15/12/2017

HPC-UGENT USER MEETING

MULTISCALE MODELING IN CHEMICAL ENGINEERING ON TIER-2 AND TIER-1

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HPC UGENT

VSC Vlaams Supercomputer Centrum

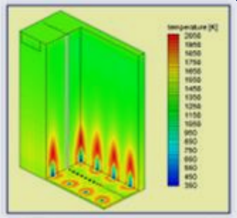
MULTISCALE MODELING IN CHEMICAL ENGINEERING

Reaction engineering

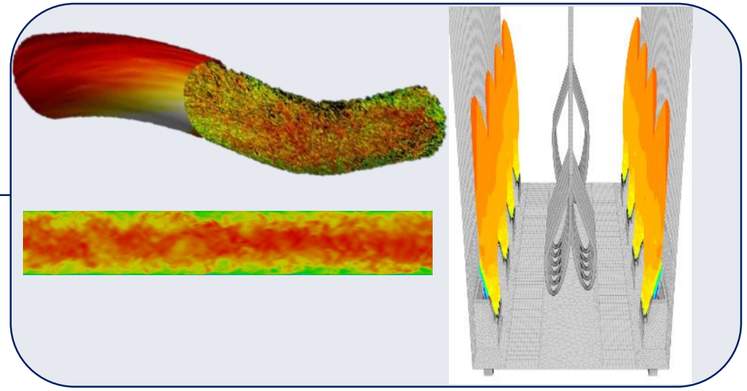
Separation units

Process

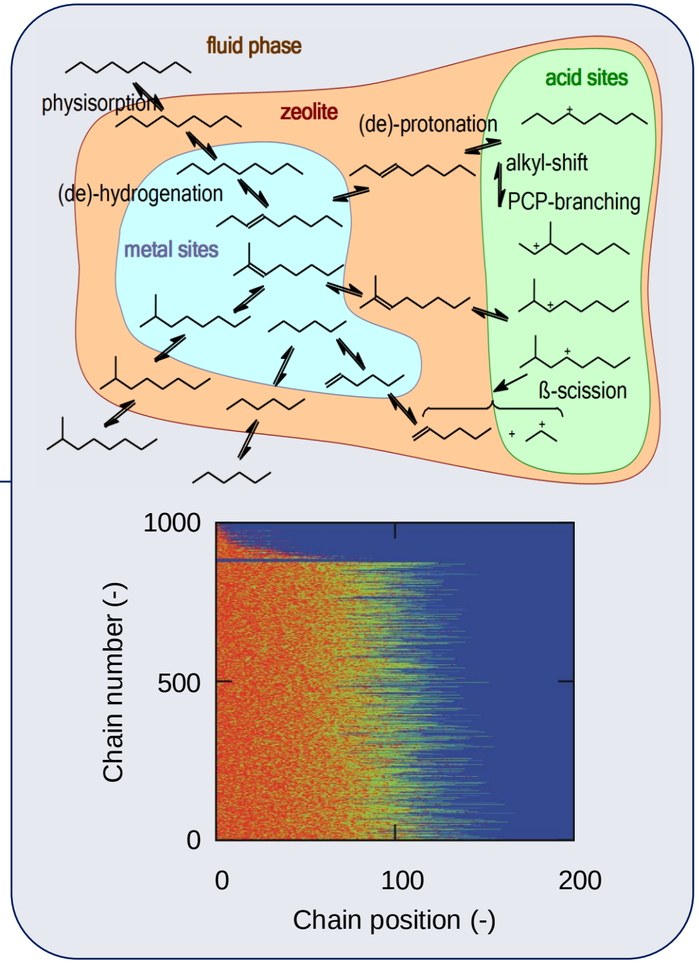
Reactor



Transport phenomena



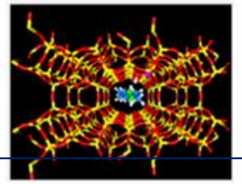
Kinetics

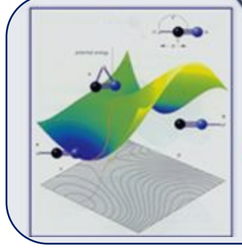


Materials design

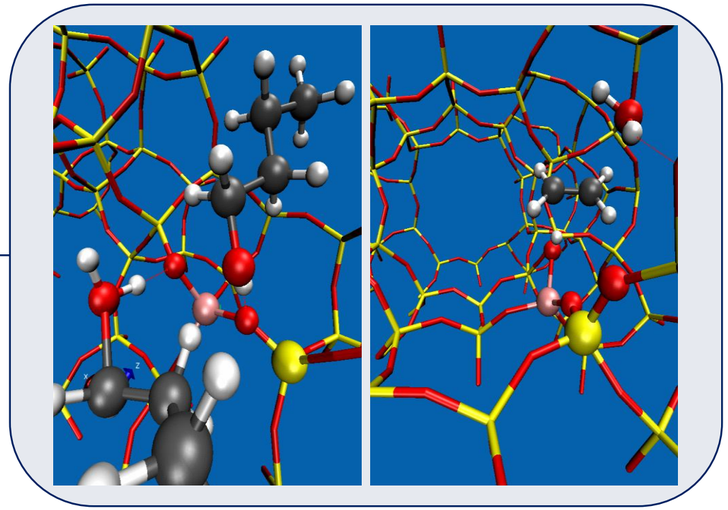
Surface phenomena

Mechanism





Ab initio



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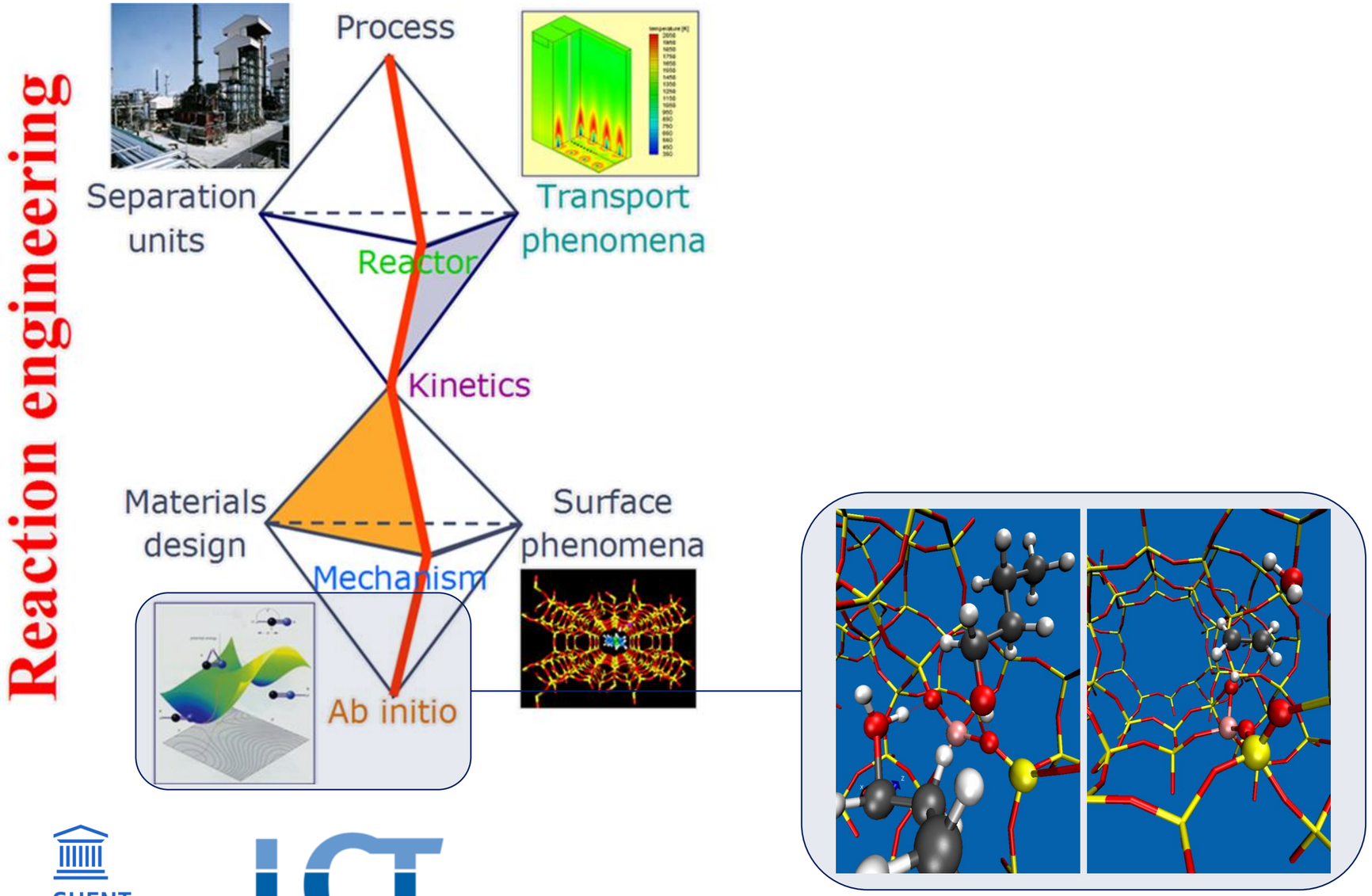
MULTISCALE MODELING IN CHEMICAL ENGINEERING



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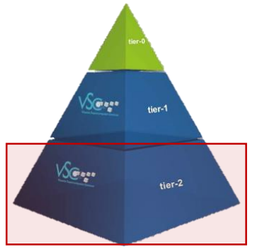
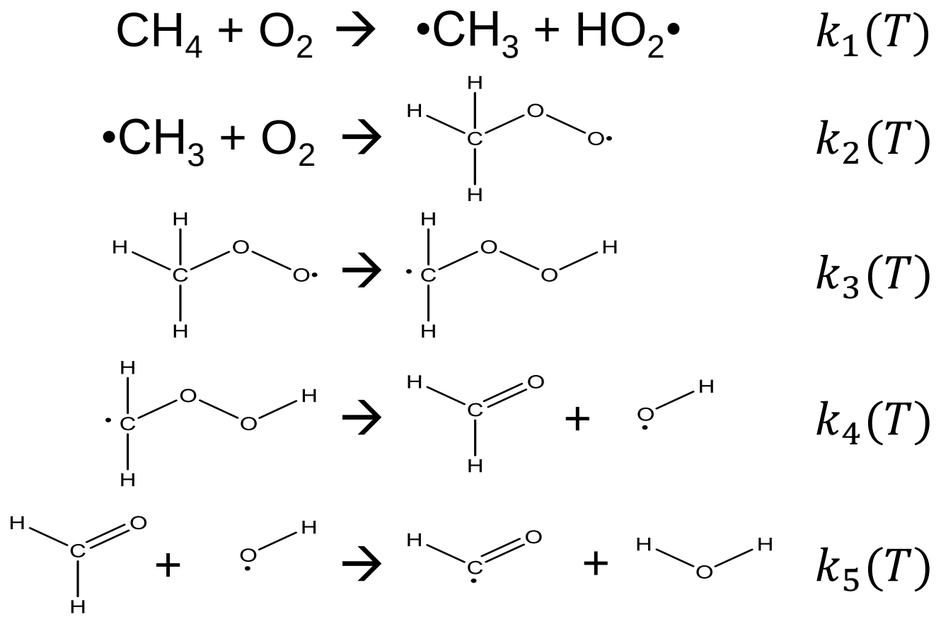
AUTOMATIC AB INITIO CALCULATIONS



Kinetic model: **List of chemical reactions** that are important for a chemical process, including a **rate coefficient** for each reaction.



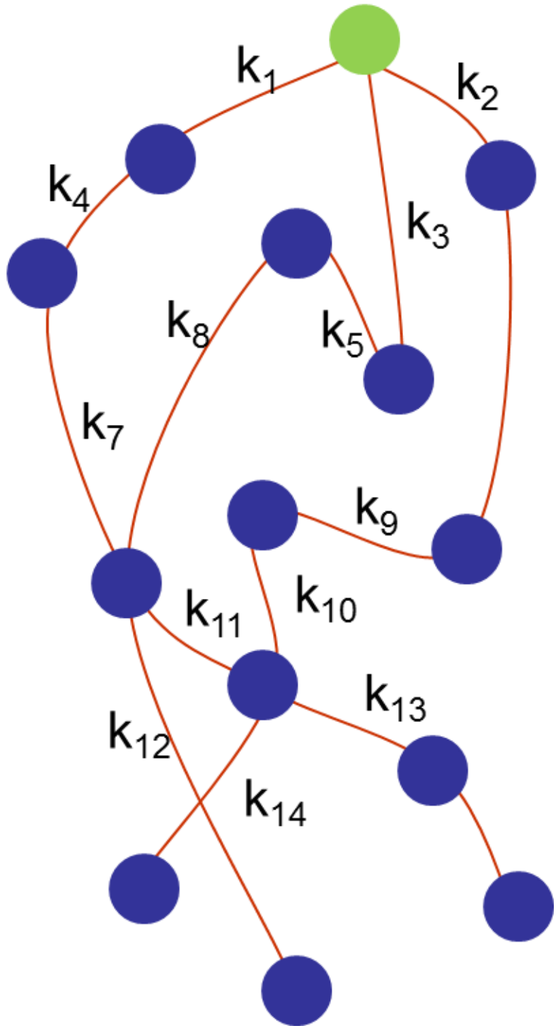
$k_1(T)$

$k_2(T)$

$k_3(T)$

$k_4(T)$

$k_5(T)$



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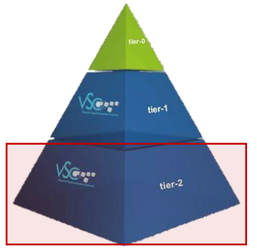
Van de Vijver, R. *et al. Int. J. Chem. Kinet.* **2015**, 47, 199-231.
Van de Vijver, R. *et al. Curr. Opin. Chem. Eng.* **2016**, 13, 142-149.

AUTOMATIC AB INITIO CALCULATIONS

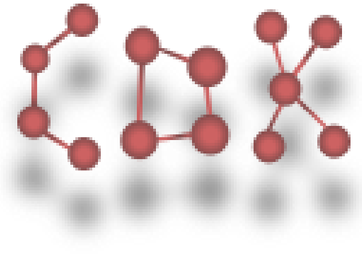


Genesys: Use of chemoinformatics

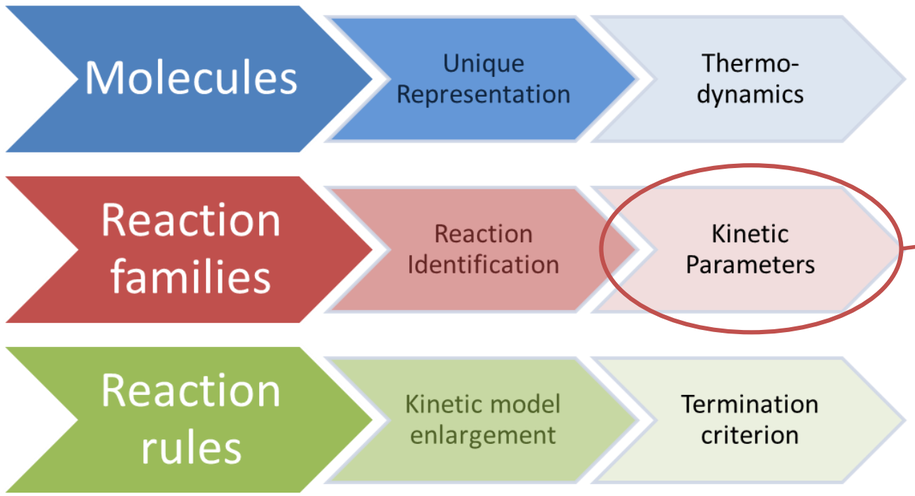
- Molecular representation
- Graph and group theory
- Not tailored to specific applications

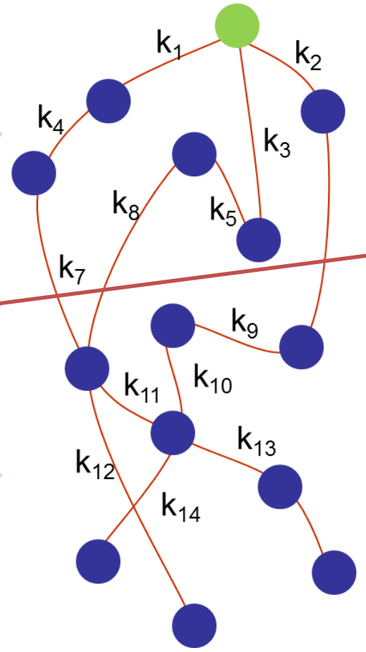
RDKit
Open-Source Cheminformatics and Machine Learning

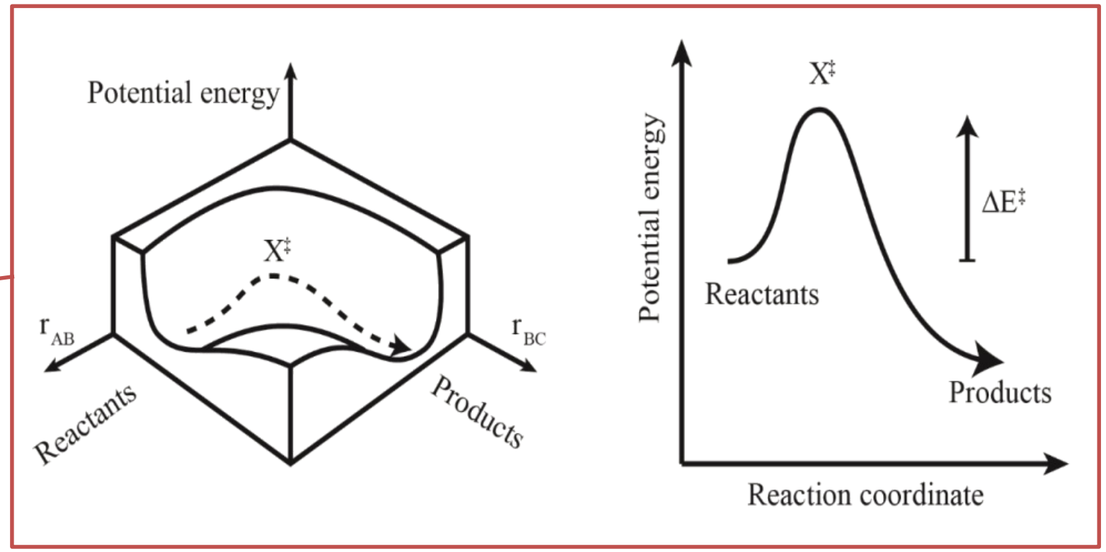
OpenBabel

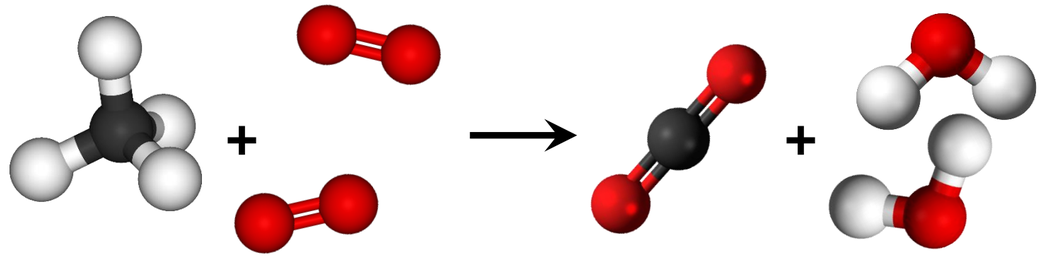


CDK









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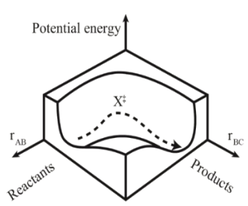
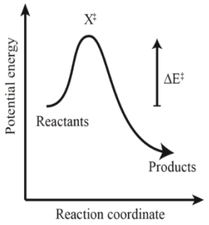
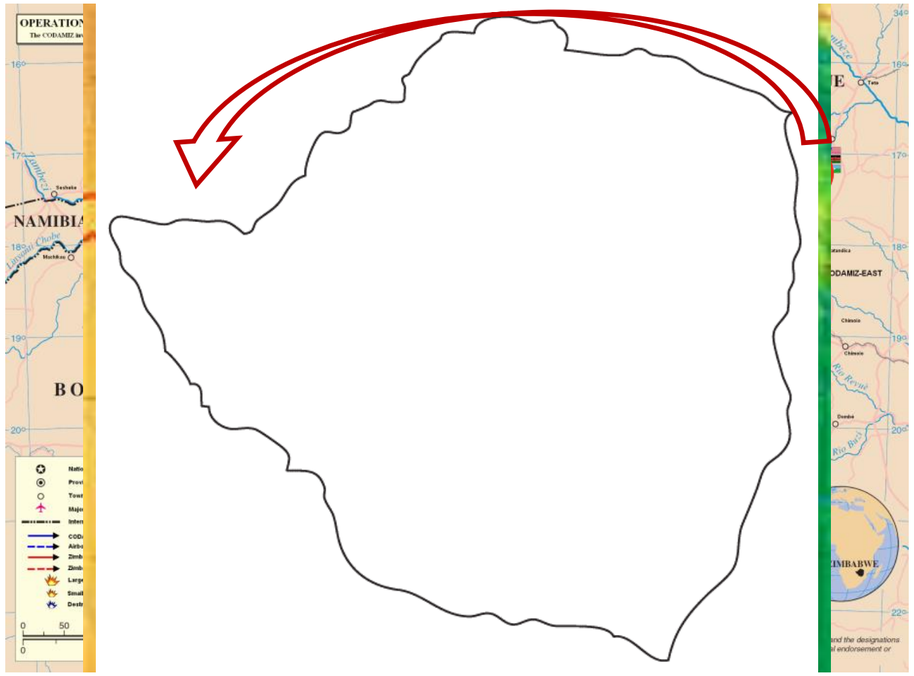
AUTOMATIC AB INITIO CALCULATIONS





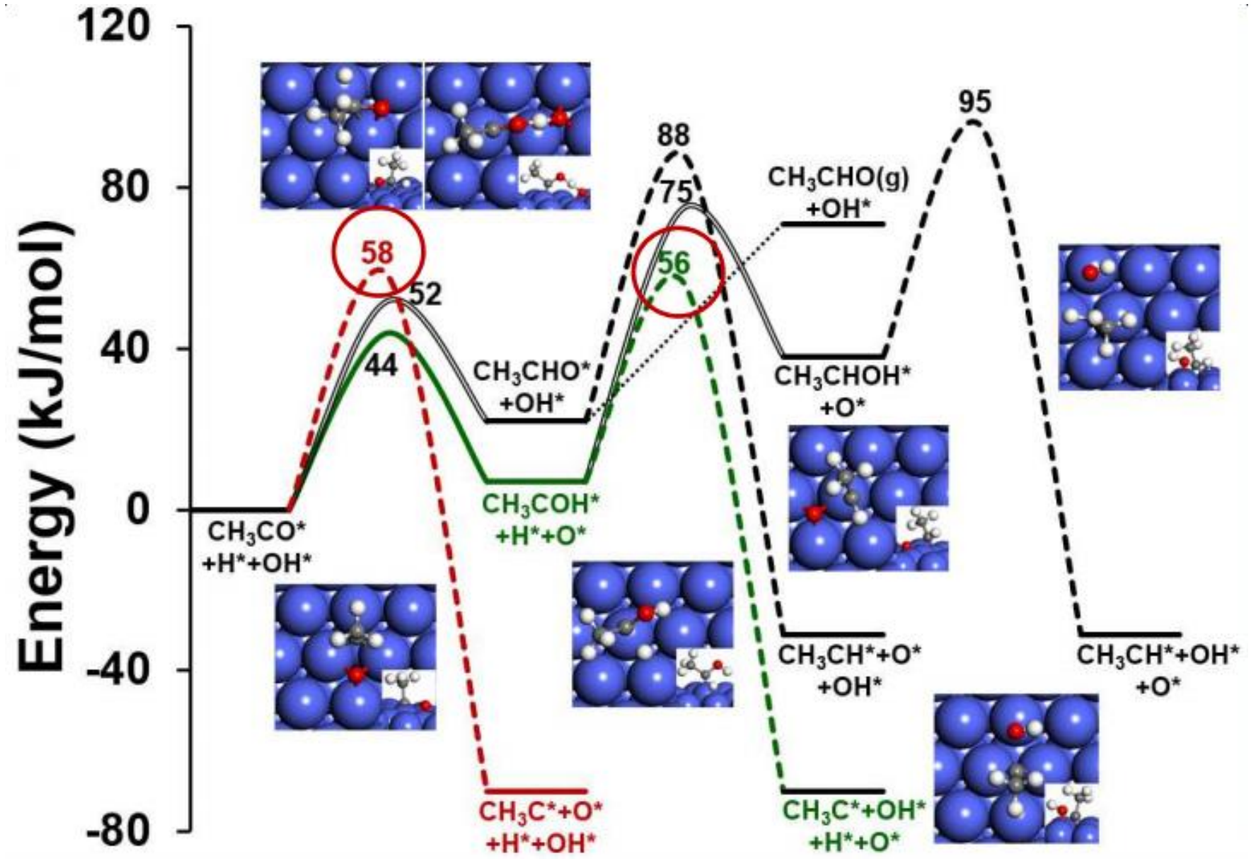


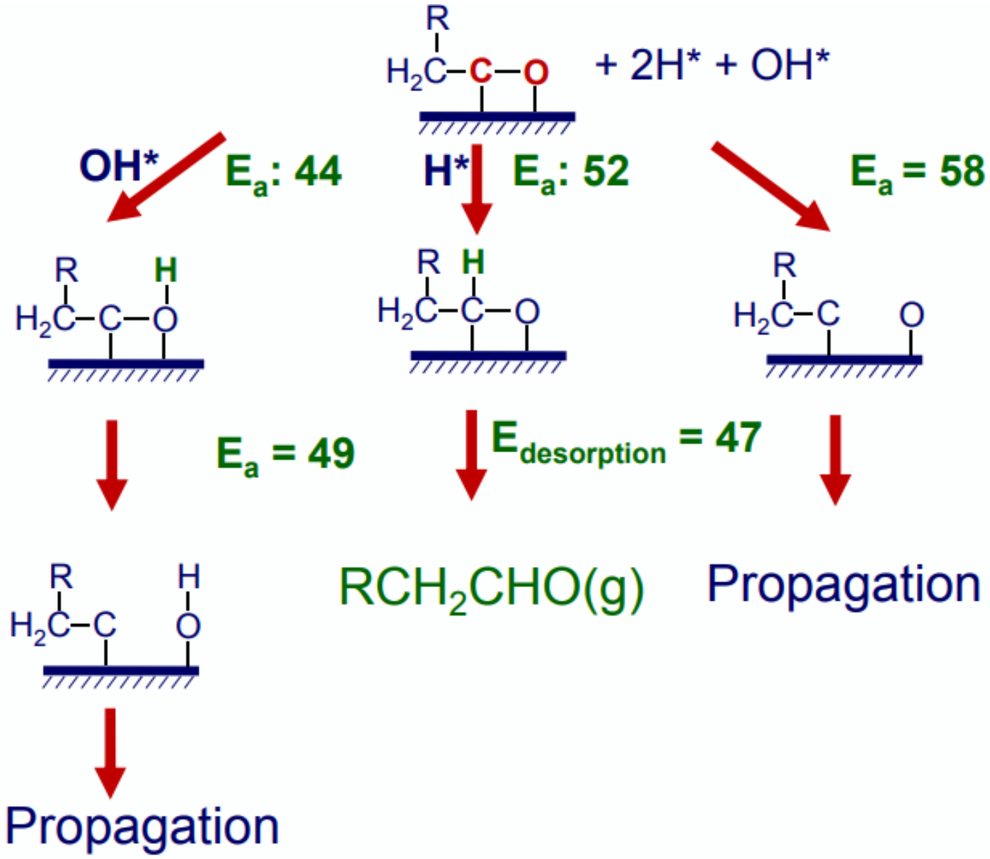
Automatic ab initio calculations via **Genesys** to complete missing thermodynamic and kinetic data in chemical networks

AB INITIO CALCULATIONS

Elucidate reaction mechanisms

Fischer-Tropsch synthesis: natural gas to liquid fuels





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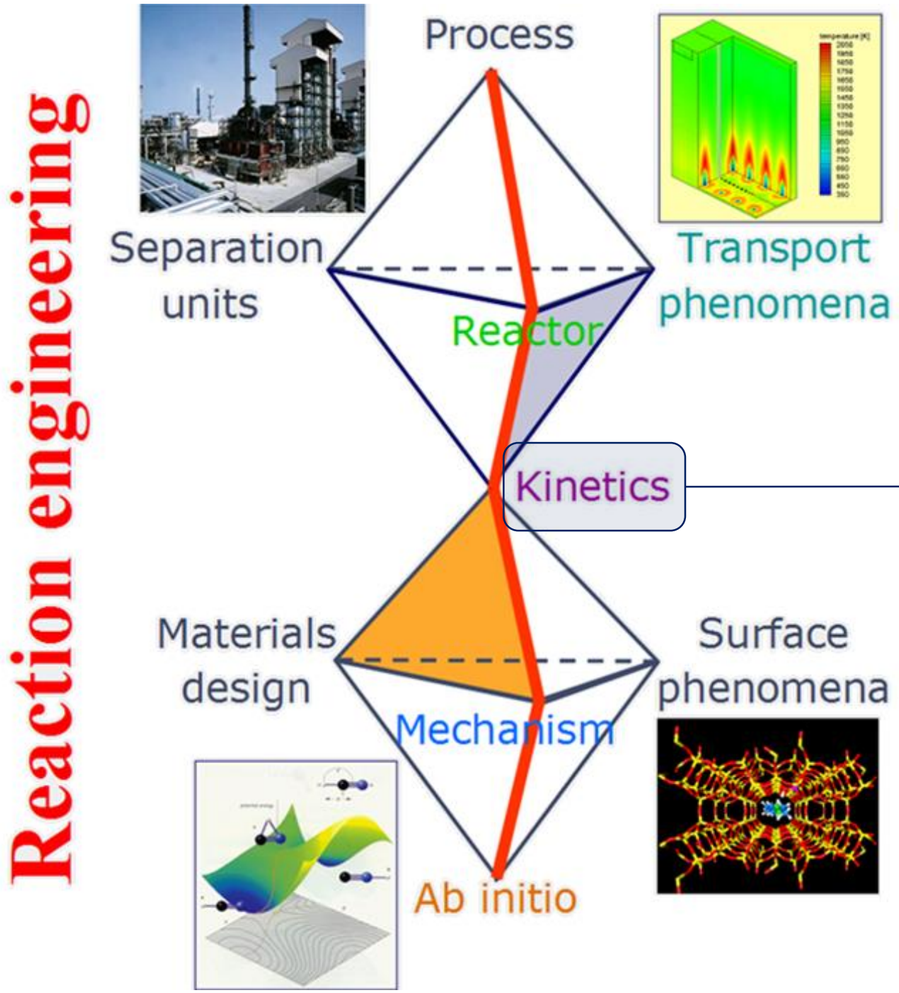
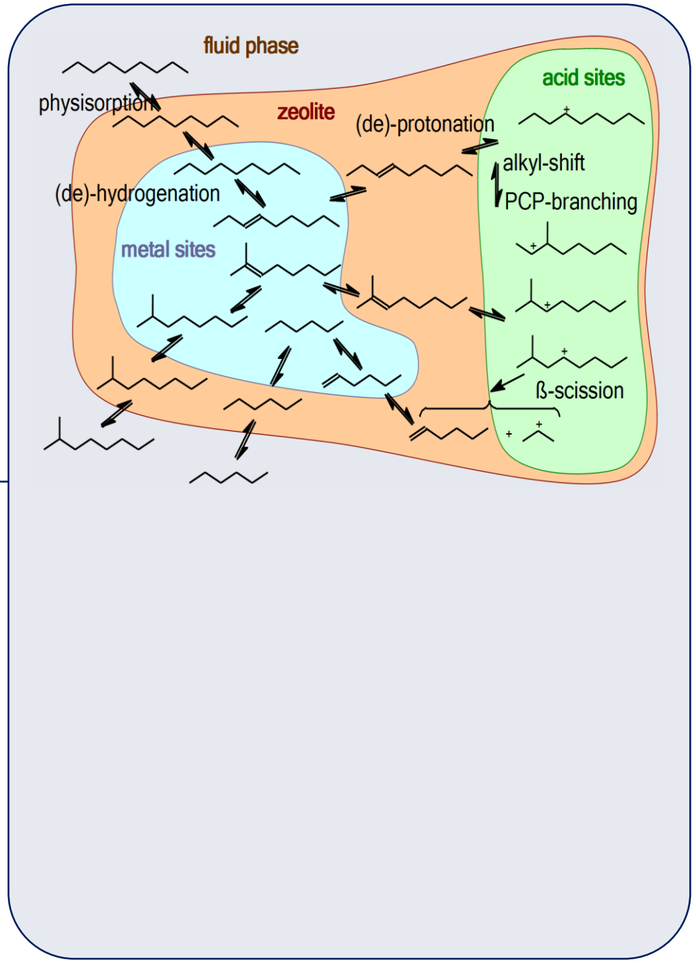
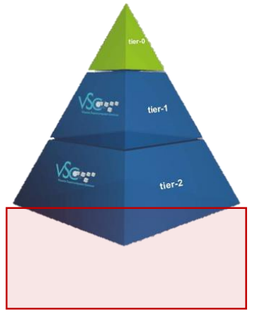
MULTISCALE MODELING IN CHEMICAL ENGINEERING



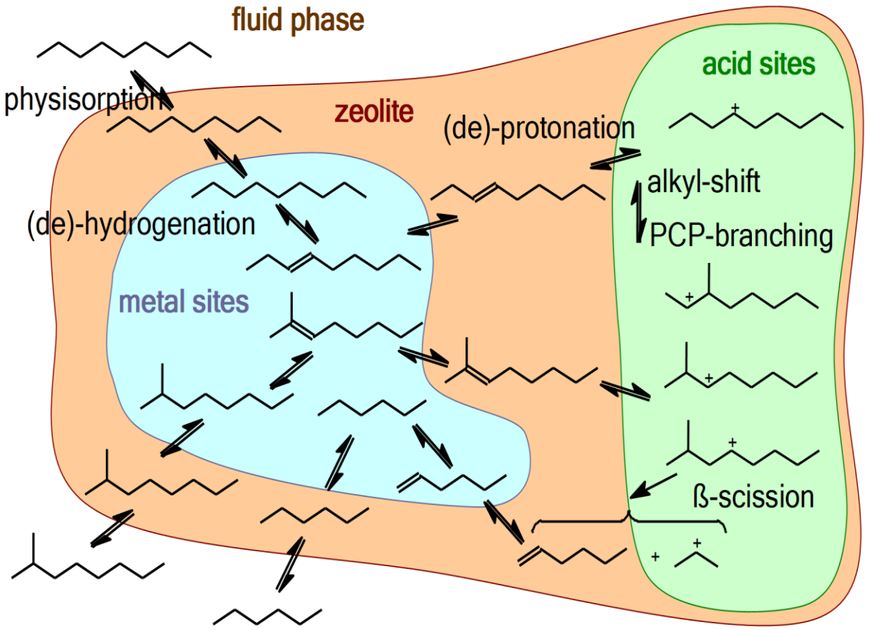


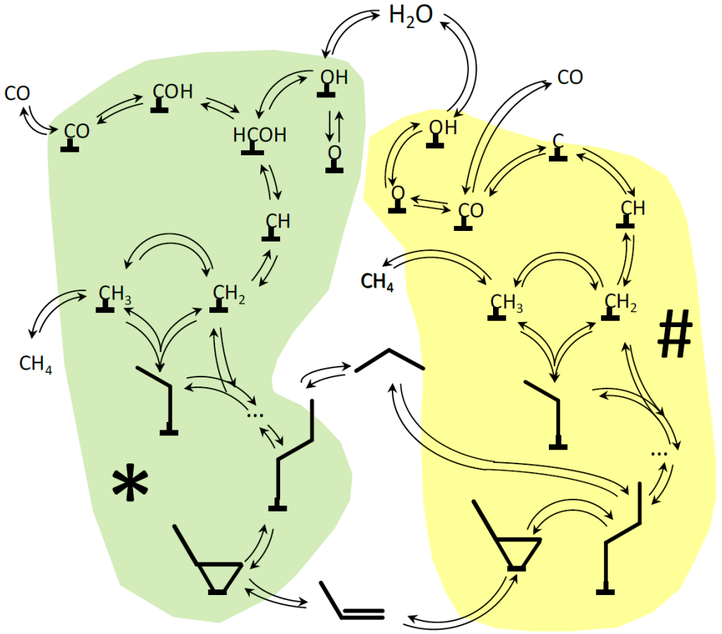
KINETIC MECHANISM DEVELOPMENT - CONTEXT

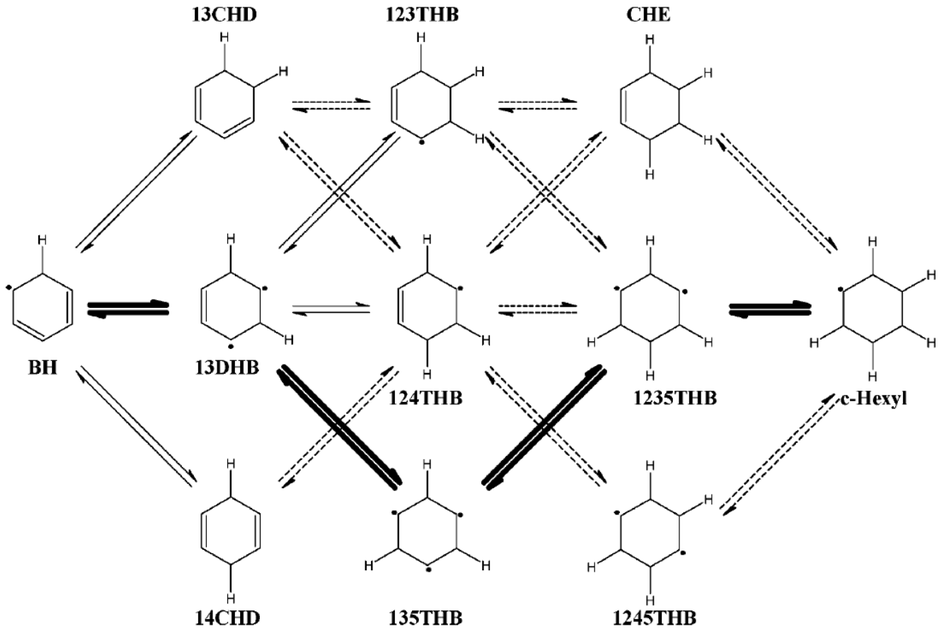


Kinetic networks form the bridge between the molecule scale and the reactor scale

Combine information from experiments and theoretical calculations







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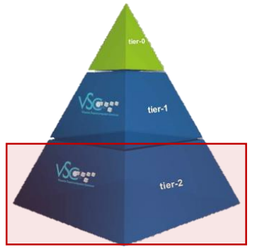
LCT DRIVING CHEMICAL TECHNOLOGY

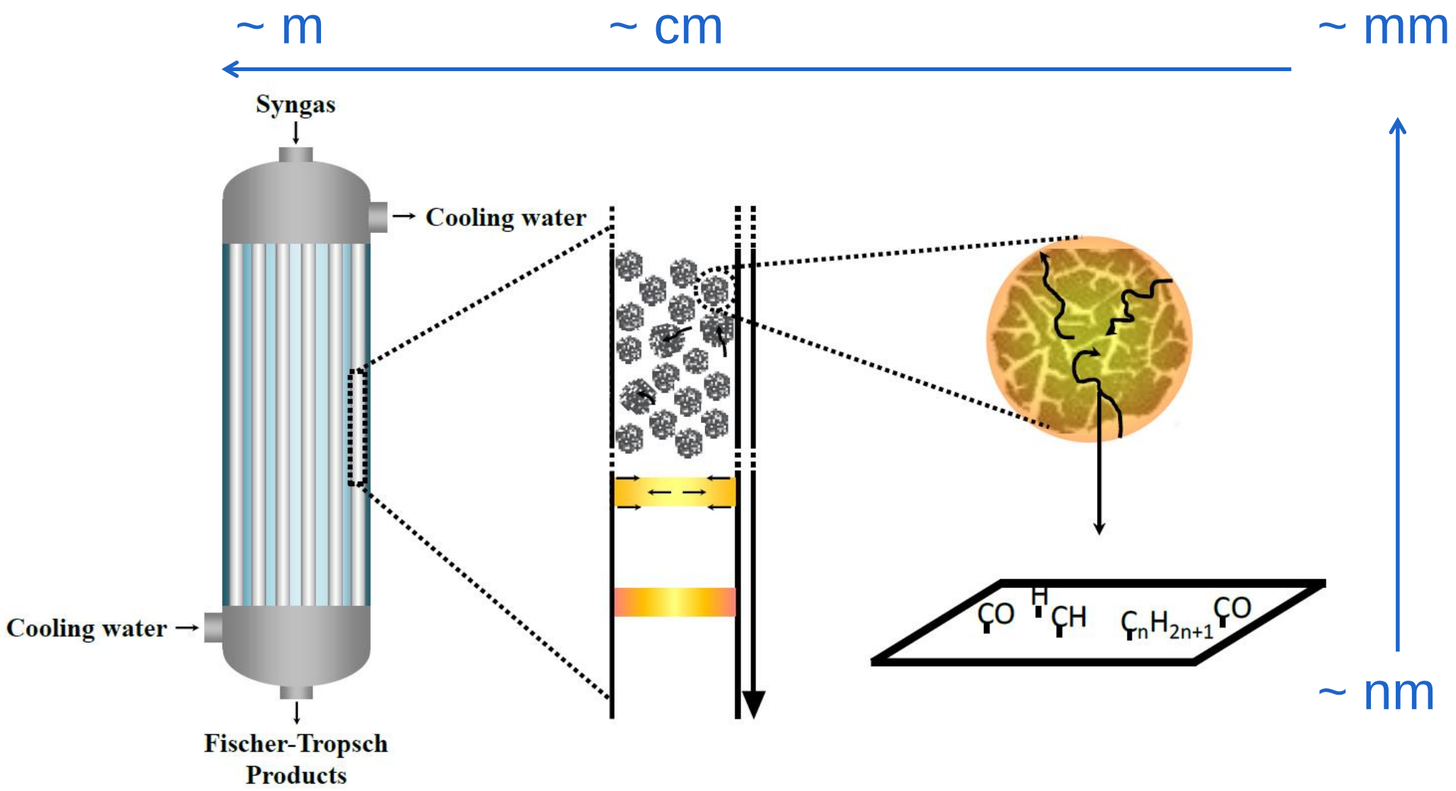
Saeys, M. *et al., J. Phys. Chem. B* **2005**, 109, 2064
Van Belleghem, J. Ghent University, **2017**.
Toch, K. *et al., AIChE J.* **2015**, 61, 880.

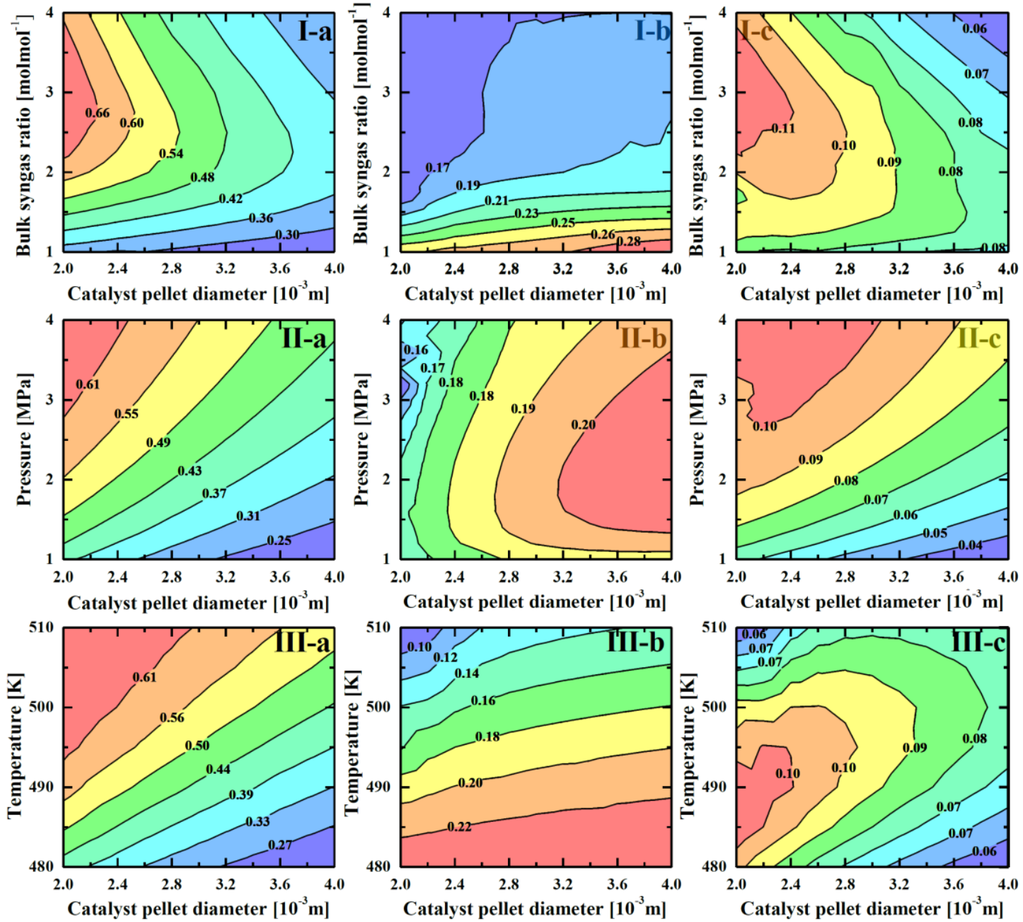
KINETIC MECHANISM DEVELOPMENT



Multiscale modelling of chemical reactors

Goal: *in silico* optimization of full-scale industrial reactor





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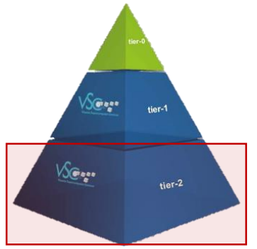
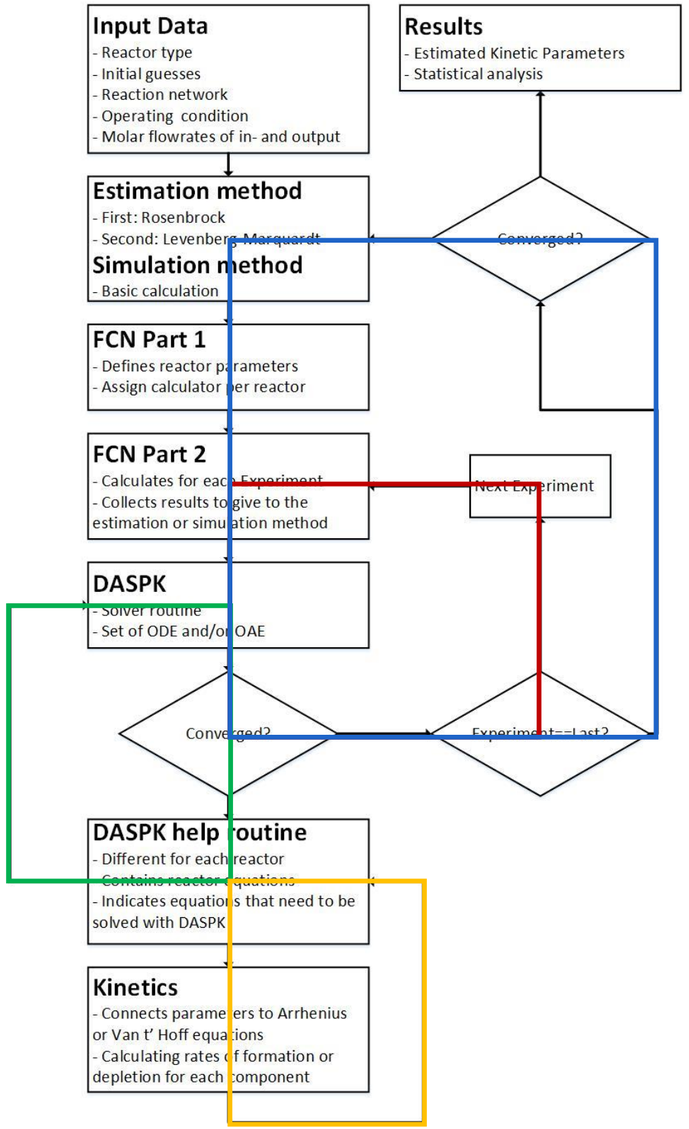
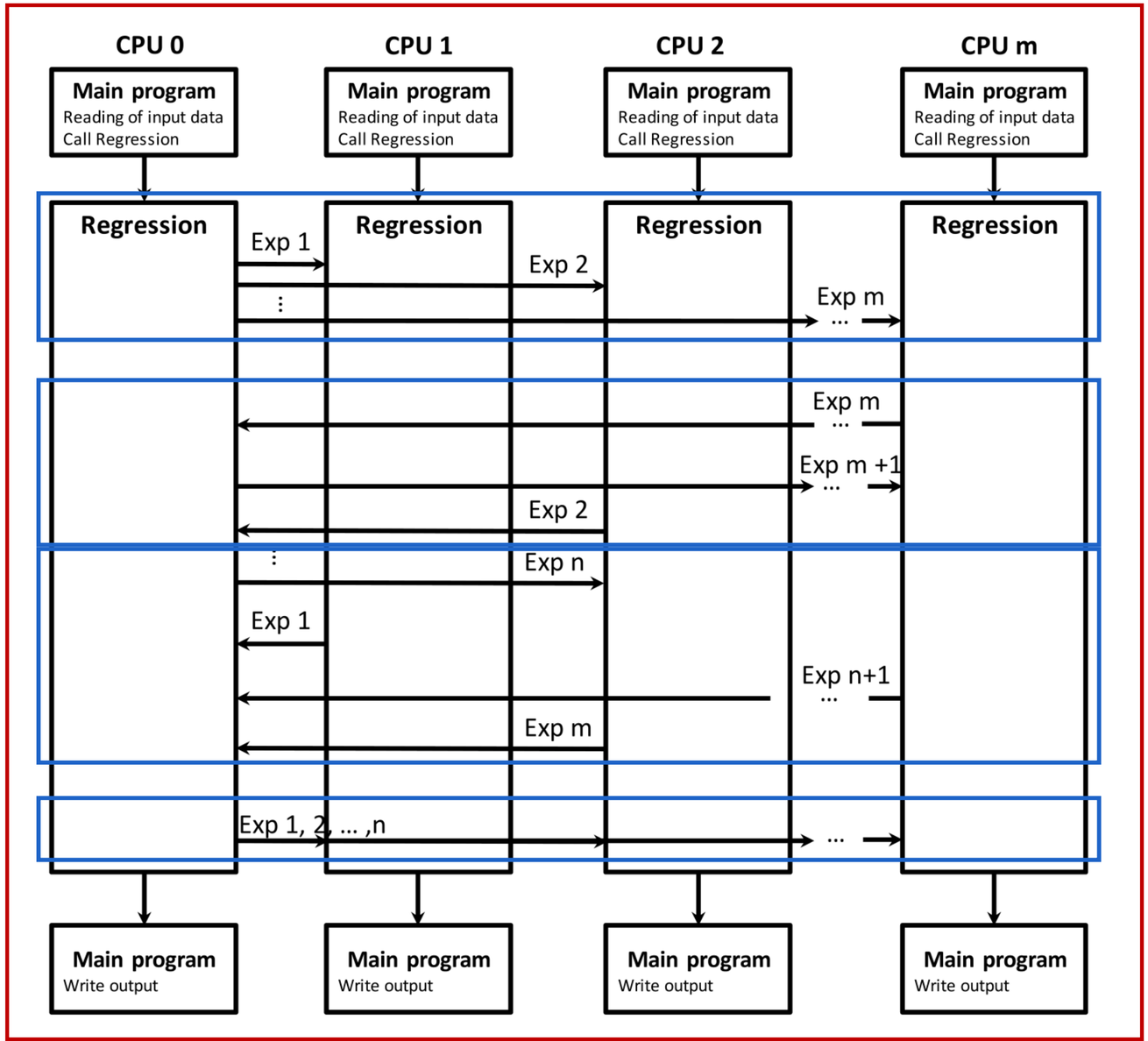
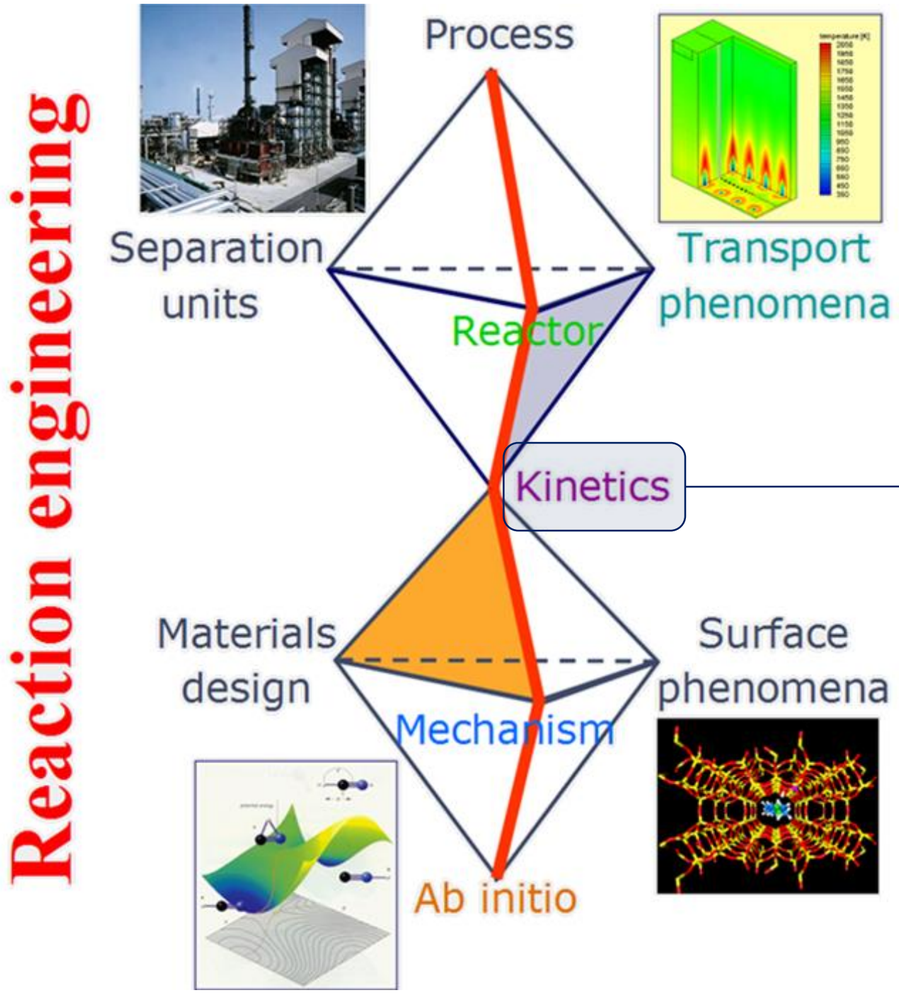


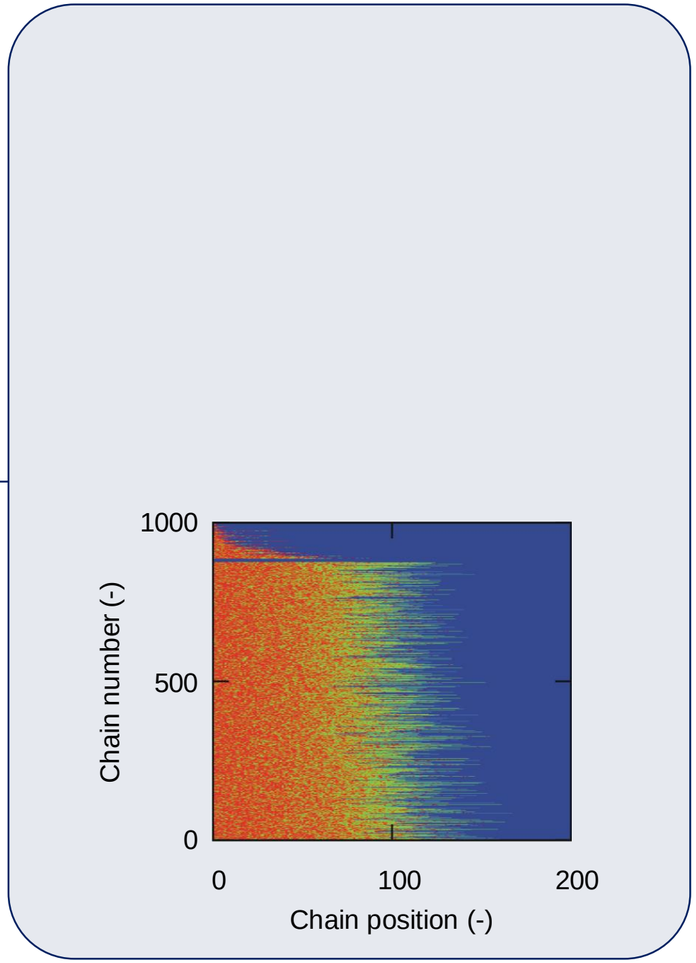
MPI based simulation framework for parallellization of n independent realizations on HPC





MULTISCALE MODELING IN CHEMICAL ENGINEERING

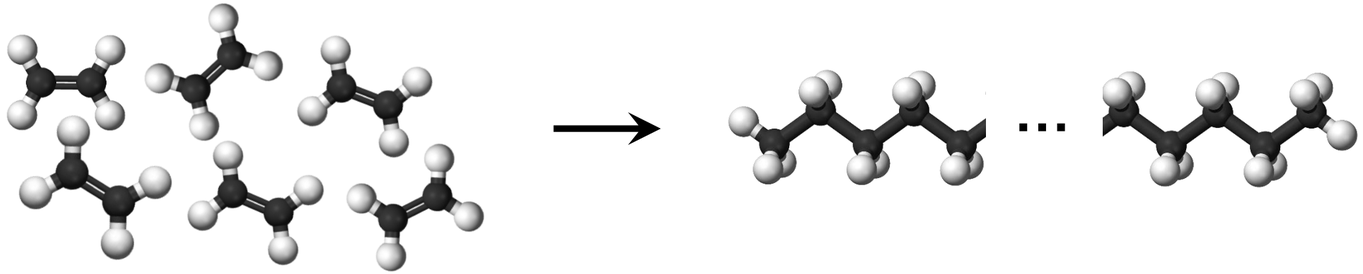


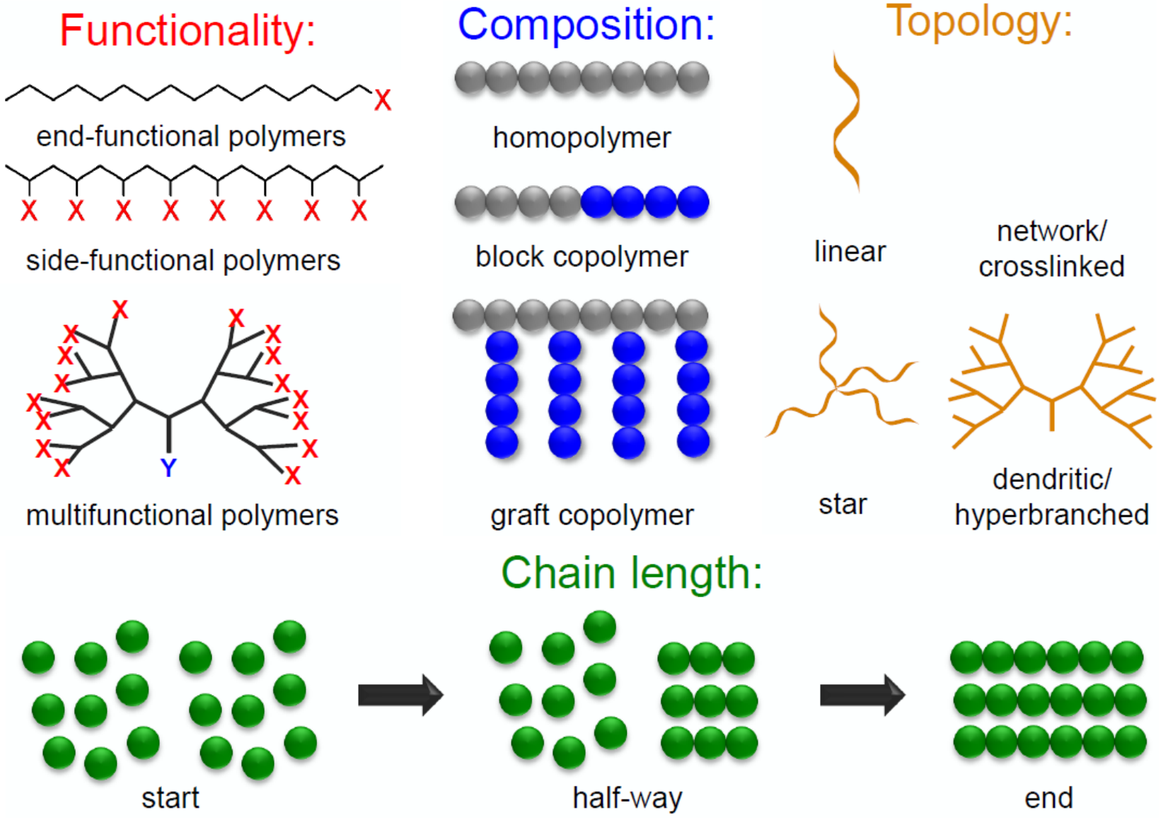


POLYMER DESIGN – CONTEXT

Model guided design of polymers

Control over polymer properties starts during polymerization





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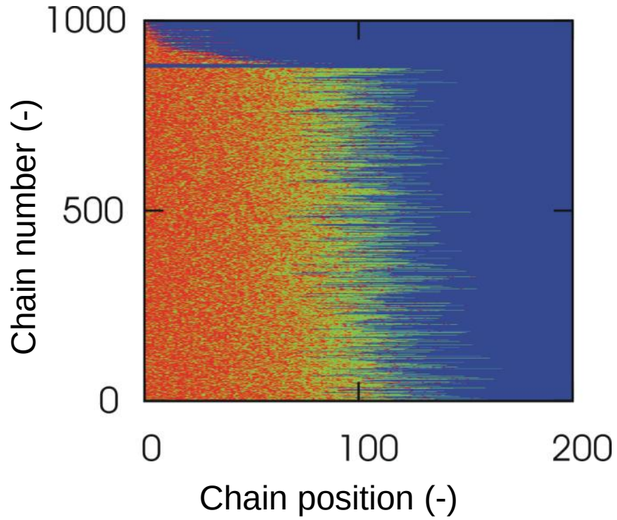
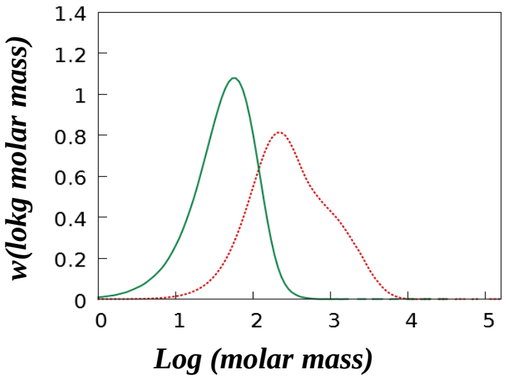
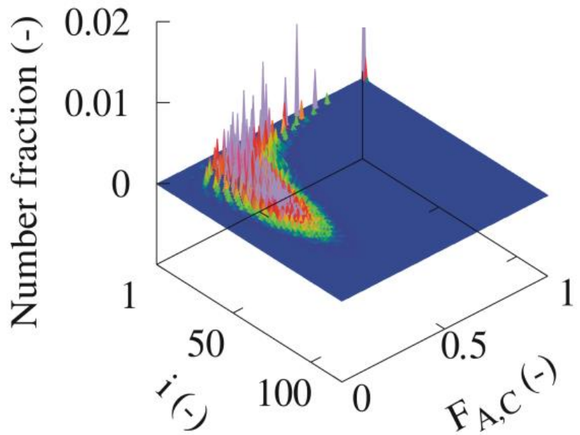
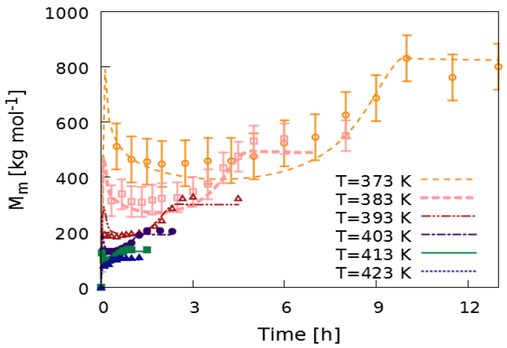






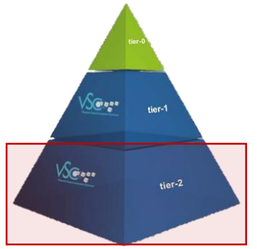


Van Steenberge P.H.M. *et al. Macromolecules* **2011**, 44, 8716
Van Steenberge P.H.M. *et al. Macromolecules* **2012**, 45,8519.
Van Steenberge P.H.M. *et al. Chem. Eng. Sci.* 2014, 11, 185
D'hooge D.R. *et al. Polym. Chem.* **2015**, 6, 7081.
Derboven P. *et al. Macromol. Rapid Commun.* **2015**, 36, 2149
D'hooge D.R. *et al. Prog. Polym. Sci.* **2016**, 58, 59

Model complexity

Macromolecular structural detail

POLYMER DESIGN – KINETIC MONTE CARLO



Event-per-event simulation of polymerization: embarrassingly parallel

Start t=0

Input:
- ✓ Reactions
- ✓ Temperature **T**
- ✓ Initial number of molecules $n_{Ao}, n_{Bo,...}$
- ✓ Intrinsic kinetic parameters k_{chem}, f_{chem}
- ✓ Diffusion parameters for calculation of D_{AB}
- ✓ Total polymerization time t_{Tot}

Calculation of:
- ✓ Volume $V=f(T, n_{Ao}, n_{Bo,...})$
- ✓ Concentrations

$$C=f(n_{Ao}, n_{Bo,...}, V, N_A)$$

- ✓ Apparent "*Monte Carlo* rate coefficients " for each reaction v

$$k^v_{app,MC} = f(k_{chem}, D_{AB}, V, N_A)$$

Calculation of:
- ✓Monte Carlo reaction rates:

$$R(v) = k^v_{app,MC} n_A n_B$$

- ✓Time between two reactions:

$$\tau = -ln(r_1)\left[\sum_v R(v)\right]^{-1}$$

- ✓Reaction probabilities:

$$P(v) = R(v)\left[\sum_v R(v)\right]^{-1}$$

Random selection of
- ✓ reaction channel (μ)

$$\sum_{v=1}^{v=\mu-1} P(v) \le r_2 \le \sum_{v=1}^{v=\mu} P(v)$$

Random selection of
- ✓ chain length

Update of:
- ✓Number of molecules: $n_A, n_{B,...}$
- ✓$t = t+\tau$

$t=t_{Tot}$?
- yes → **End**
- no → back to Calculation of:

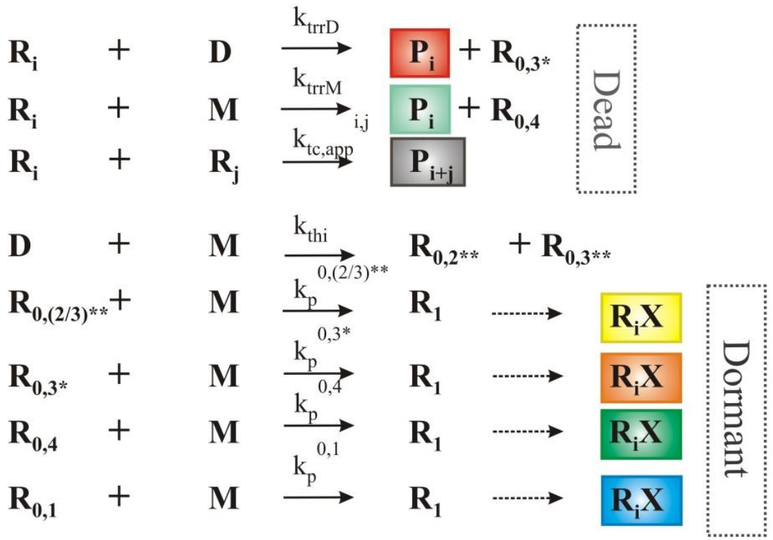
Van Steenberge P.H.M. *et al. Chem. Eng. Sci.* **2014**, 11, 185
Brandao A.L.T. *et al. Macromol. React Eng.* **2015**, 9, 141

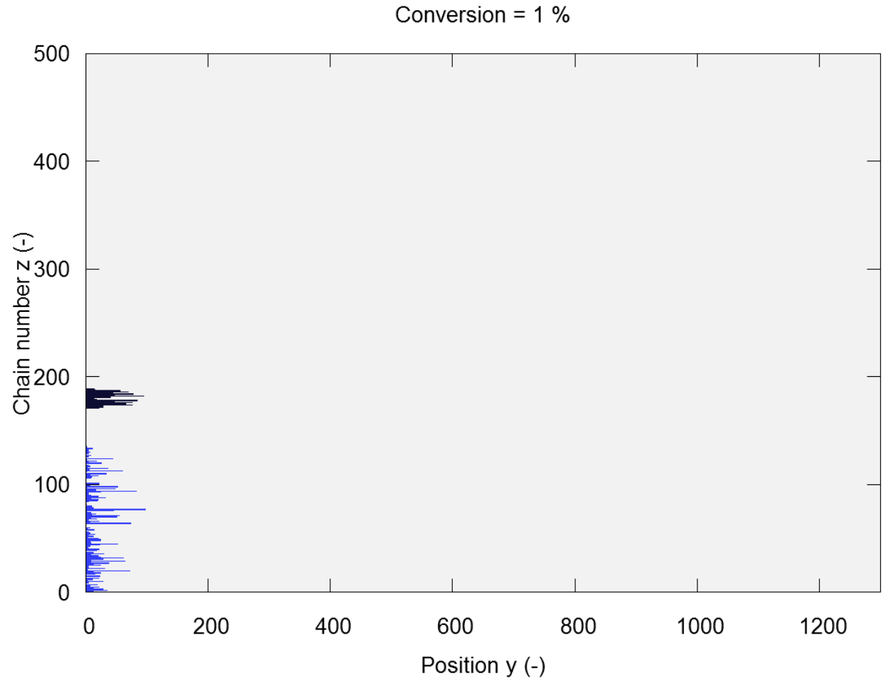
POLYMER DESIGN – MICROSTRUCTURAL CONTROL

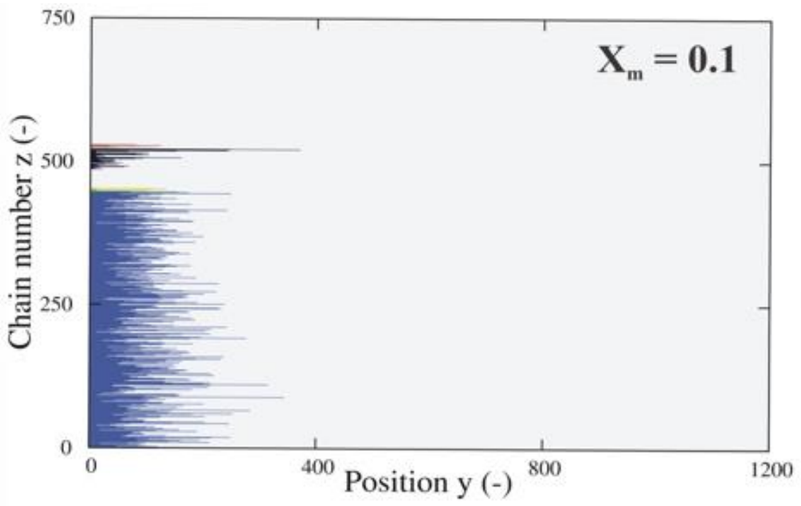
Event-per-event simulation of polymerization

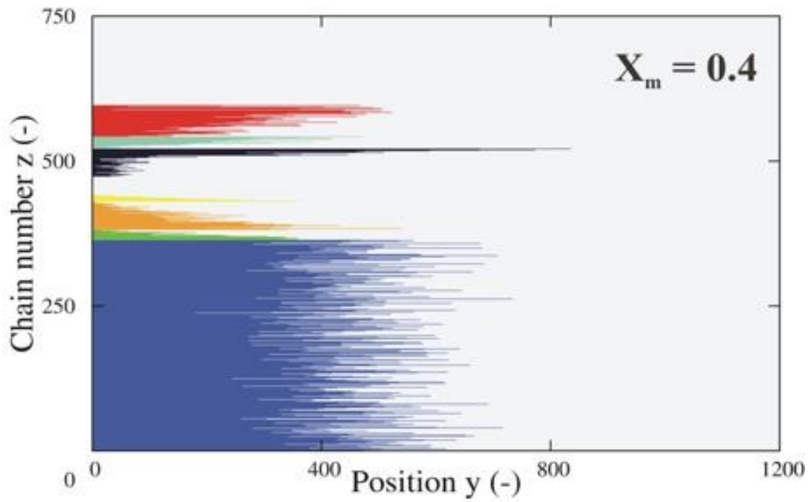
troxide /mediating agent

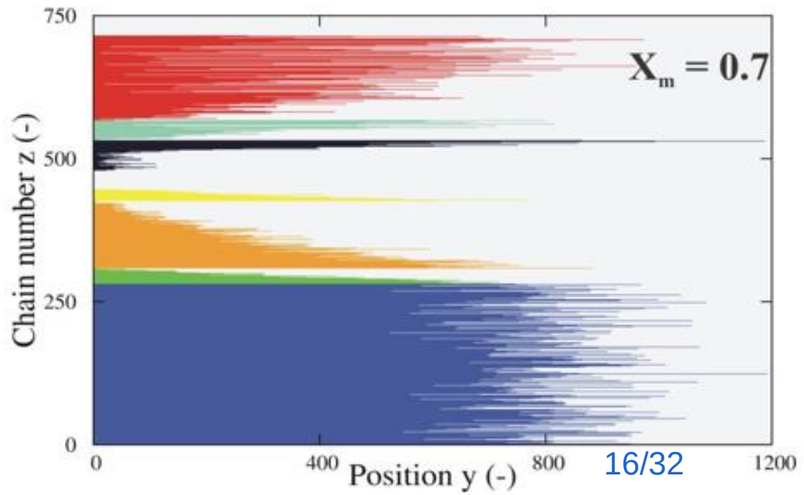
olymer





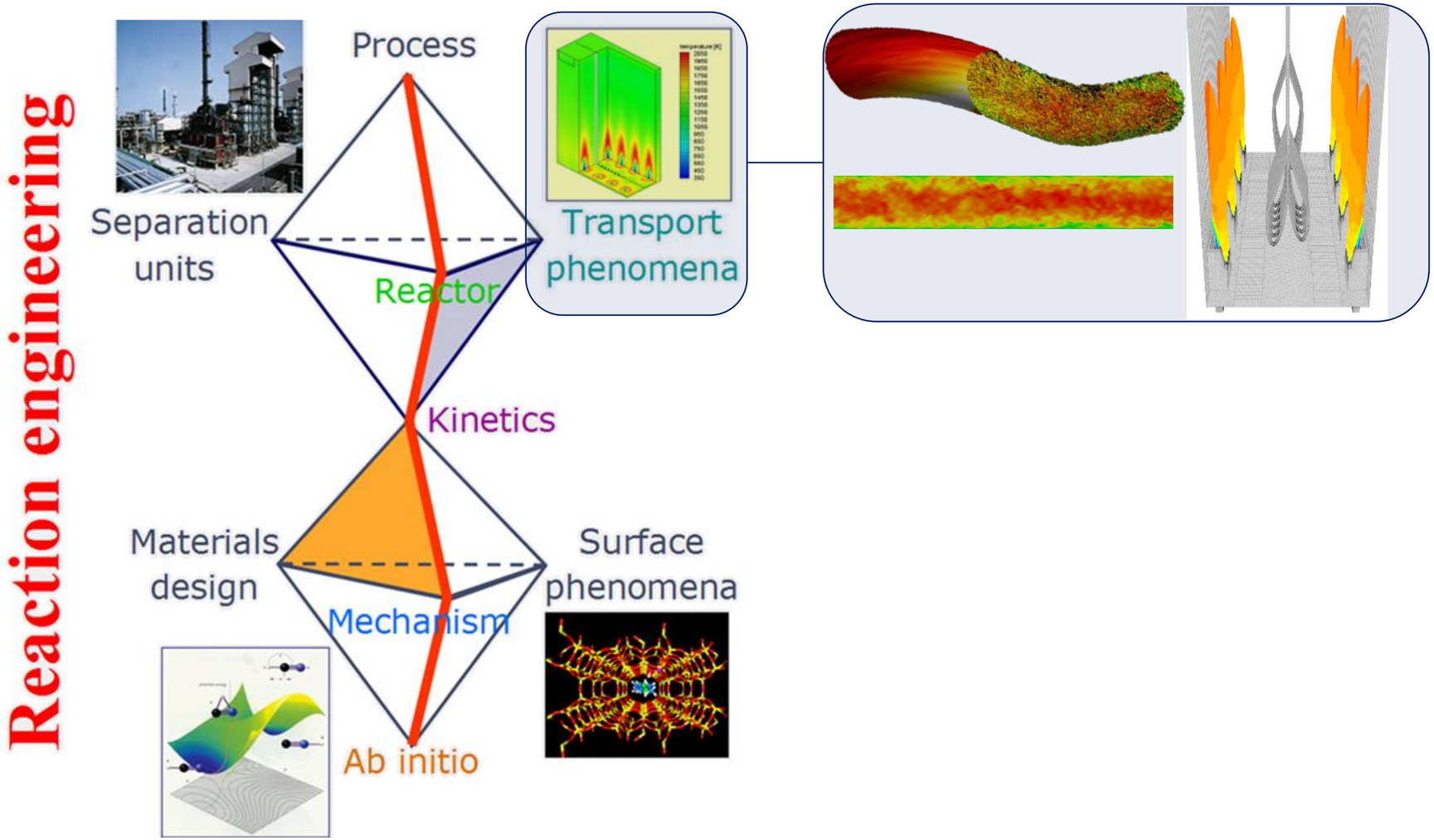




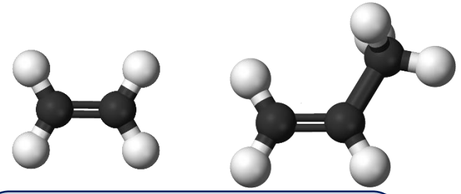


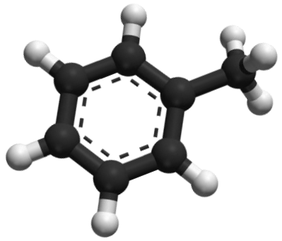
Fierens, S. K. *et al. Chem. Eng. J.* **2015**, 278, 407-420.

MULTISCALE MODELING IN CHEMICAL ENGINEERING



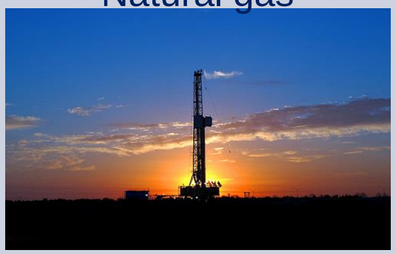
STEAM CRACKING



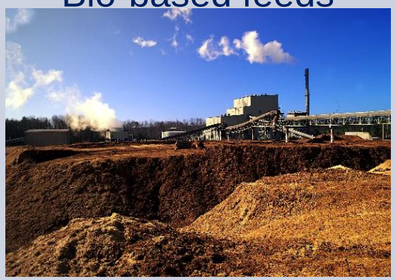


Crude oil

Natural gas

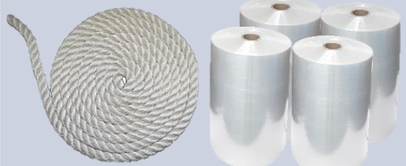


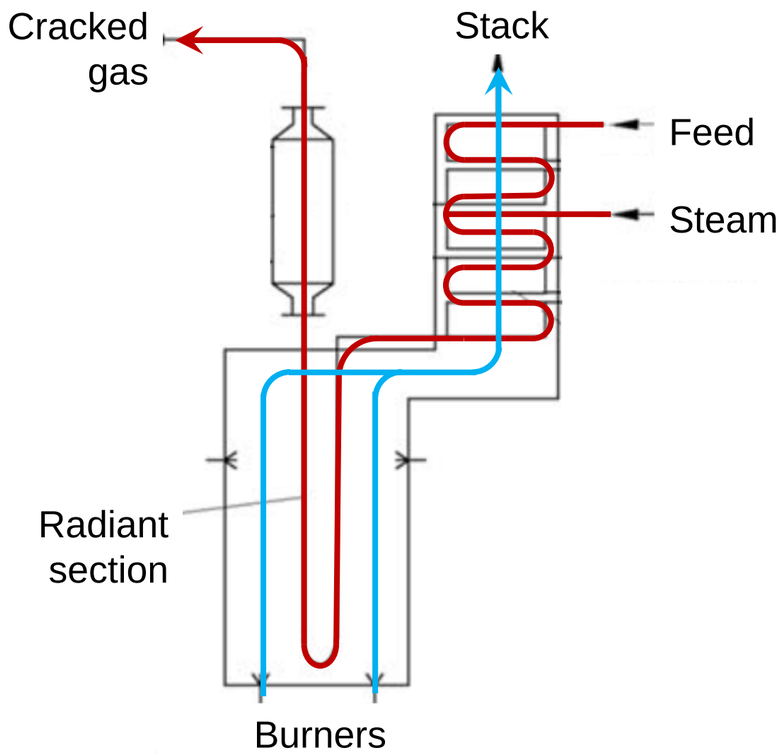
Bio-based feeds



Steam cracking

Consumer goods from chemical industry





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atozforex.com; pnnl.org; districtenergy.org; scade.fr; schmidt-clemens.de; Linde Group; IHS Chemical Insight

COKE FORMATION IN STEAM CRACKING

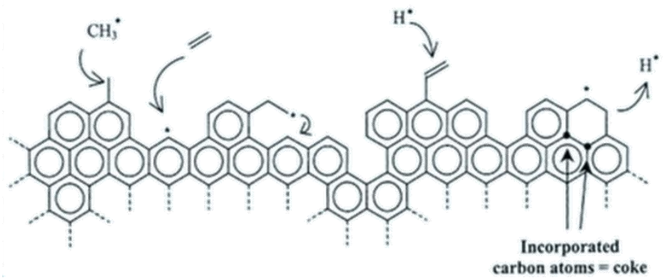
Endothermic process at temperatures of 800–900 °C

Deposition of a carbon layer on the reactor surface

⇒ Reduced thermal efficiency

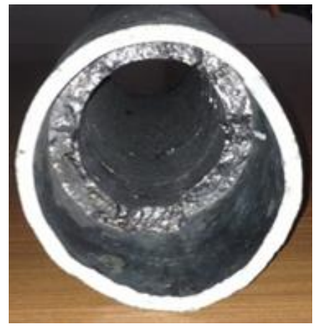
⇒ High pressure causes loss of product selectivity

⇒ Coil carburization and thermal stress



$$r_C = \sum_i c_i \cdot A_i \cdot \exp\left(\frac{-E_{a,i}}{R T_{int}}\right)$$

Coke reduction method: 3D reactor technology



Coil cracking due to differences in thermal expansion rate

Hot spots due to inhomogeneous coke formation

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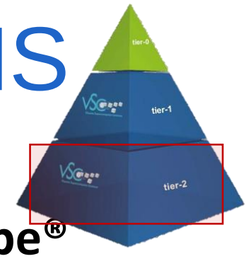
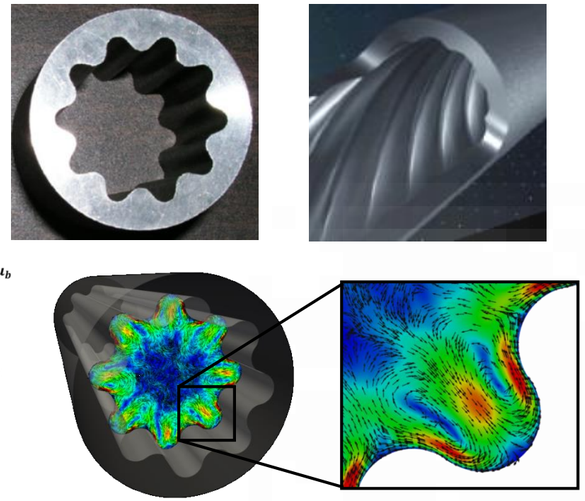
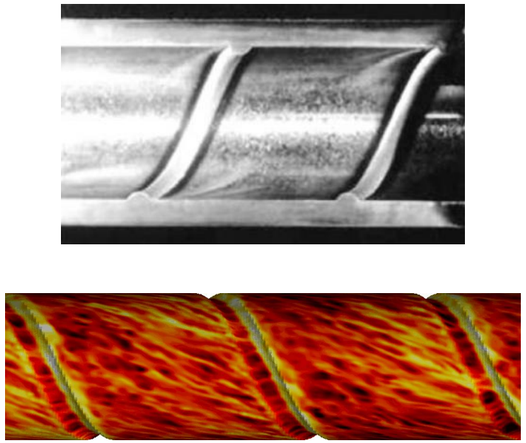
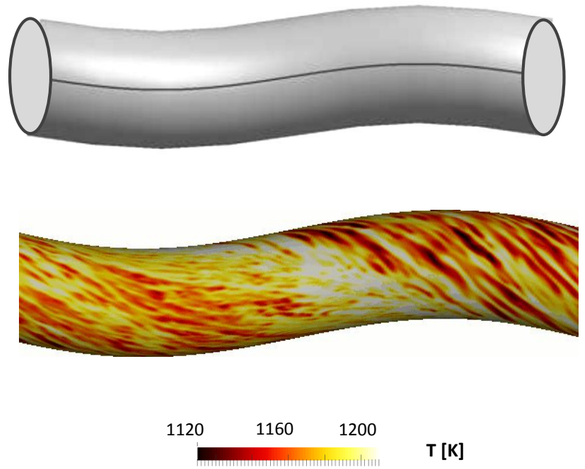
Nova Chemicals, **2002**; Linde Group; Muños et al., **2013**; Albright et al., **1988**; Muños et al., **2014**

ENHANCED STEAM CRACKING REACTOR DESIGNS



KBR / S+C **Straight / rifled fins**	Kubota **(Slit- / X-) MERT®**	Lummus/Sinopec **IHT®**	Technip **Swirl Flow Tube®**
1988, 2002, 2011	1996, 2003, 2009	2009	2011
			
			

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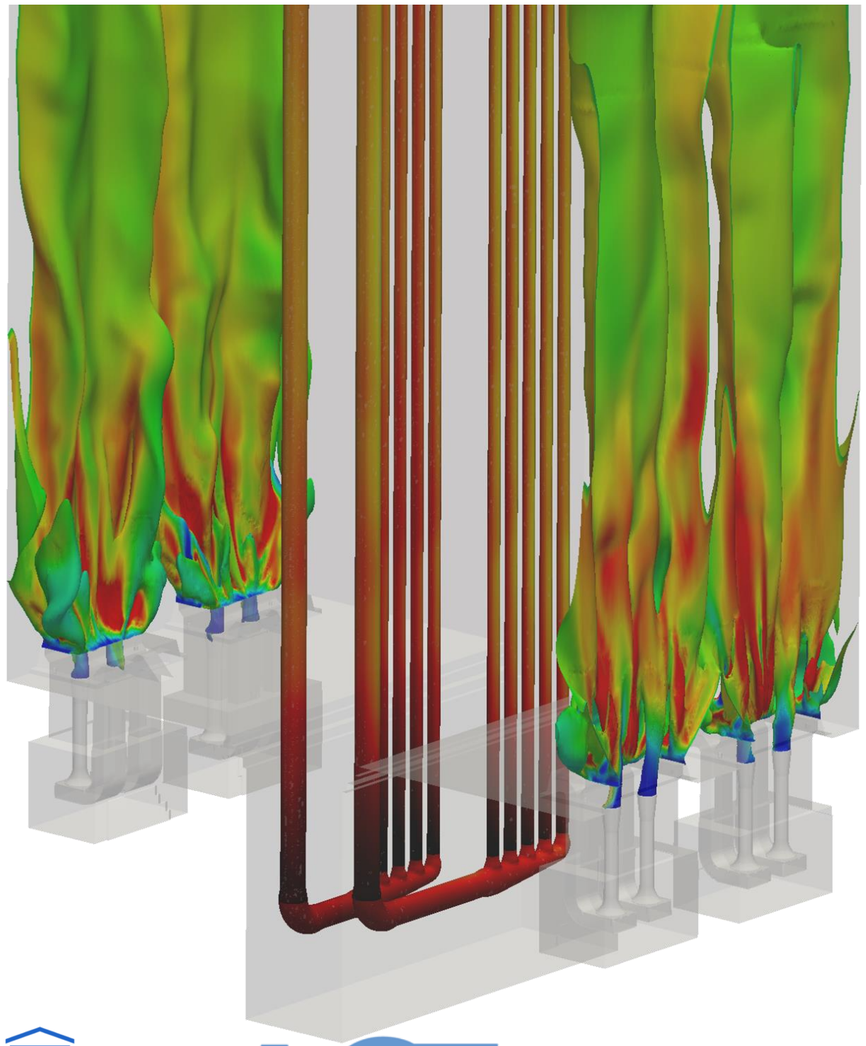
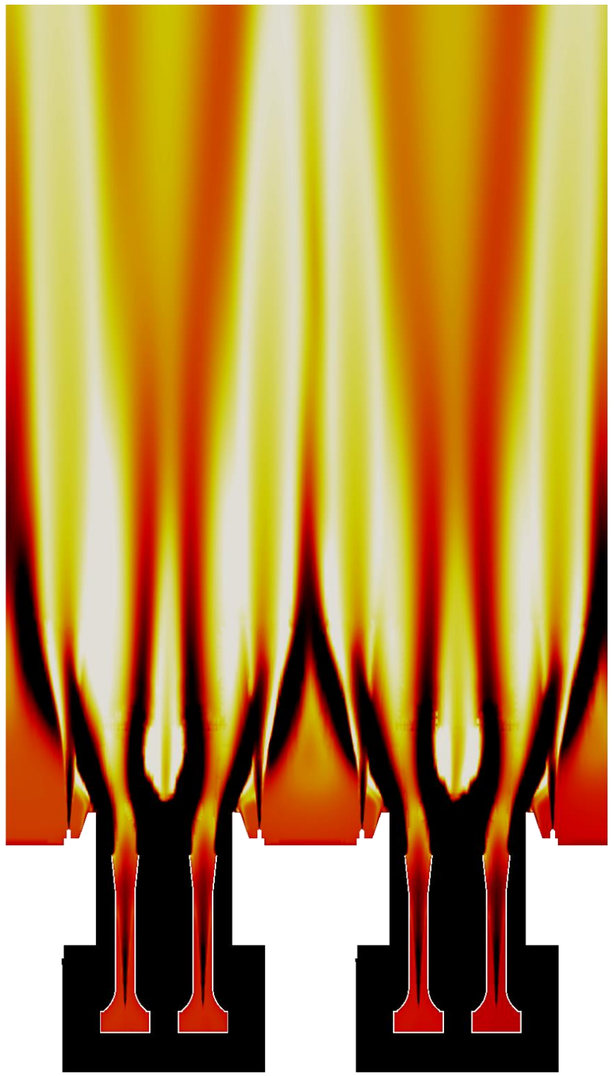
Van Cauwenberge, D. J. et al. Chem. Eng. J. **2015**, 282, 66-76.

FURNACE MODELLING USING CFD





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PREDICTION OF TURBULENT REACTIVE FLOWS

PRETREF: http://www.pretref.ugent.be/

Contact: dr. Georgios Maragkos (Georgios.Maragkos@UGent.be)

A project by **Ghent University** which aims to develop a flexible, open source **Large-Eddy Simulations (LES) Computational Fluid Dynamics (CFD)** code-base for multiscale modelling of several multidisciplinary applications.

Objectives defined in the following fields

1. Reduced chemistry
2. Sprays
3. Turbulent steady spray flames
4. Unsteady sprays, in internal combustion engines
5. Fire dynamics

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HPC-UGENT HARDWARE

	#nodes	CPU	Mem/node	Diskspace/node	Network	Online since…
 **Raichu**	64	2 x 8-core Intel E5-2670 (Sandy Bridge @ 2.6 GHz)	32 GB	400 GB	GbE	January 2013
 **Delcatty**	160	2 x 8-core Intel E5-2670 (Sandy Bridge @ 2.6 GHz)	64 GB	400 GB	FDR IB (6.5 GB/s)	November 2013
 **Phanpy**	16	2 x 12-core Intel E5-2680v3 (Haswell-EP @ 2.5 GHz)	512 GB	3 x 400 GB (SSD)	FDR IB (6.5 GB/s)	July 2015
 **Golett**	200	2 x 12-core Intel E5-2680v3 (Haswell-EP @ 2.5 GHz)	64 GB	500 GB	FDR-10 IB (5.0 GB/s)	July 2015
 **Swalot**	128	2 x 10-core Intel E5-2660v3 (Haswell-EP @ 2.5 GHz)	128 GB	1000 GB	FDR IB (6.5 GB/s)	August 2016

HPC-UGENT +TIER-1 HARDWARE

	#nodes	CPU	Mem/node	Diskspace/node	Network	Online since…
 **Raichu**	64	2 x 8-core Intel E5-2670 (Sandy Bridge @ 2.6 GHz)	32 GB	400 GB	GbE	January 2013
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 **Swalot**	128	2 x 10-core Intel E5-2660v3 (Haswell-EP @ 2.5 GHz)	128 GB	1000 GB	FDR IB (6.5 GB/s)	August 2016
 **Tier-1a Muk**	528	2 x 8-core Intel E5-2670 (Sandy Bridge @ 2.6 GHz)	64 GB	500 GB	FDR IB (6.5 GB/s)	July 2013
 **Tier-1b BrENIAC**	580	2 x 14-core Intel E5-2680v4 (Broadwell @ 2.4 GHz)	128 GB/256 GB	128 GB (SSD)	EDR IB (11.75 GB/s)	January 2017

THE NEXT STAGE: USING TIER-1

Information on project access
https://www.vscentrum.be/en/access-and-infrastructure/project-access-tier1.

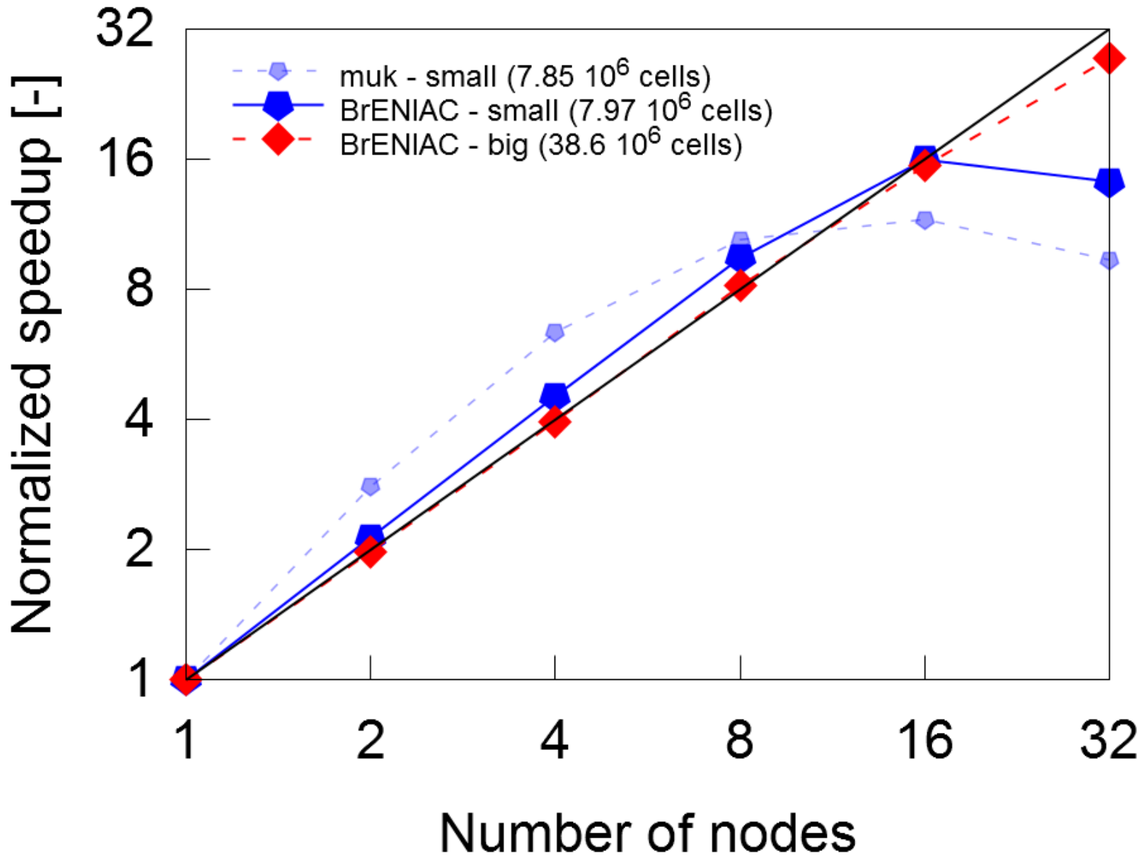
- Project proposal in a single document (maximum 17 pages)
- Scientific relevance is demonstrated by framing the calculation time in an approved project
- Next cut-off date for proposals: February 5th, 2018.
- Possibility of requesting a starting grant (continuous call)
- FWO bears all the cost but the number of nodedays is limited

- Nearly identical in use compared to UGent Tier-2 machines (modules, scheduler, job-scripts)
- Major difference: accounting system to keep track of consumed nodedays
- Connection between BrENIAC (@KULeuven) and UGent via BelNet (1 Gbps).
- Request software (well in advance) via hpcinfo@icts.kuleuven.be

SCALING OF OPENFOAM ON TIER-1

Scaling on Tier-1b

muk – small: OpenFOAM/2.2.0-ictce-4.1.13 / Intel MPI v4.1.0
BrENIAC – small: OpenFOAM/2.2.0-intel-2016a / Intel MPI v5.1.3
BrENIAC – big: OpenFOAM/2.2.0-intel-2016a / Intel MPI v5.1.3



Better scaling compared to Tier-1a – Muk

Fast interconnect (EDR IB) reduces wall-clock time and maintains efficiency while scaling on more cores

Bottleneck: pre- and postprocessing

Remote desktop on Tier-1b login node with GPU via NoMachine client.

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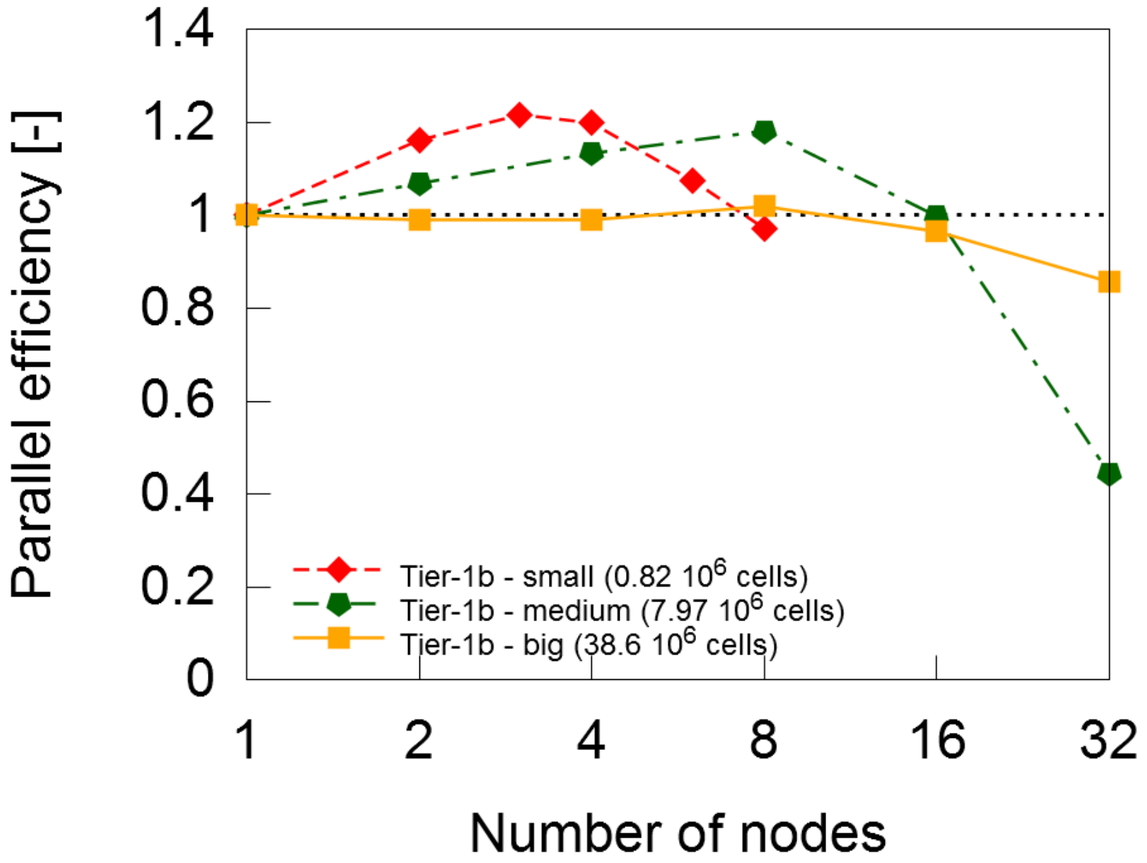
OPENFOAM ON TIER-1

Scaling on Tier-1b

BrENIAC – small: OpenFOAM/2.2.0-intel-2016a / Intel MPI v5.1.3
BrENIAC – medium: OpenFOAM/2.2.0-intel-2016a / Intel MPI v5.1.3
BrENIAC – big: OpenFOAM/2.2.0-intel-2016a / Intel MPI v5.1.3



Super-linear scalability due to cache effect and better accomodation of memory patterns across multiple nodes

The choice of decomposition method (scotch, simple, metis, etc.) is important for the number of processor faces

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Axtmann, G. et al. *High Performance Computing in Science and Engineering ´16,* ***2016***
Nagel, W. E. et al., Eds. Springer International Publishing, **2016,** 413-424.

GENERAL BEST PRACTICES

Use modules compiled with recent compiler toolchains (UGent Tier-2)

```
------------------------------------ /apps/gent/CO7/sandybridge/modules/all ---------------
   OpenFOAM/2.2.2-intel-2017a    OpenFOAM/2.4.0-intel-2017a    OpenFOAM/4.0-intel-2016b
   OpenFOAM/2.3.1-intel-2017a    OpenFOAM/3.0.1-intel-2016b    OpenFOAM/4.1-intel-2017a (D)

------------------------------------ /apps/gent/SL6/sandybridge/modules/all ---------------
   OpenFOAM-Extend/3.2-intel-2016a    OpenFOAM/2.3.1-intel-2015a
   OpenFOAM/2.1.1-ictce-4.0.10        OpenFOAM/2.4.0-intel-2015b
   OpenFOAM/2.2.0-ictce-4.1.13        OpenFOAM/3.0.0-intel-2015b-eb-deps-Python-2.7.10
   OpenFOAM/2.2.2-intel-2015a         OpenFOAM/3.0.1-intel-2016b
   OpenFOAM/2.2.2-intel-2016a         OpenFOAM/4.0-intel-2016b
   OpenFOAM/2.3.0-intel-2014b
```

Run your job from the appropriate location, excessive I/O on low-bandwidth locations will seriously slow down your job

$VSC_DATA: not meant for calculations, only long-term storage

$VSC_SCRATCH: default scratch on 15k disks

$VSC_SCRATCH_NODE: /tmp location on local node, only accessible as long as the jobs is running, suited for single-node jobs

DOCUMENTATION AND TRAINING

Documentation is available at

- https://www.ugent.be/hpc/en/support/documentation.htm
- https://www.vscentrum.be/en/user-portal
- (http://hpc.ugent.be/userwiki, being phased out)

Regular training sessions (HPC-UGent intro, Introduction to Linux,…)

- https://www.ugent.be/hpc/en/training
- https://www.vscentrum.be/en/education-and-trainings

Support and new software installations

- hpc@ugent.be

ACKNOWLEDGEMENTS

HPC-UGent staff!

Stijn De Weirdt
technical lead

Ewald Pauwels
team lead

Kenneth Hoste
user support & training

Wouter Depypere
sysadmin, hardware

Jens Timmerman
sysadmin, security

Kenneth Waegeman
sysadmin, storage

Andy Georges
sysadmin, tools & testing

Alvaro Simon Garcia
cloud, user support

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Colleagues @LCT

fwo

M2D2R2C Methusalem programma

VSC Vlaams Supercomputer Centrum

HPC UGENT

PRETREF

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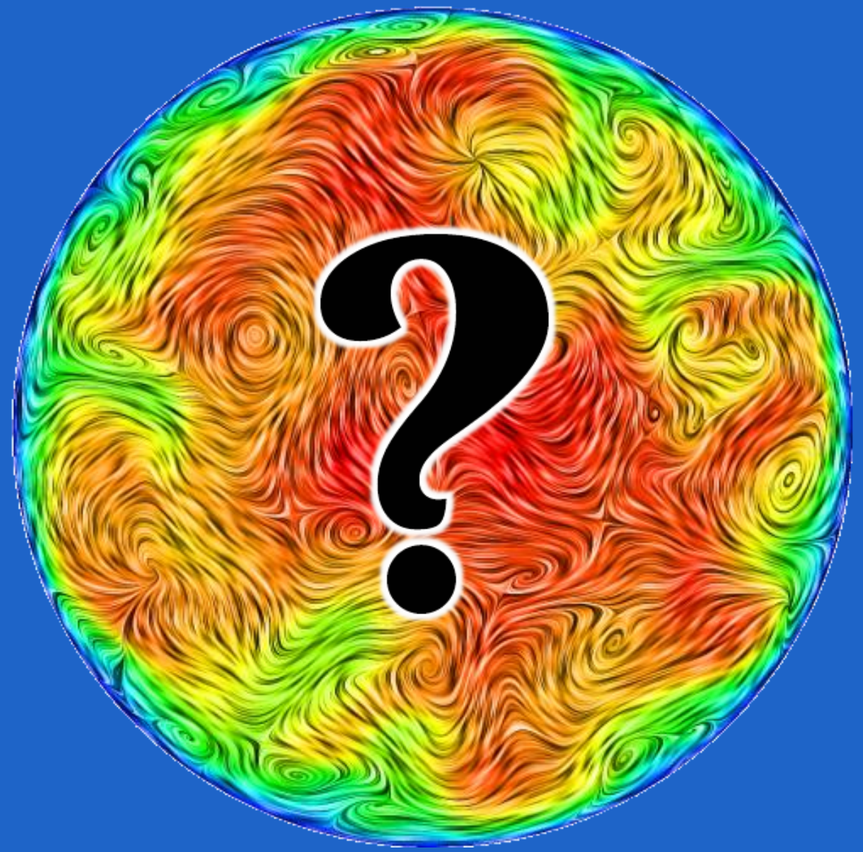
https://www.lct.ugent.be



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