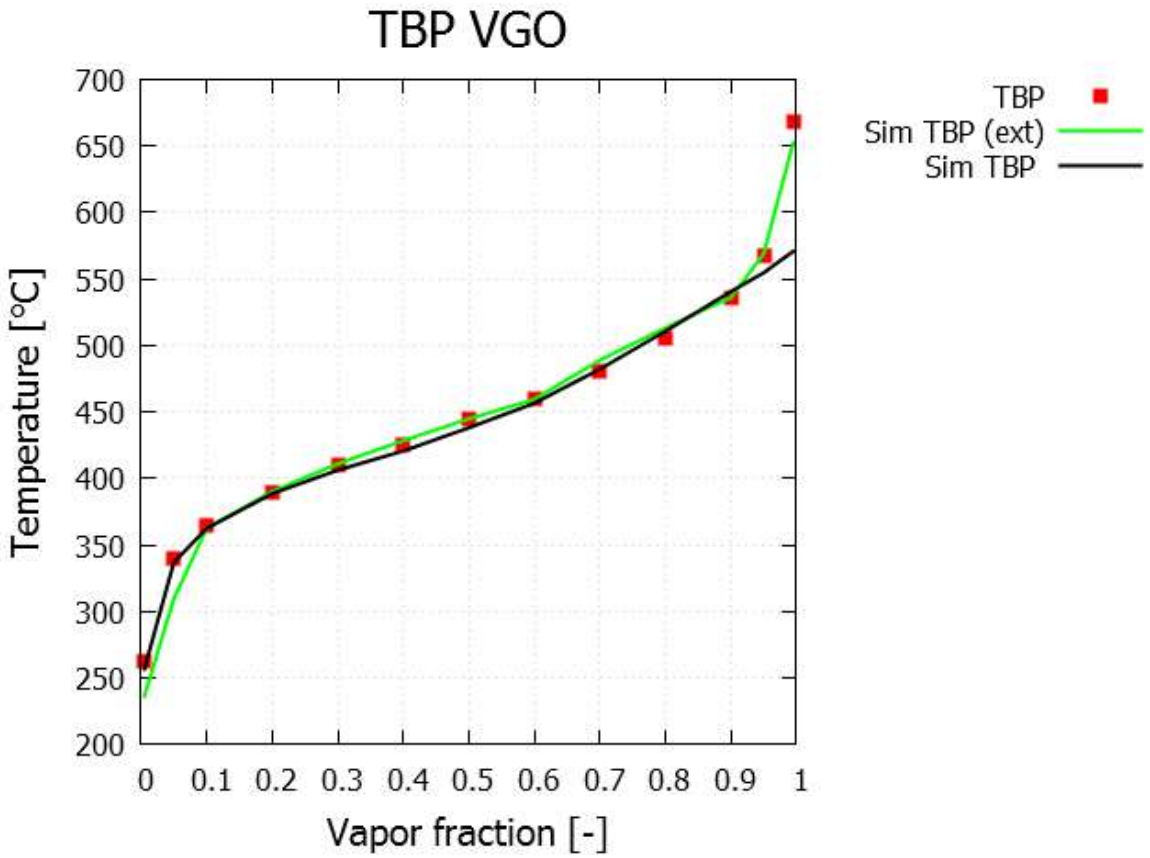
Dijkmans T, Djokic MR, Van Geem KM, Marin GB. Comprehensive compositional analysis of sulfur and nitrogen containing compounds in shale oil using GC × GC – FID/SCD/NCD/TOF-MS. Fuel. 1/15/ 2015;140:398-406.

# Example: Vacuum Gas Oil (VGO)

Molecular library extended from $C_{33}$ to $C_{60}$

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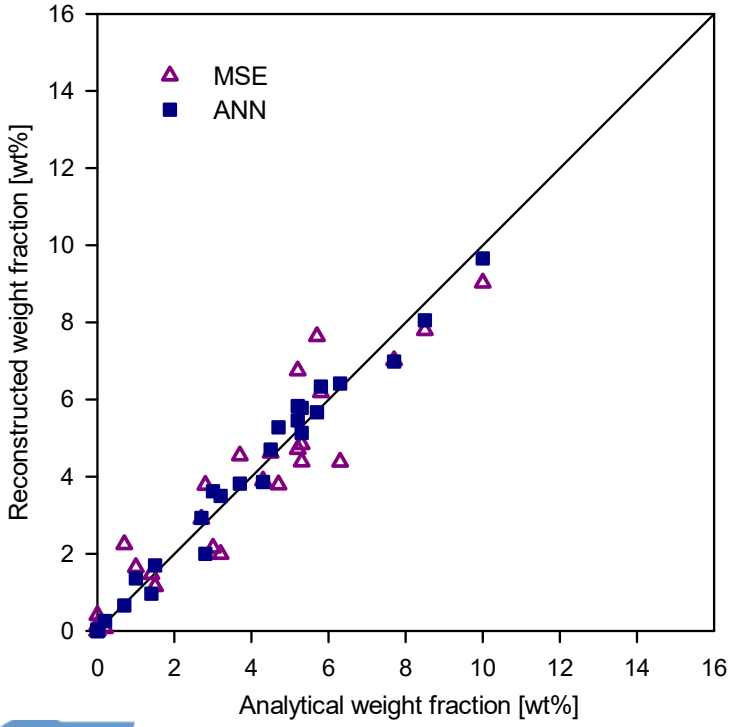
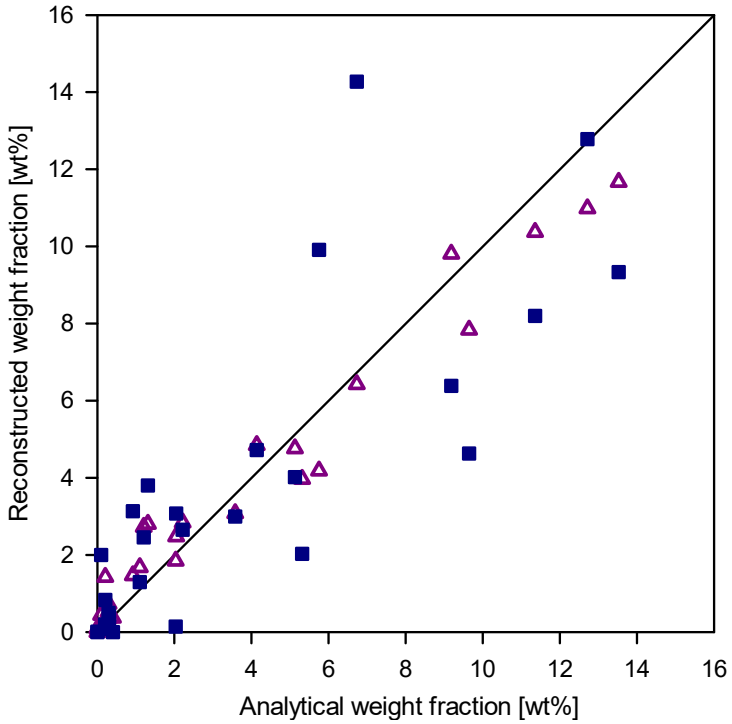
# Example: naphtha

**Naphtha A – in range of ANN training set**




**Naphtha B – out of range of ANN training set**

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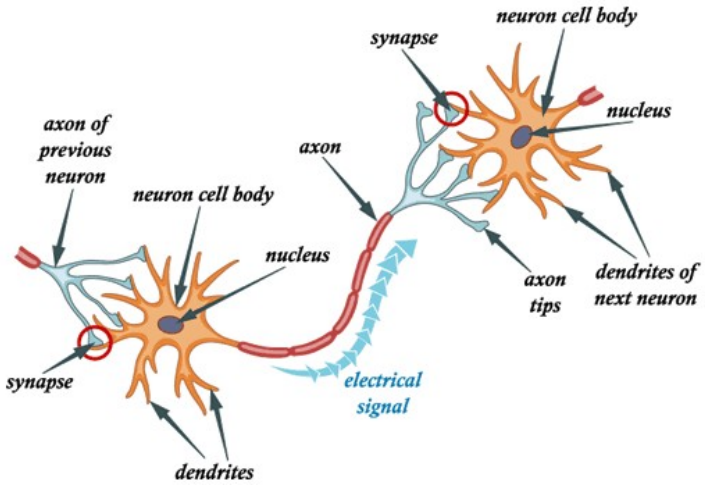
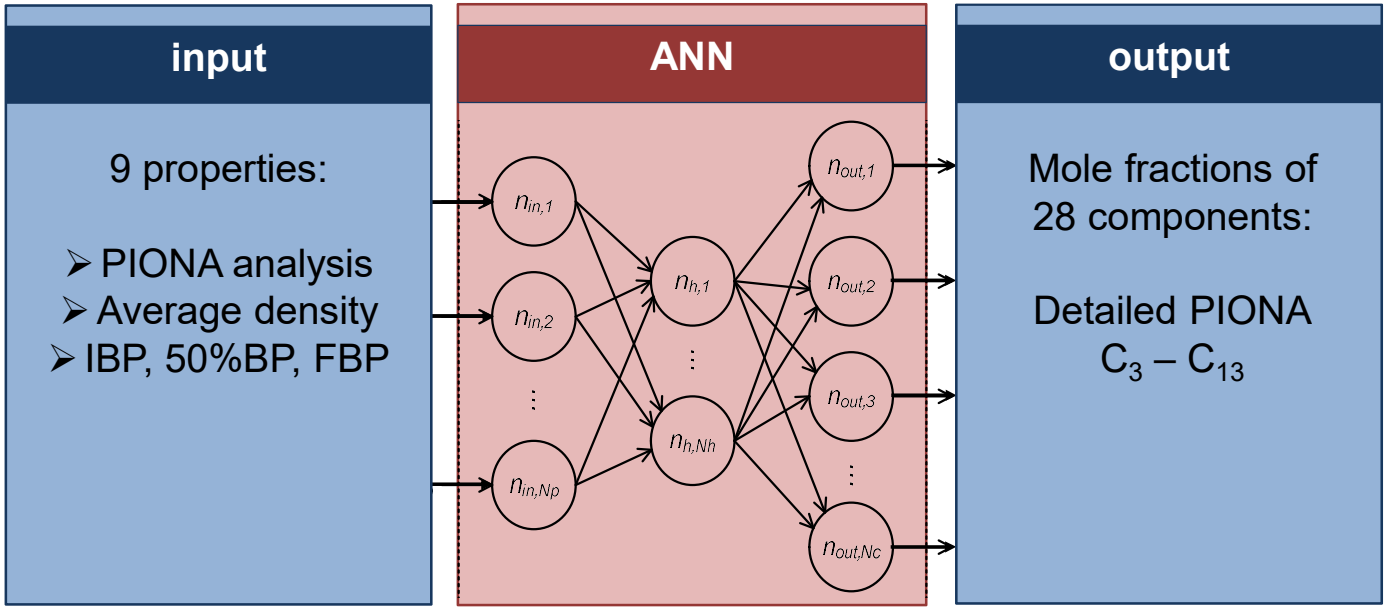
# Artificial neural network (ANN): e.g. naphtha




ANN = nodes + weighted links

Weights and activation functions from **training data set**

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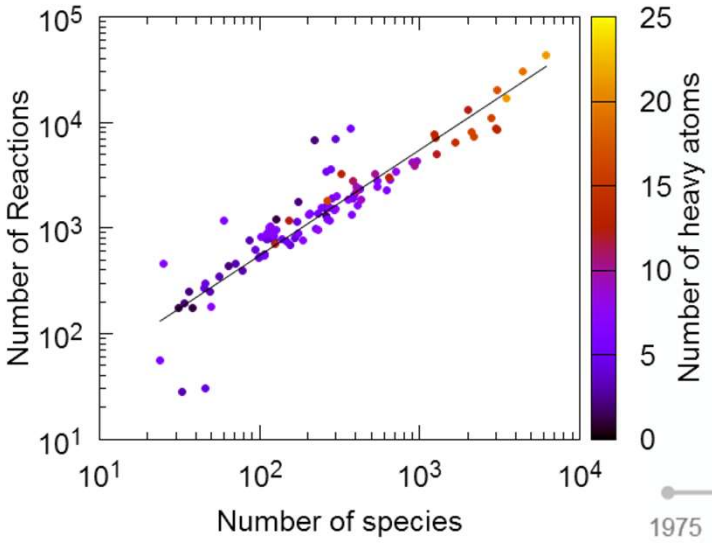
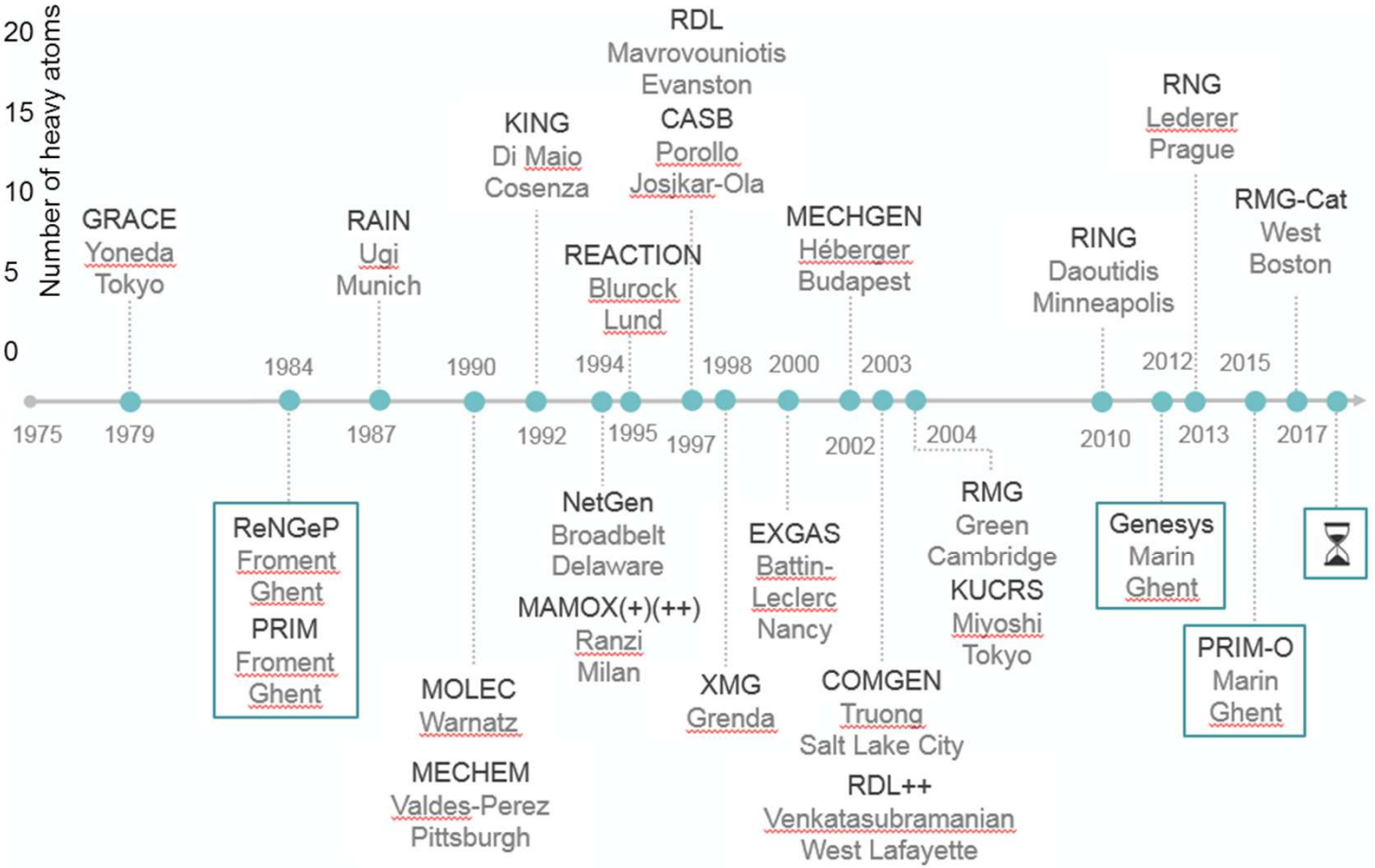
# Outline

- Introduction
- Complex feedstocks: ideal hydroconversion
- Feedstock characterization and reconstruction
- Reaction-network generation
- Complex chemistry: parameter determination
- Reactor design
- Conclusions

# Network generation

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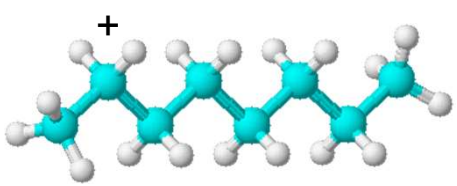
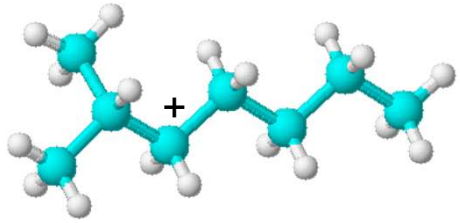
# RENGEP: Matrix operations





| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| 1 | | 1 | | | | | | |
| 2 | 1 | | 1 | | | | | |
| 3 | | 1 | | 1 | | | | |
| 4 | | | 1 | | 1 | | | |
| 5 | | | | 1 | | 1 | | |
| 6 | | | | | 1 | | 1 | |
| 7 | | | | | | 1 | | 1 |
| 8 | | | | | | | 1 | |
| | 2 | | | | | | | |
| | 1 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |
| | 26 | 26 | 26 | 26 | 26 | 26 | 26 | 26 |

+2

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| 1 | | 1 | | | | | | |
| 2 | 1 | | 1 | | | | | 1 |
| 3 | | 1 | | 1 | | | | |
| 4 | | | 1 | | 1 | | | |
| 5 | | | | 1 | | 1 | | |
| 6 | | | | | 1 | | 1 | |
| 7 | | | | | | 1 | | |
| 8 | | 1 | | | | | | |
| | 4 | | | | | | | |
| | 1 | 3 | 2 | 2 | 2 | 2 | 1 | 1 |
| | 26 | 26 | 26 | 26 | 26 | 26 | 26 | 26 |

+2

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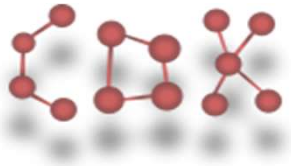
Clymans P.J., Froment G.F., *Comput Chem. Eng.* 1984, 8, 137-142

# GENESYS : GENEration of reacting SYStems

CDK

OpenBabel

- Computer sciences, chemistry and mathematics
- Open source projects
- Advanced species representation
- Advanced algorithms
  - Substructure matching
  - Transition state identification
  - 3D representation
    - Chirality

Vandewiele, N.M. et al., Chem. Eng. J., 207-208, 526-538, 2012
Van de Vijver, R. et al. Int. J. Chem. Kinet., 47 (4), 199-231, 2015
Vandewiele, N.M. et al., J. Comput. Chem., 36 (3), 181-192, 2015
Van de Vijver, R. et al., “Automatic kinetic model generation for heterogeneous catalysis”, ISCRE 2018

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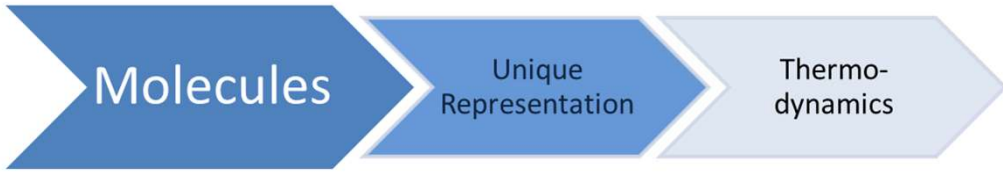
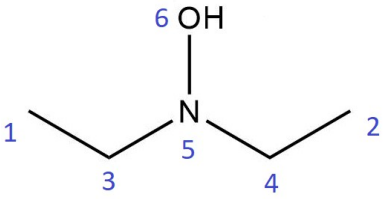
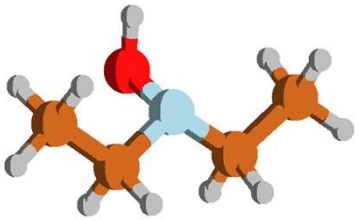
# Molecules



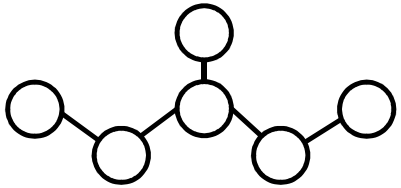

**Structural formula**



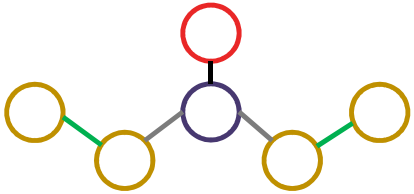

**3D structure**



**Graph structure**



**Weighted graph structure**



- Molecular identifiers
  - SMILES:
    CCN(O)CC
  - InChI:
    InChI=1S/C4H11NO/c1-3-5(6)4-2/h6H,3-4H2,1-2H3
- Graph Theory

"Kinetics of Chemical Reactions : Decoding Complexity"
G.B. Marin,G.S. Yablonsky, D. Constales Wiley-VCH Verlag, 2nd edition, 2018

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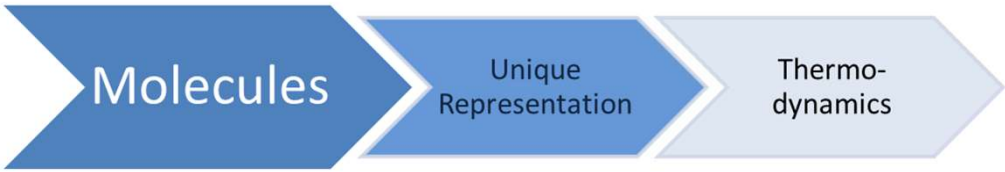
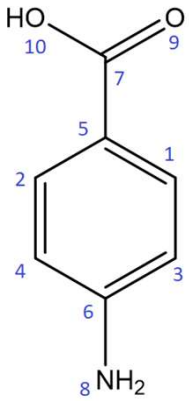
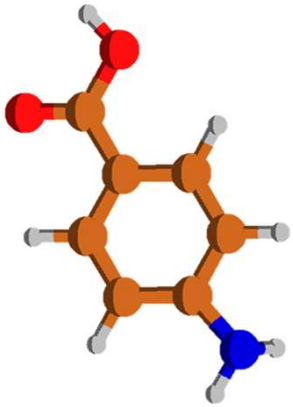
# Molecules



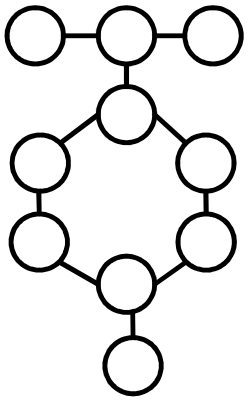

**Structural formula**

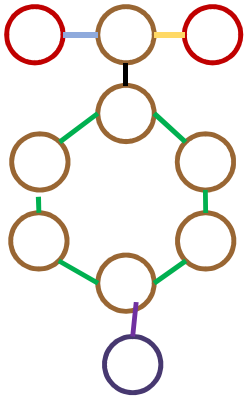



**3D structure**



**Graph structure**





**Weighted graph structure**

- Molecular identifiers
  - SMILES:
    NC1=CC=C(C(O)=O)C=C1
  - InChI:
    InChI=1S/C7H7NO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,8H2,(H,9,10)

- Graph Theory

"Kinetics of Chemical Reactions : Decoding Complexity"
G.B. Marin,G.S. Yablonsky, D. Constales Wiley-VCH Verlag, 2nd edition, 2018

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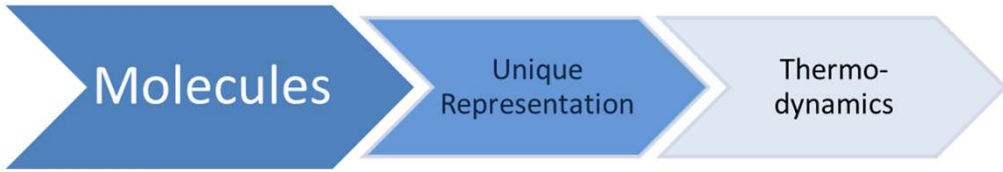
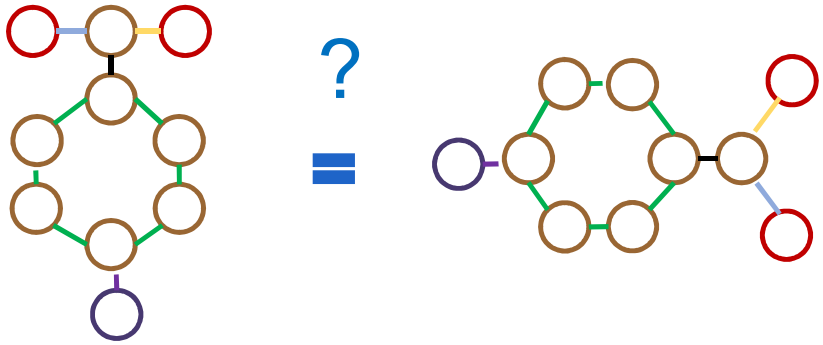
Vandewiele, N.M. et al., Chem. Eng. J., 207-208, 526-538, 2012
Van de Vijver, R. et al. Int. J. Chem. Kinet., 47 (4), 199-231, 2015
Vandewiele, N.M. et al., J. Comput. Chem., 36 (3), 181-192, 2015

# Graph theory

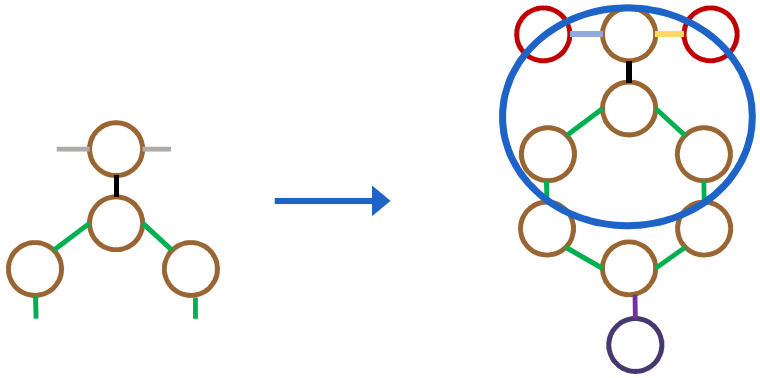



- Graph isomorphism

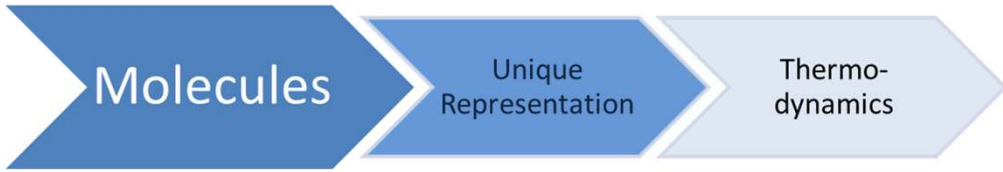


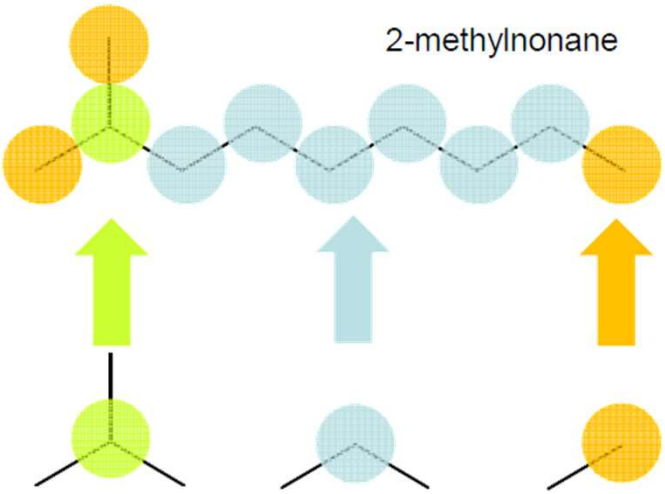

- Subgraph recognition

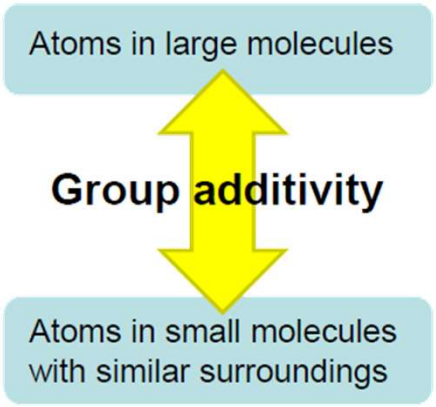
SMARTS c(:c)(:c)-[C;X3]



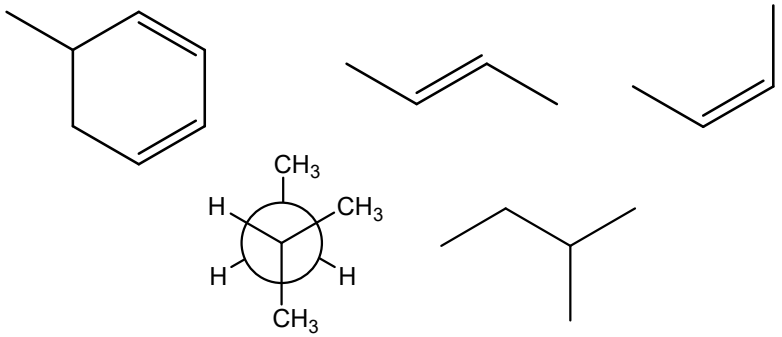
# Group additivity



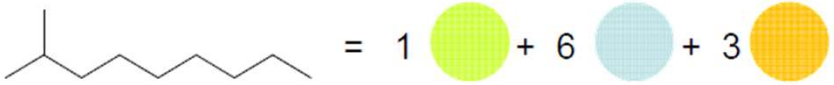




- Ring strain corrections
- Non-nearest neighbor interactions
  - Gauche interactions
  - Trans interactions
- Symmetry contribution




**Group** definition based on surroundings (ligands)

**Additivity:**




$$S = S_{int} - R \ln \sigma$$

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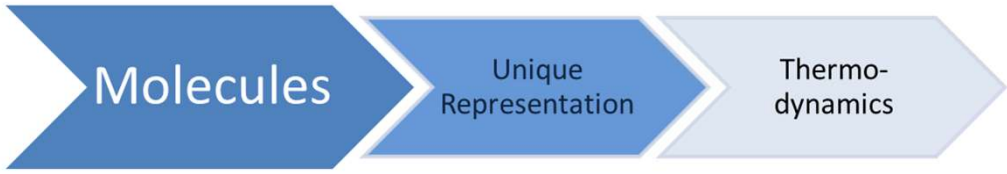
Pappijn, C. et al., “Ab initio group additivity model for the free radical reactions of nitrogen-containing compounds”, ISCRE 2018

# Thermodynamics




- "SpeciesThermo" database
  - Single entry per species
  - Originates from experimental work or high level quantum chemistry calculations
  - Limited in size
  - Database search via isomorphisms or InChI identifiers
- "BensonThermo" database
  - Group additive values
  - Originate from high level quantum chemical calculations (CBS-QB3)
  - Database search via SMARTS

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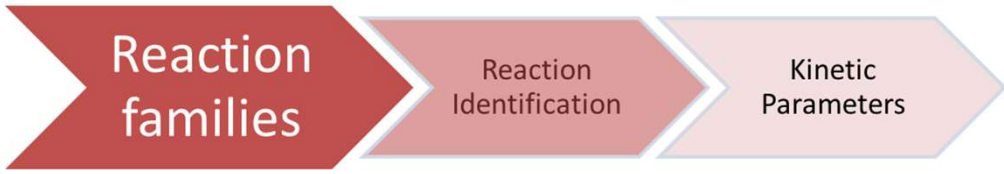
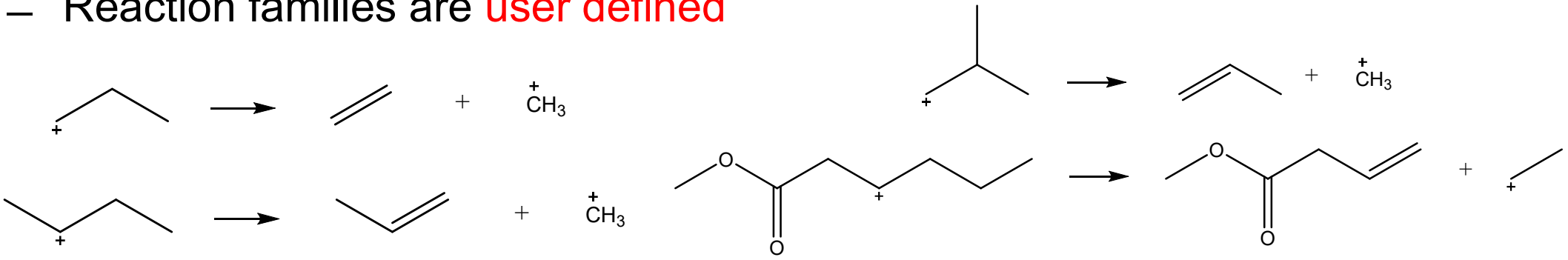
# Reactions




- Thousands of reactions can be classified in only a few reaction families
- All reactions within one reaction family have a very similar change in electronic structures of the atoms
- The reaction is mainly governed by a few atoms rather than the reactants in their entirety
- Reaction families are user defined

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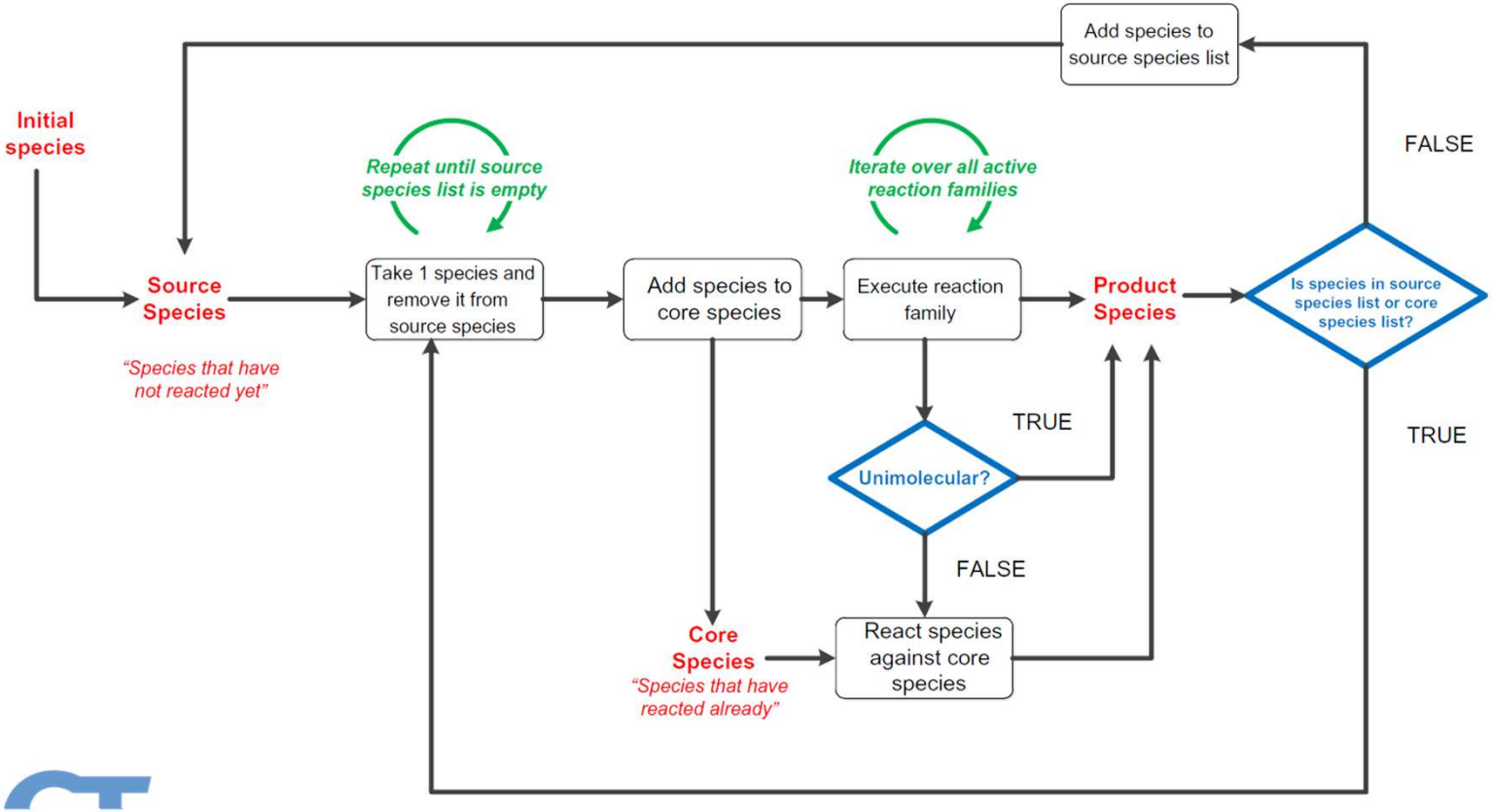
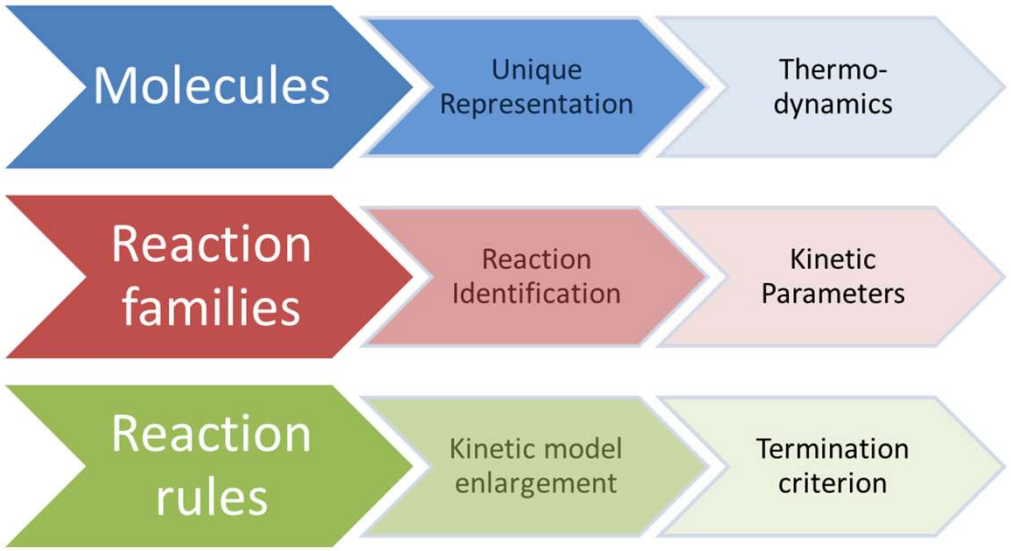
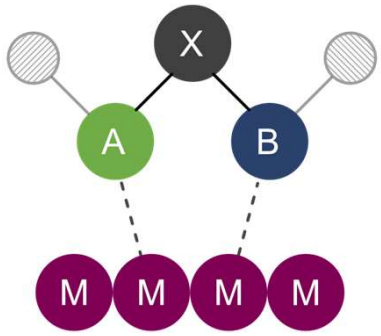
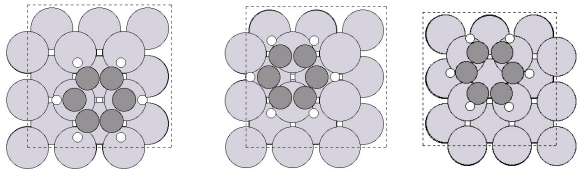
# Network Generation

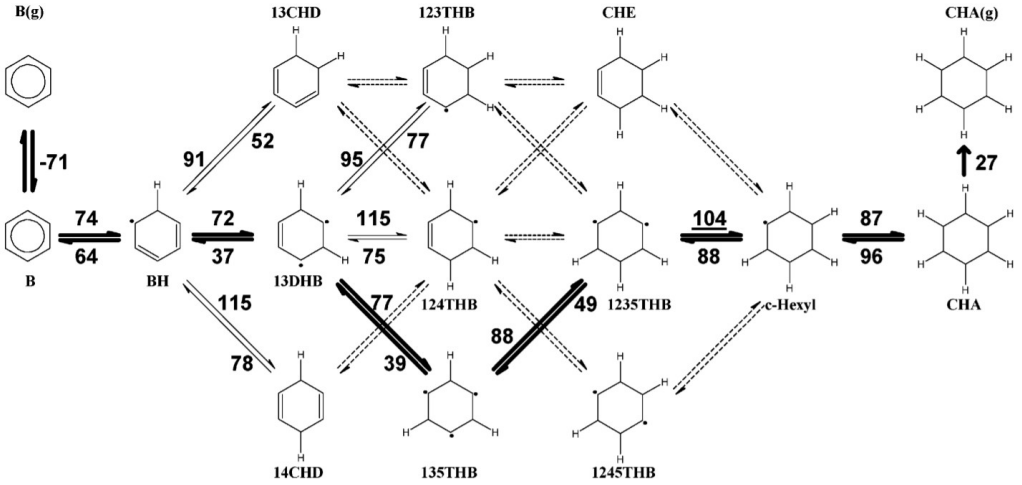



# Genesys: Catalytic Systems



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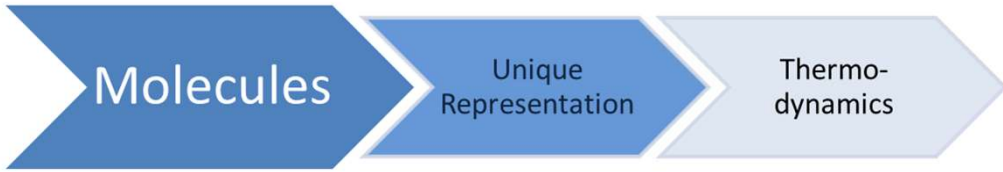
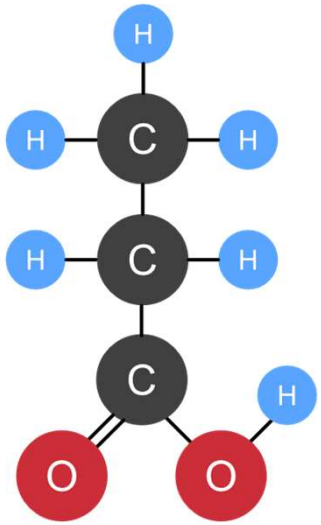
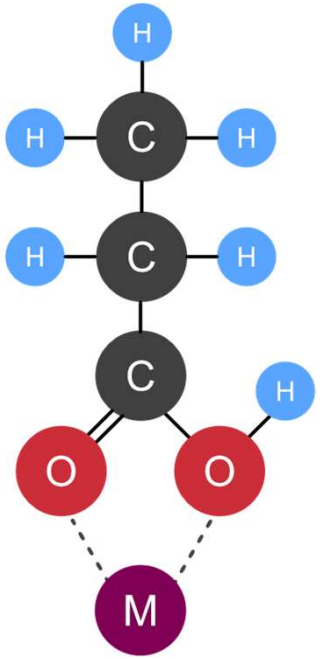
Saeys, M., et al., *The Journal of Physical Chemistry B* **2005,** 109, (6), 2064-2073.

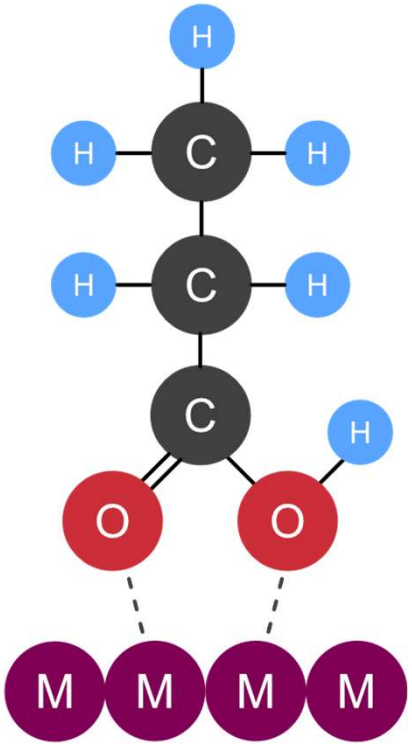
# Molecules: Catalysis




- Dummy atoms for representation of surface
- No specific metal atoms: generation of general mechanism
- Properties of surface in separate input file
- Active site = multiple dummy atoms

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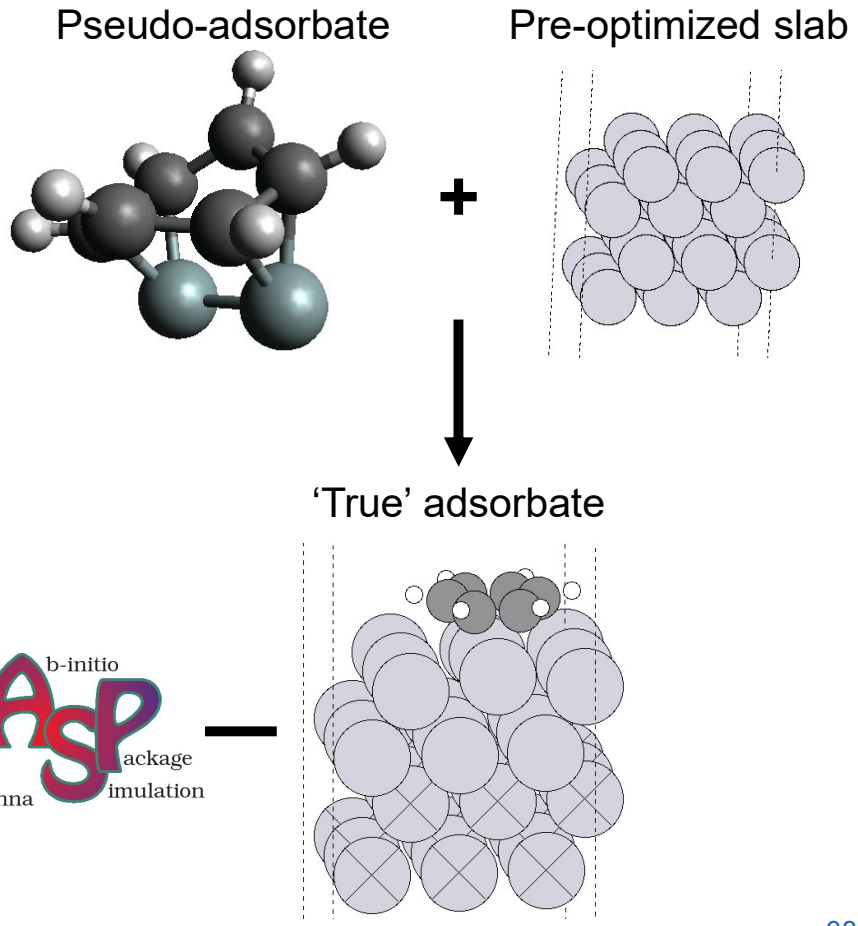
# Reaction Kinetics: catalysis

Reaction families → Reaction Identification → Kinetic Parameters

- Automated Ab-Initio calculations
  - Pre-optimized catalyst geometries
  - Pseudo-adsorbate
  - Combine + re-optimize
- Use obtained reaction (activation) energies to develop fast estimation methods

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# Outline

- Introduction
- Complex feedstocks: ideal hydroconversion
- Feedstock characterization and reconstruction
- Reaction-network generation
- Complex chemistry: parameter determination
- Reactor design
- Conclusions

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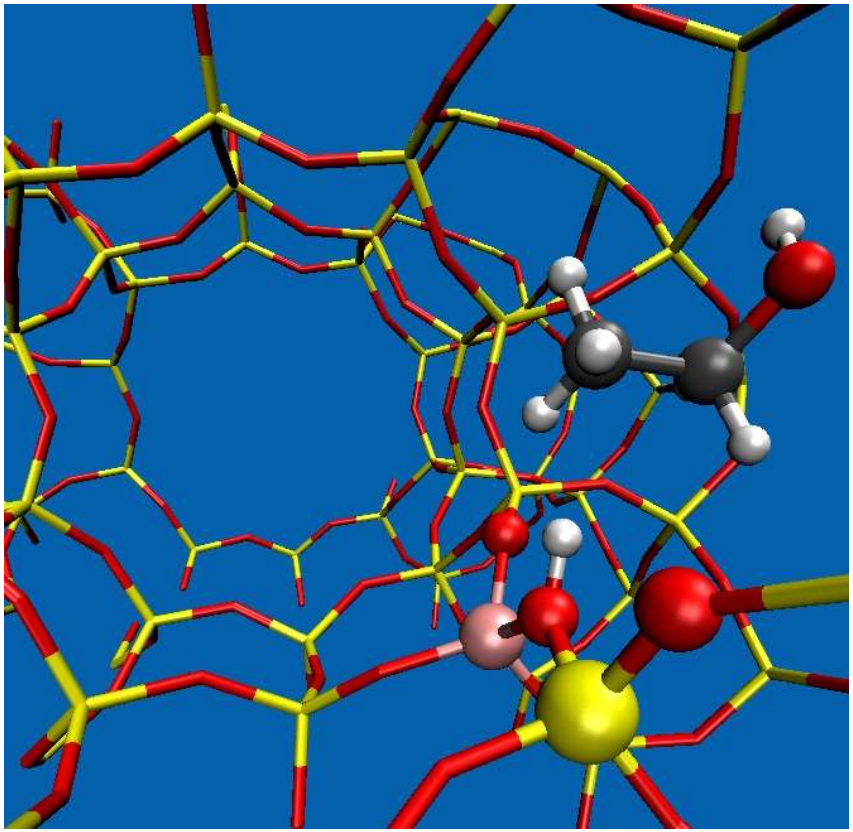
# Alcohol conversion in zeolites: e.g. $C_2H_5OH \rightarrow C_2H_4 + H_2O$

Ethanol physisorption in H-ZSM-5



- van der Waals:
  - dipole-dipole
  - dipole-induced dipole
  - dispersive
- H-bonding
- electrostatic interactions

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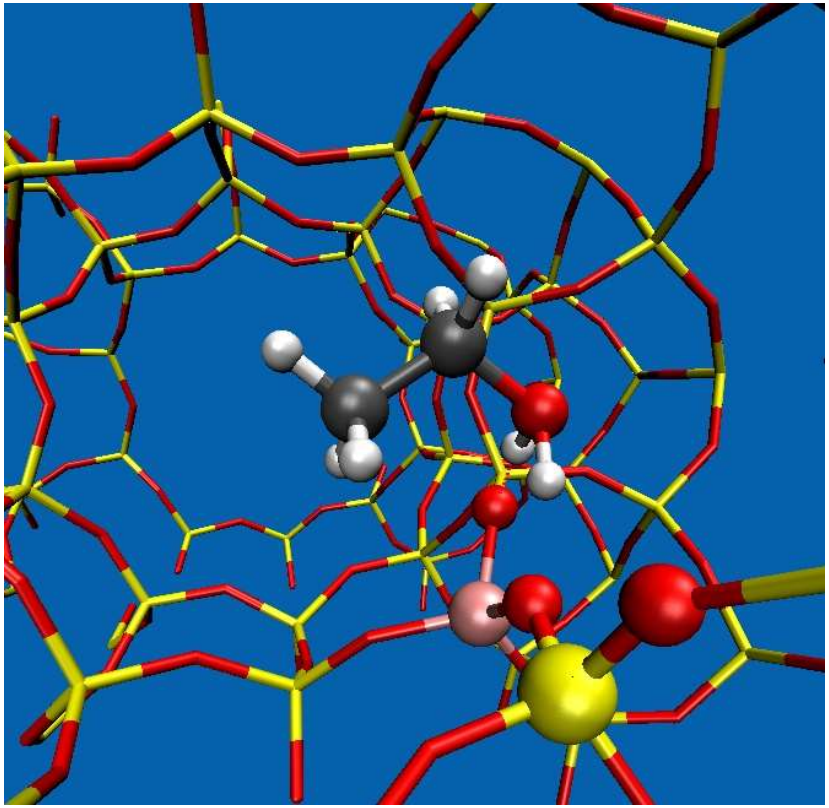
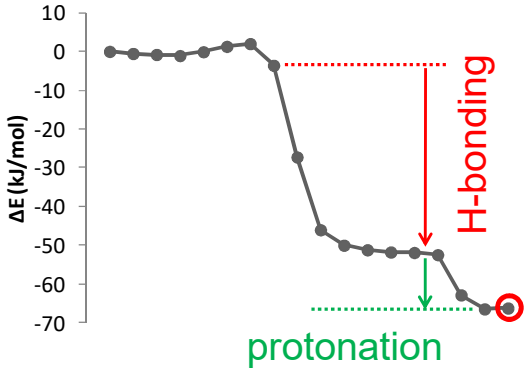
# H-bonding and protonation: chemisorption

Ethanol adsorption and protonation in H-ZSM-5



Nudged Elastic Band calculation with PBE-D2 functional

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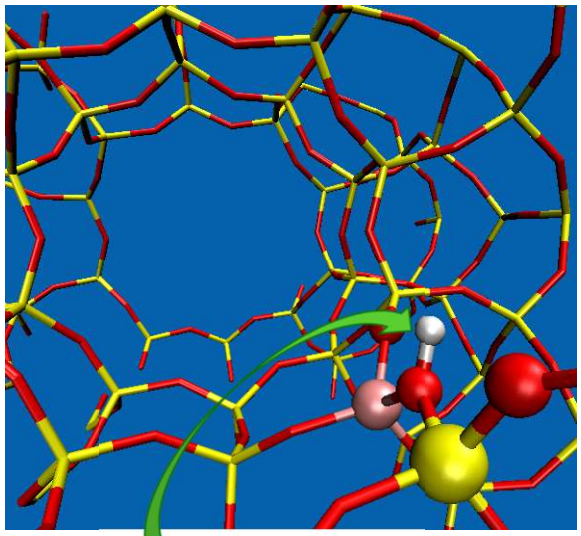
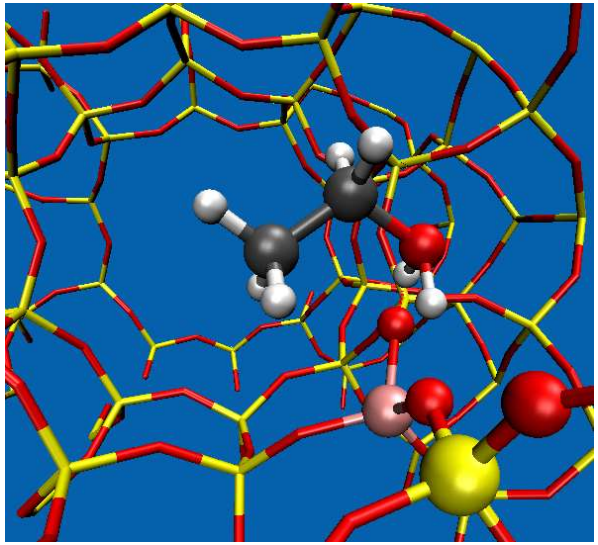
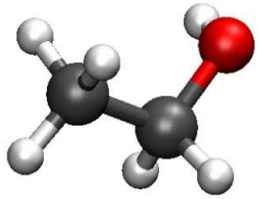
# Alcohol adsorption & reaction in zeolites







$$r = k\,\theta_{ads,alcohol} = k\,K_{ads}\,p_{alcohol}$$

Ab initio calculation of:

$$K_{\text{ads}} = \exp\left(-\frac{\Delta G^0_{ads}}{RT}\right) = \exp\left(-\frac{\Delta H^0_{\text{ads}} - T\Delta S^0_{\text{ads}}}{RT}\right)$$

thermodynamics

$$k = \frac{k_b T}{h}\exp\left(\frac{\Delta S^{0,\#}}{R}\right)\exp\left(-\frac{\Delta H^{0,\#}}{RT}\right) = \frac{k_b T}{h}\exp\left(-\frac{\Delta G^{0,\#}}{RT}\right)$$

kinetics

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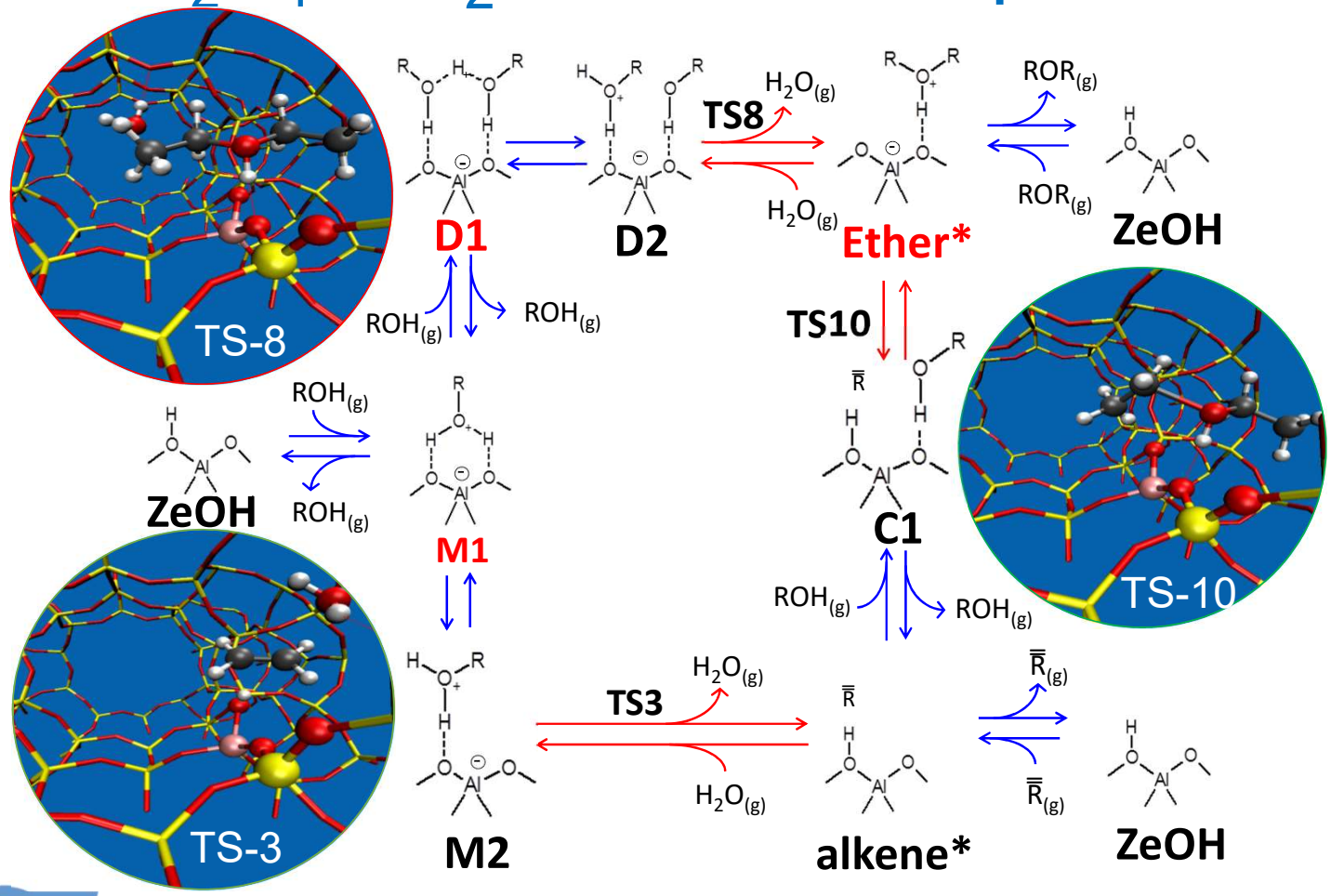
# $C_2H_5OH \rightarrow C_2H_4 + H_2O$ : dominant paths

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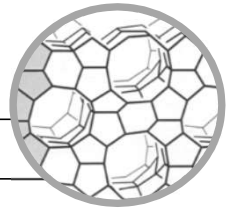
John, M. et al., J. Catal., 330, 28-45, 2015

# Experimental procedures and conditions

HZSM-5



| Properties | | |
|---|---|---|
| Si/Al | 15 | 40 |
| $c_{H+}$(mol kg$^{-1}$) | 0.77 | 0.36 |
| BET ($10^3$ m$^2$ kg$^{-1}$) | 430 | 436 |
| $V_{micro}$($10^{-5}$ m$^3$ kg$^{-1}$) | 1.1 | 1.1 |

| Experimental conditions | |
|---|---|
| Temperature (K) | 453 – 523 |
| $p_{EtOH,in}$ (kPa) | 8 – 50 |
| $W/F_{EtOH,in}$ (kg s mol$^{-1}$) | 1.5 – 17.0 |

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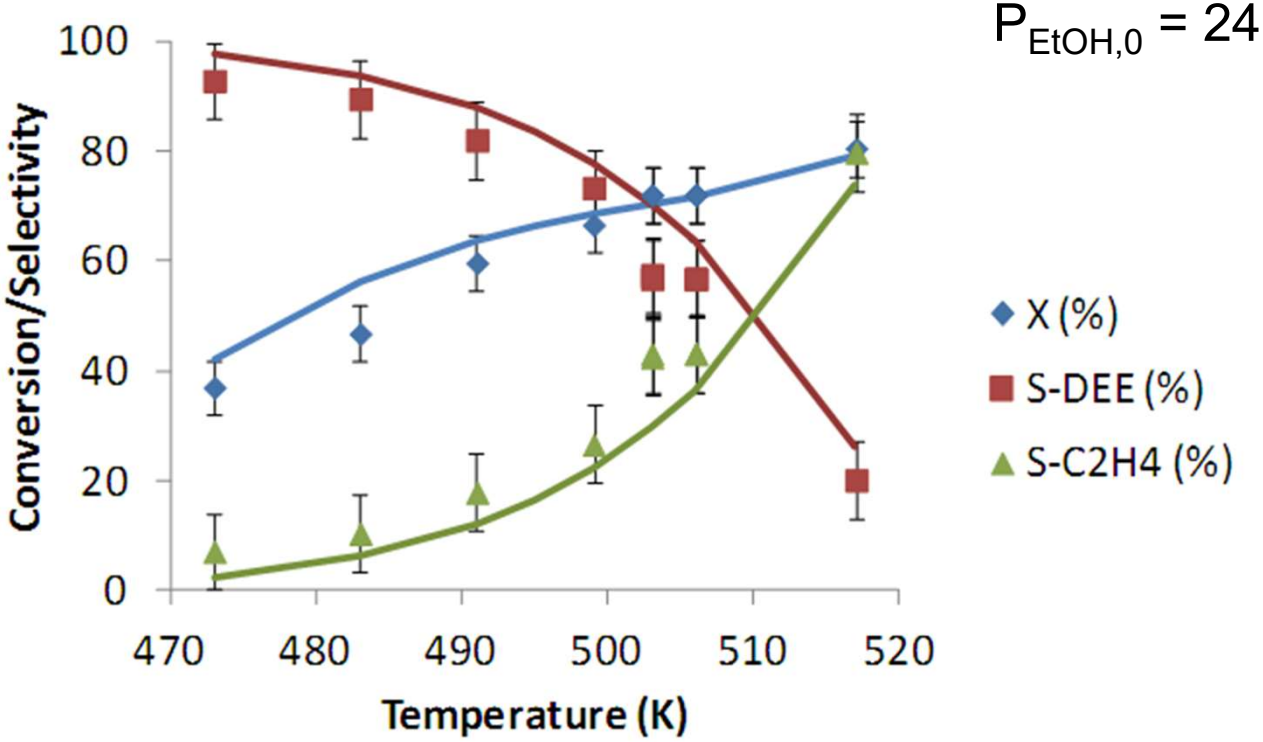
# Conversion and selectivities

HZSM-5

$W_{cat}/F_{EtOH,0}$ = 6.5 kg s / mol

$P_{EtOH,0}$ = 24 kPa

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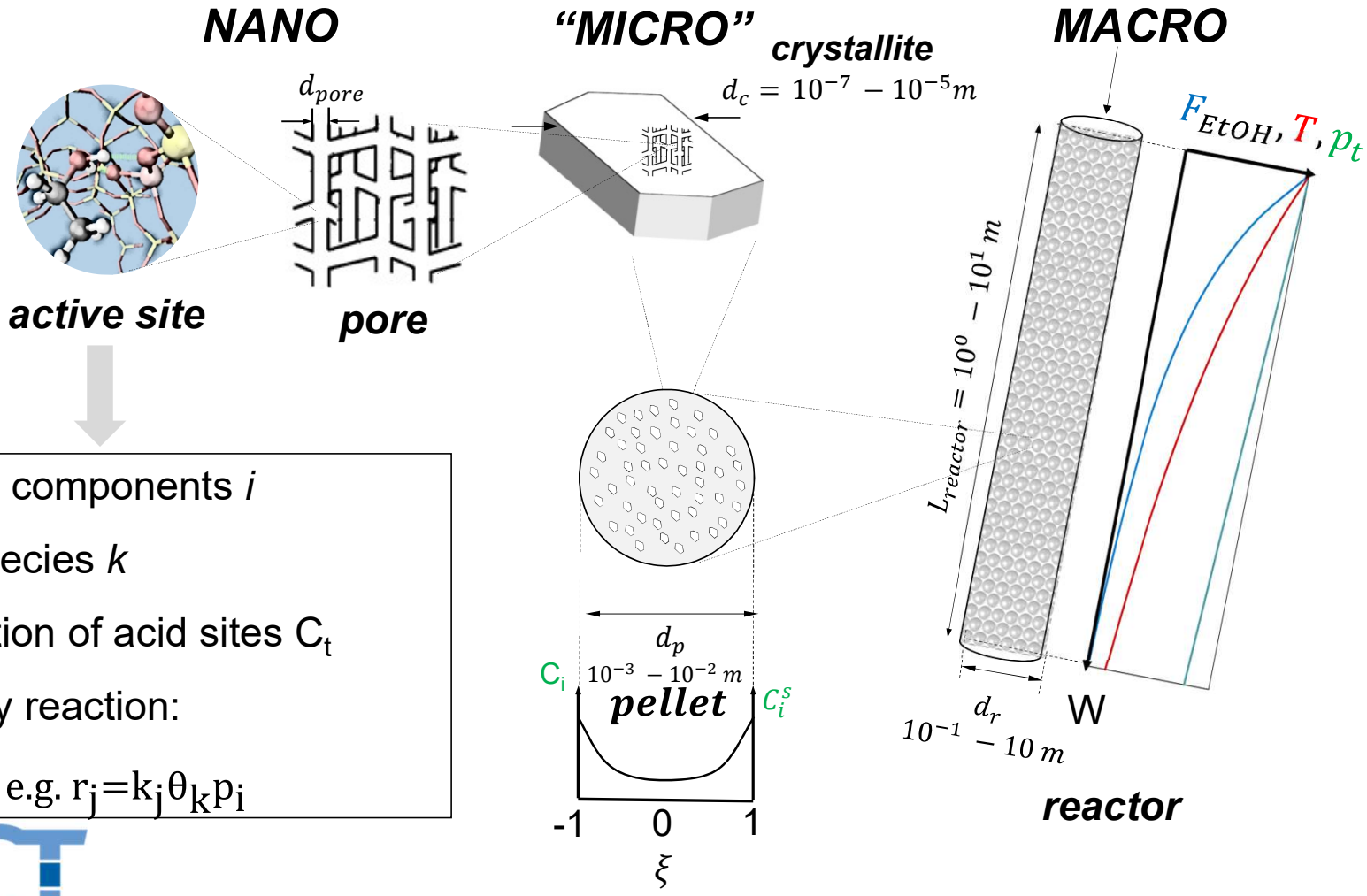
# Outline

- Introduction
- Complex feedstocks: ideal hydroconversion
- Feedstock characterization and reconstruction
- Reaction-network generation
- Complex chemistry: parameter determination
- Reactor design
- Conclusions

# Multiscale modeling of an industrial reactor




gas phase components *i*

surface species *k*

concentration of acid sites $C_t$

elementary reaction:

e.g. $r_j = k_j \theta_k p_i$

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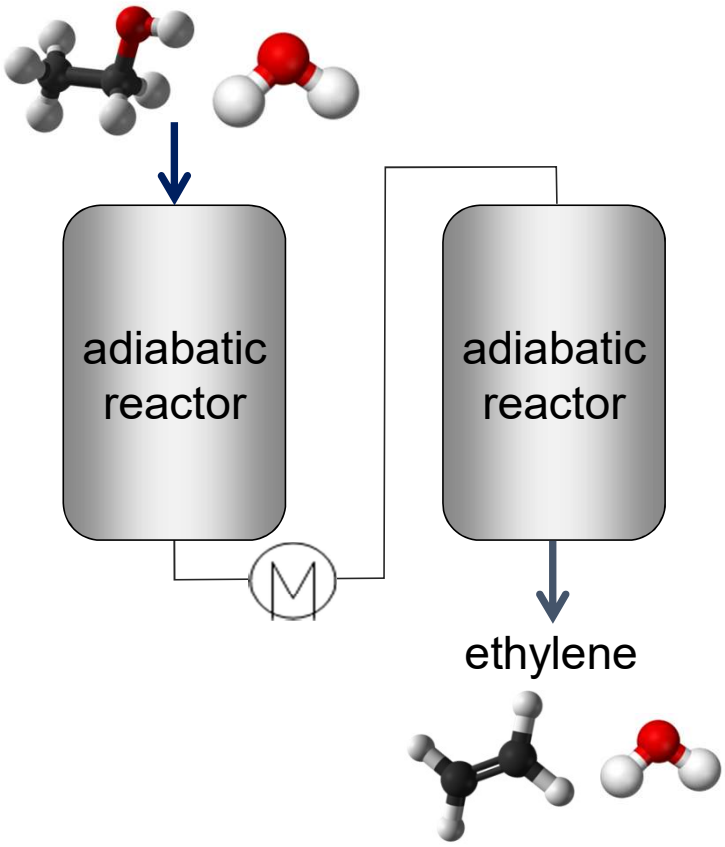
Van der Borght, K. et al., Angew. Chem. Int. Ed., 55(41), 12817-12821, 2016

# Industrial dehydration reactor

bio-ethanol (aqueous ethanol solution)




| Design specifications[1] | |
|---|---|
| $T^0$ (K) | 673 |
| $P^0$ (kPa) | 590 |
| Ethylene production (kT $y^{-1}$) | 220 |
| Ethanol content (wt.%) | 26 |
| HZSM-5 mass (ton) | 6 |

$C_2H_5OH \rightarrow C_2H_4 + H_2O$ $\quad \Delta H = 46\ kJ/mol_{EtOH}$

$2\ C_2H_5OH \rightarrow (C_2H_5)_2O + H_2O$ $\quad \Delta H = -12\ kJ/mol_{EtOH}$

$(C_2H_5)_2O \rightarrow C_2H_4 + C_2H_5OH$ $\quad \Delta H = 70\ kJ/mol_{EtOH}$

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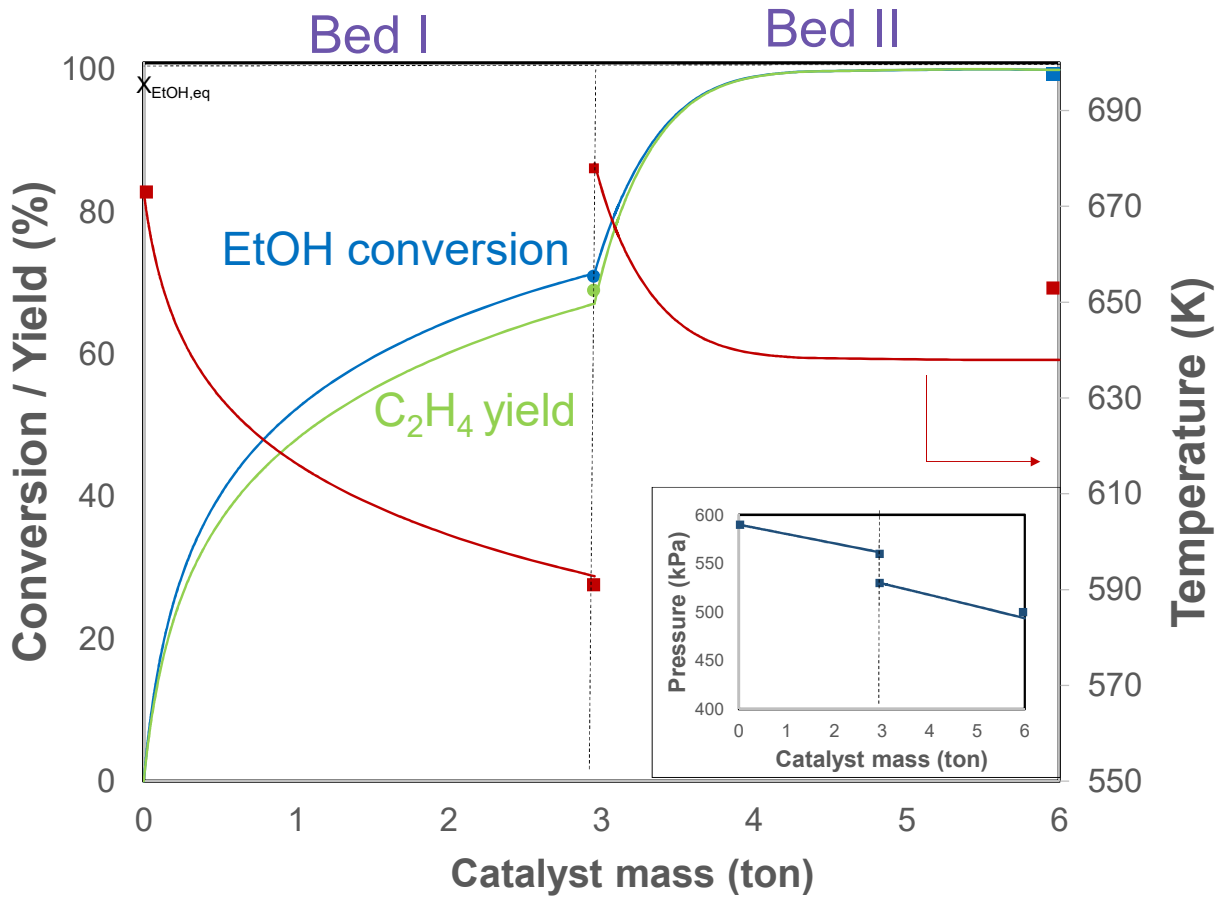
[1]US Patent 2013/0090510 A1 assigned to IFP Energies Nouvelles and Total Research & Technology

# Industrial multibed adiabatic operation

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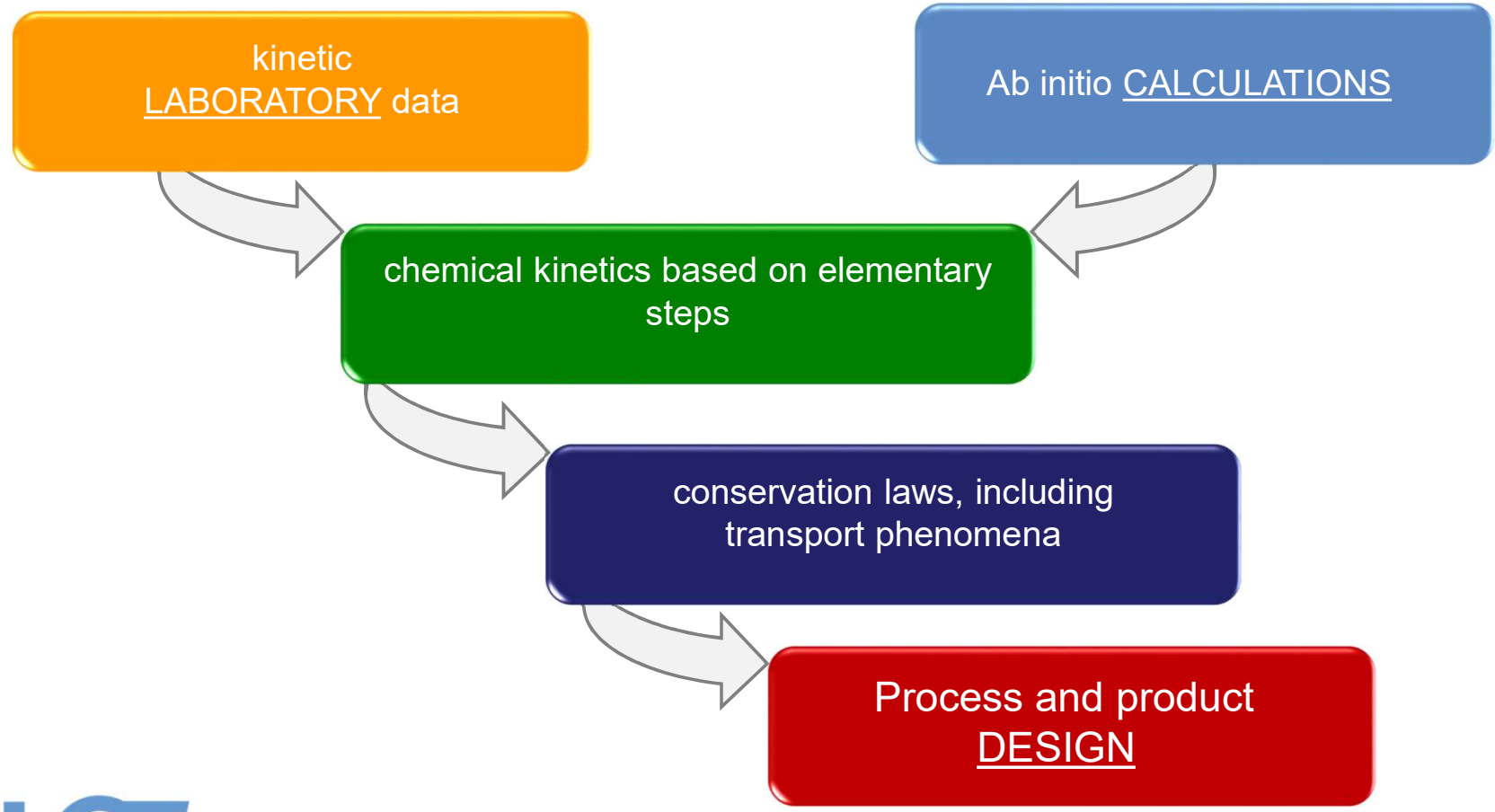
- Conclusions

# Kinetics: From Molecules to Process/Products

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*M.-F. Reyniers & G.B. Marin, Annu. Rev. Chem. Biomol. Eng. 5 (2014) 563*

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# Glossary

| | |
|---|---|
| GPC | Gel permeation chromatography |
| FBP | Final boiling point |
| FT-NIR | Transform-near infrared |
| FT-NMR | FT-nuclear magnetic resonance |
| GC | Gas chromatography |
| GC × GC | Comprehensive two-dimensional gas chromatography |
| HPLC | High-performance-liquid-chromatography |
| IBP | Initial boiling point |
| CE | Capillary electrophoresis |
| MS | Mass spectrometry |
| GFC | Gel Filtration Chromatography |
| PIONA | Paraffins Isoparaffins Olefins Naphthenes and Aromatics |
| SFC | Supercritical fluid chromatography |
| IC | Ion Chromatography |

# Glossary

| | |
|---|---|
| Roof-tile | In GCxGC: ascending band of components with similar features |
| TOF-MS | Time-of-Flight Spectrometry |
| SSL | Split/Splitless |
| PTV | Programmable Temperature Vaporizing |
| COC | Cold on Column |
| NP | Normal Phase |
| RP | Reversed Phase |
| SCD | Sulfur Chemiluminescence Detector |
| NCD | Nitrogen Chemiluminescence Detector |
| DAD | Diode-Array Detector |
| ELSD | Evaporative Light Scattering Detector |
| FPD | Flame Photometric Detector |
| SARA | Saturates Aromatics Resins Asphaltenes |
| FID | Flame Ionization Detector |

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# Glossary

- **SMILES** (Simplified Molecular Input Line Entry System): line notation for representing chemical structures. By making use of a canonicalization algorithm, a “unique SMILES” can be generated. SMILES are also quite compact compared to other methods for representing chemical structures (making them more human readable) and they allow isotopic and chiral specifications.

- **SMARTS** (SMiles ARbitrary Target Specification): line notation that allows to specify substructures using rules that are straightforward extensions of SMILES. In addition to the atomic and bond symbols, wildcard atoms and bonds can be specified and logical operators can be used, allowing an extremely precise sub structural specification. Using SMARTs flexible and efficient substructure-search specifications can be made (database searching, reactive center identification ...)

# Glossary

- **InChI** (IUPAC International Chemical Identifier): InChI encodes a chemical structure into “layers”, with each layer holding a distinct class of structural information (main layer, charge layer, stereochemical layer, isotopic layer, fixed-H layer and reconnected layer). Only the main layer specifying the chemical formula, atoms, and bonds between them, is required for all InChIs. The InChI is open-source and the software for generating InChI strings is freely available (in contrast to SMILES). However, they are less human readable compared to SMILES strings, because InChI was developed as a “machine-readable” chemical identifier.

- **Fixed H-layer**: When potentially mobile hydrogen atoms are present and the user specifies that they should be immobile (e.g. tautomerism not allowed), this layer binds these hydrogen atoms to the atoms specified in the input structure.

- **Reconnected layer:** when e.g. all metal atoms are disconnected in the main layer. The user can request to add a “reconnected” layer that generates an InChI containing all bonds given in the input structures.

# Glossary

- **CDK** (Chemistry Development Kit): collection of modular Java libraries for processing chemical information (Cheminformatics). The modules are free and open-source and are easy to integrate with other open-source of in-house projects. Functionalities include: molecule and reaction valence bond representation, reading and writing file formats such as SMILES and InChI, canonical identifiers for fast exact searching, substructure and SMARTS pattern searching…

- **RDKit**: cheminformatics toolkit similar to CDK, with the same core functionalities, but written in another language (C++ versus Java).

- **OpenBabel**: software mainly used to interconvert chemical file formats or representations. Other functionalities include generation of 3D molecular structure, generation of molecular fingerprints, calculation of partial charges …

# Glossary

- **Benson group**: polyvalent atom, i.e. a central atom with ligancy ≥ 2, together with all of its ligands. The corresponding notation is $X\text{-}(A)_i(B)_j(C)_m(D)_l$ , in which X represents the central atom surrounded by *i* ligands of atom A, *j* ligands of atom B and so on.

- **(Un)weighted graph:** An unweighted graph object consists of a set of nodes or vertices representing the atoms, connected by edges representing the chemical bonds. A weighted graph introduces additional information. The vertices can bear information about the atom type, its electronic configuration etc. The edges can refer to single, double, triple, transition-state etc. bonds.