

REVCNOSTICS  
Science & Engineering

REVCNOSTICS

UNDERSTAND YOUR  
**CATALYST**

OPTIMIZE YOUR  
**REACTOR**

REVCNOSTICS  
Science & Engineering

REACtor diagNOSTICS

# REACNOSTICS

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REACNOSTICS specializes in reaction engineering with a primary focus on enhancing the efficiency and sustainability of catalytic reactors.

Catalytic reactors are central to numerous industrial processes, with approximately 80% of chemical reactions in industry relying on catalysts, most of which are heterogeneous. Catalytic reactors typically operate under high temperature and pressure, handling toxic, flammable, or even explosive chemicals.





Despite the crucial role of heterogeneous catalytic reactions in the chemical industry, the processes within catalytic reactors often remain elusive. Heterogeneous catalysts are dynamic systems that change properties based on local conditions, much like a chameleon adapting to its environment. Since reactors are typically non-transparent, optimizing them poses a significant challenge.

REACNOSTICS offers reactor hardware and services that provide insights into catalytic reactors, enabling knowledge-based optimization.

**Our mission is to make catalytic reactors transparent.**

A handwritten signature in black ink, appearing to read 'M. Schmidt', written in a cursive style.

**Michael Schmidt**

- CEO -





## Conventional Approach

Reactants

Black box

Reactants

Products

Waste

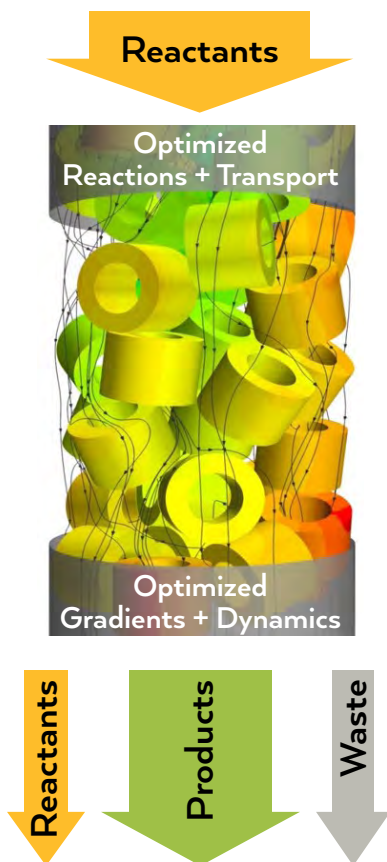
Catalytic reactors are non-transparent, they are a black box.

Measurements are restricted to inlet and outlet flows. Mathematical models are often too simplified and reactor optimization is based on trial and error.

## Making Catalytic Reactors

# Transparent

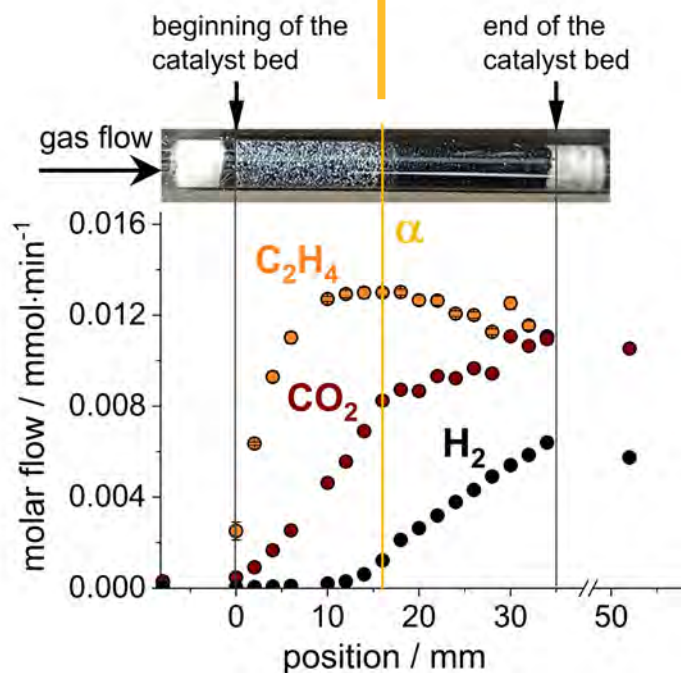
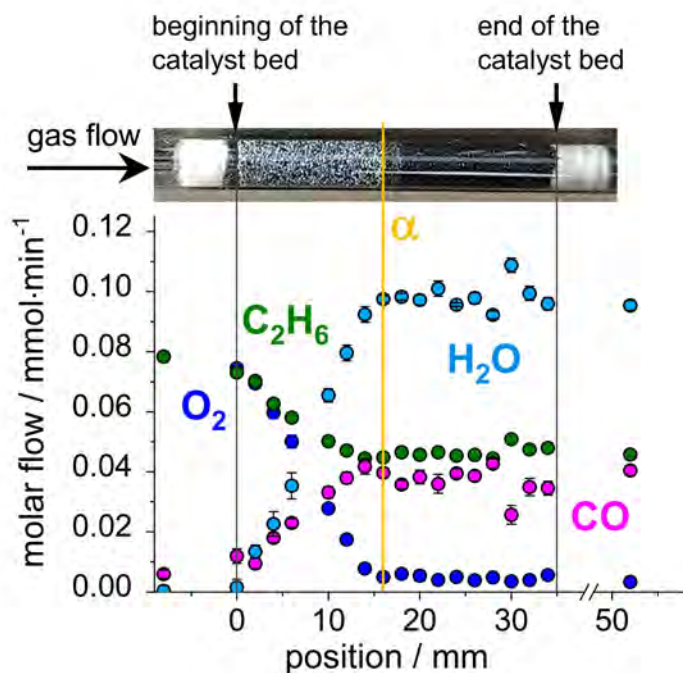
## REACNOSTICS Approach



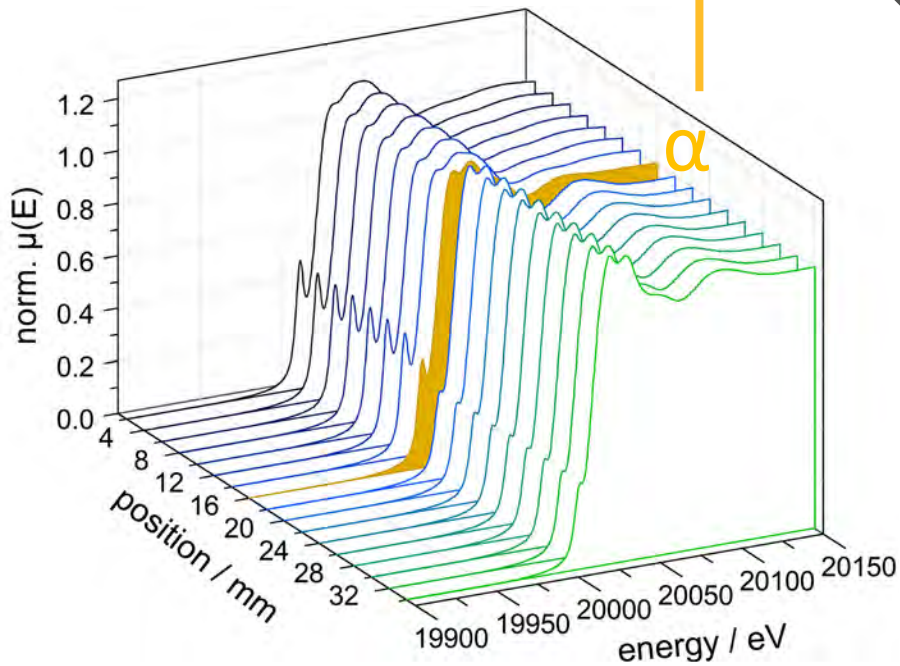
REACNOSTICS offers reactor hardware which allows measuring concentration and temperature profiles inside the reactor.

REACNOSTICS' reactor hardware enables the characterization of the local catalyst state by spatially resolved spectroscopy.

# Profile Measurements & Catalyst Dynamics



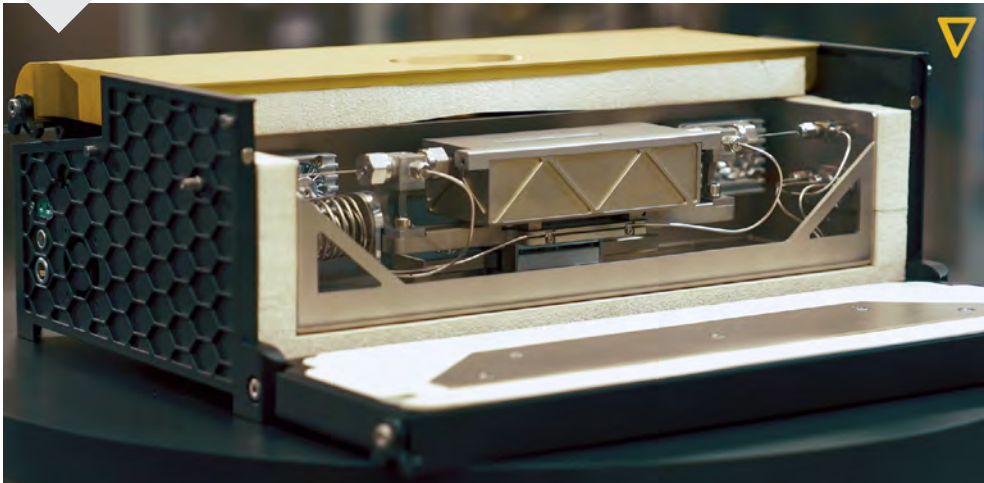
Reactor diagnostics  
– unraveling chemical  
processes inside catalytic  
reactors by measuring  
concentration, temperature  
and spectroscopic profiles.



# Products

Compact  
Profile  
Reactor  
(CPR)

CPR  
Turnkey  
Solutions

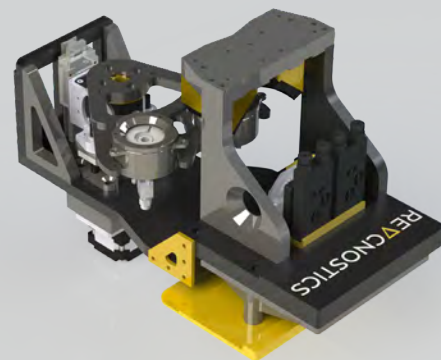






$\mu$ -DRIFTS  
Cell

Bench &  
Pilot Scale  
Profile  
Reactors





- » Compact fixed bed reactor with optional optical access (Raman, XRD)
- »  $T_{\max} = 550\text{ }^{\circ}\text{C}$
- »  $P_{\max} = 80\text{ bar}$
- » 60 mm isothermal zone for catalyst bed
- » 4 mm bed diameter
- » Up to 400 ml/min flow rate



- » Heated interior to avoid condensation
- » Trigger for external analytical devices (GC, MS, Raman)
- » Control unit
- » Browser based software included



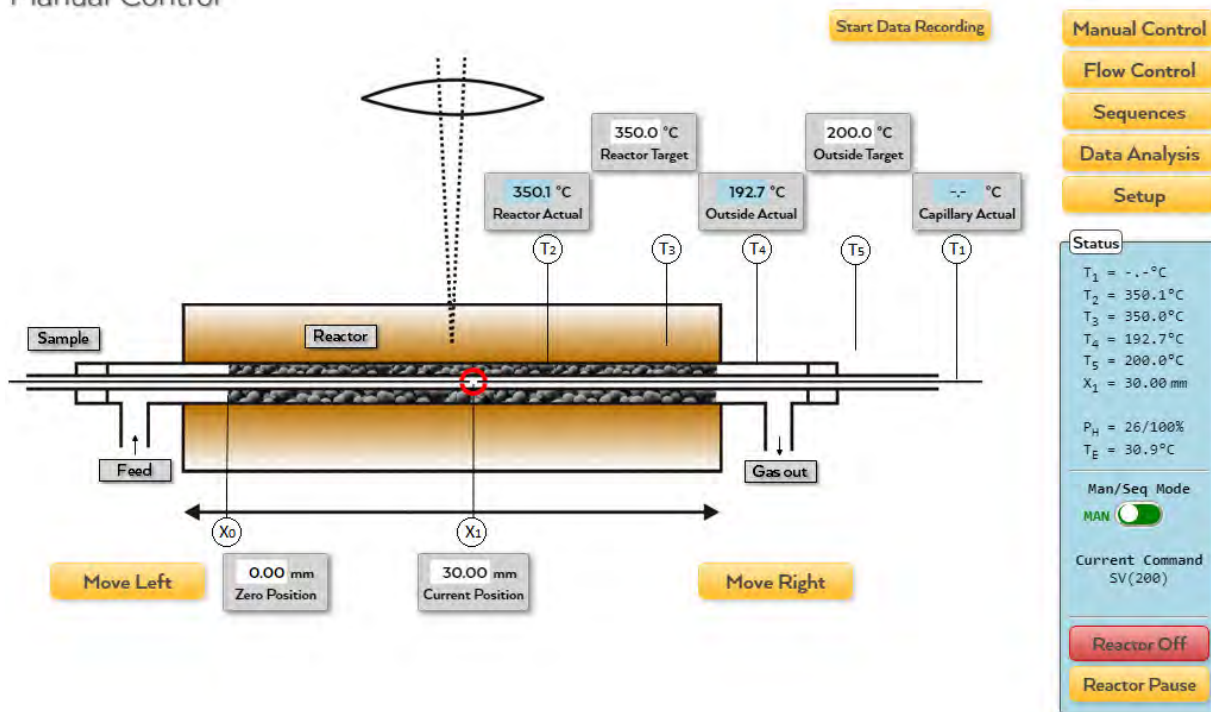
- Optional:
- » Gas and liquid feed supply
  - » Evaporator
  - » Pressure control
  - » Condensation trap
  - » Analytics
  - » Pyrometer
  - » Ventilated rack
  - » Gas warning system

# Compact Profile Reactor

## COMPACT PROFILE REACTOR

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Manual Control



# CPR Tailored - Turnkey Solutions



## Optional components:

- » Mobile rack or table
- » Exhaust system
- » Gas and liquid feed units
- » Evaporator unit
- » Compression stage
- » Compact Profile Reactor
- » Pressure control unit
- » Condensation trap
- » Analytical device
- » Process control and safety system





## Applications:

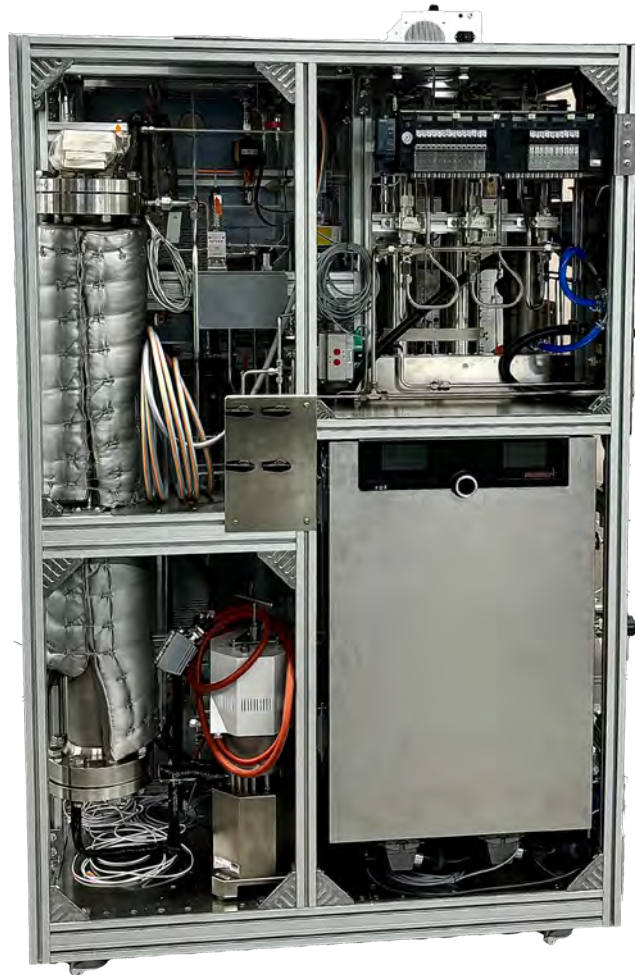
- » Methanol synthesis
- » CO<sub>2</sub> Methanation
- » DME synthesis
- » DME reforming
- » Methanol reforming
- » Methane reforming
- » Fischer-Tropsch synthesis
- » Oxidative dehydrogenation
- » MtG process
- » E-fuels
- » HPPO process
- » Ammonia oxidation
- » Ethylene oxide synthesis
- » Catalytic partial oxidation

# Bench & Pilot Scale Profile Reactors

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## E-Fuels Mini-plant

- » Profile and production reactor
- » Stand-alone system or integration between upstream & downstream units
- » Condensation trap
- » Mobile rack with integrated safety system
- » Exhaust
- » Gas sensors
- » Process control system



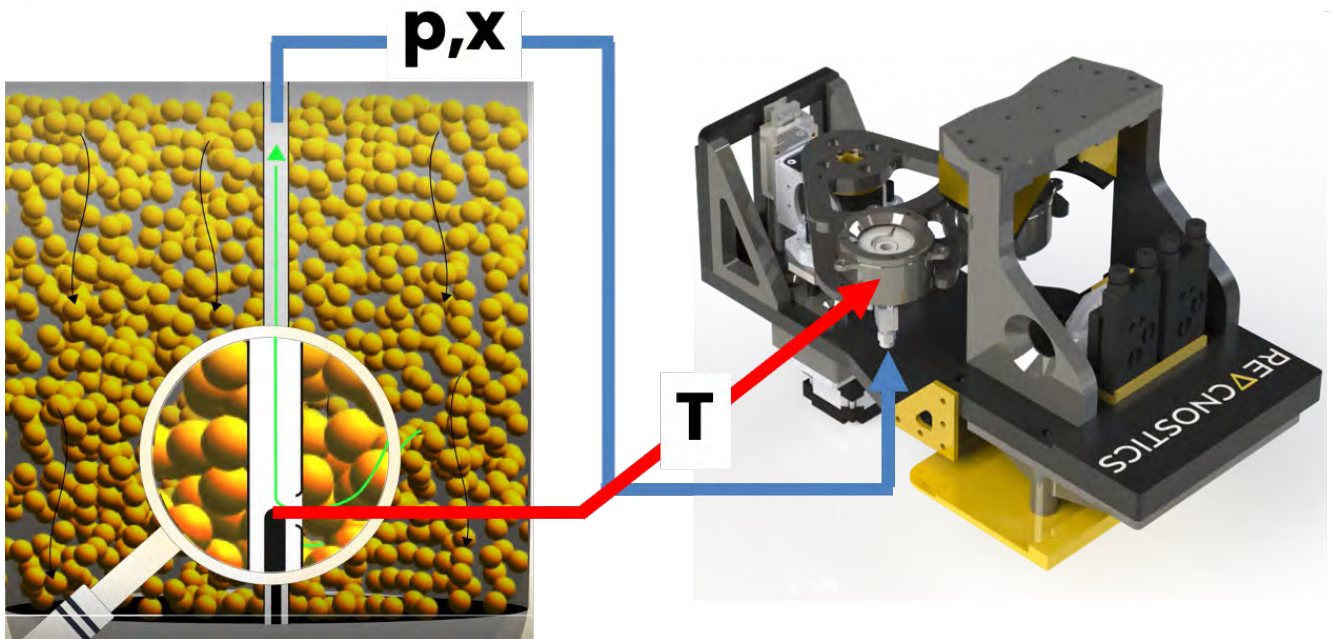


## Ethylene Oxide Pilot Plant

- » Modular gas and liquid feed supply
- » Evaporator
- » Compression stage
- » Analytics
- » Safety system



$$\mu_i(T, p, \mathbf{x}) = \mu_i^*(T, p) + RT \ln \left[ \frac{\bar{f}_i(T, p, \mathbf{x})}{f_i^*(T, p)} \right]$$





# - Potential Operando Spectroscopy (IPOS)

In IPOS the catalytic reactor is equipped with spatial profiling and the sampled reaction mixture is transferred into a spectroscopic cell containing a tiny amount of the same catalyst as in the reactor. Temperature and pressure are adjusted to the local reactor values.

The catalyst in the spectroscopic cell sees the same chemical potential as the catalyst locally in the reactor and therefore shows the same adsorbates, oxidation state, crystal structure etc.

Any spectroscopic method, which can

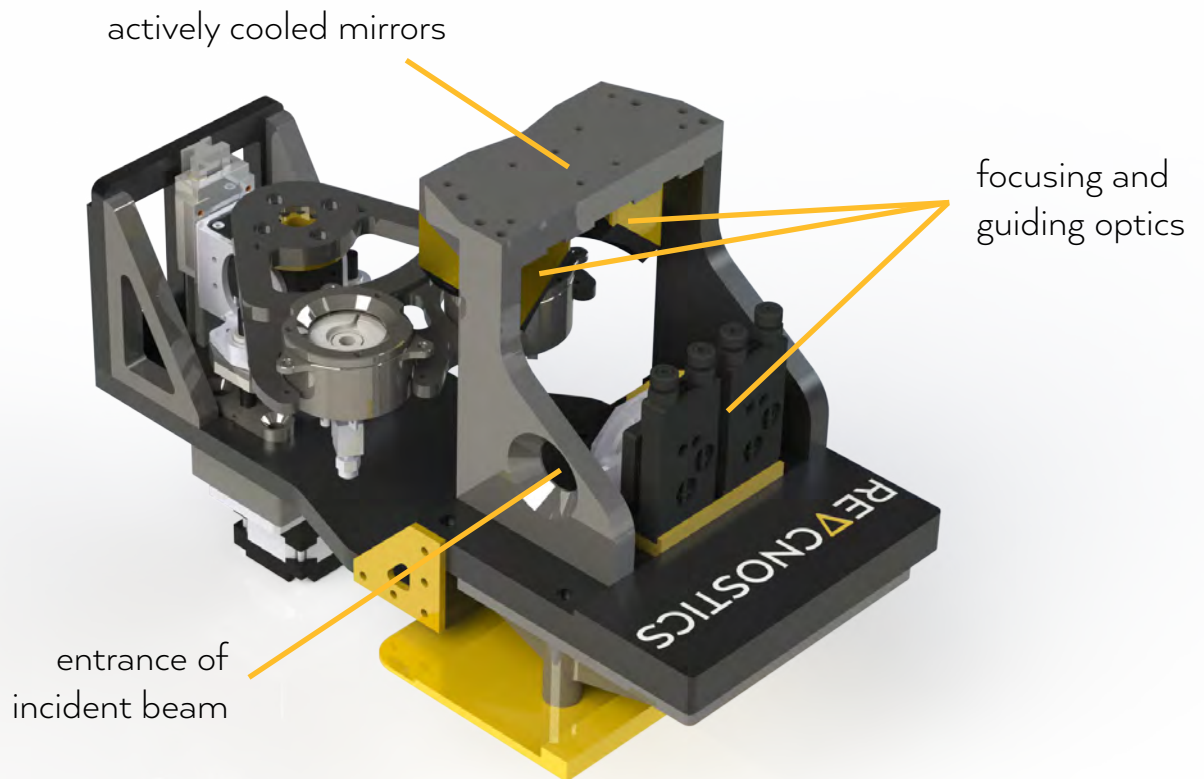
be applied at reactor conditions, can be combined with any catalytic reactor, in principle even industrial production reactors. The spectroscopic cell can be designed to meet the demands of the measurement method without that compromises have to be made resulting from the dual use as a catalytic reactor, like in traditional operando spectroscopy. The question of which reaction conditions to study is answered automatically, as the reactor sets the reaction conditions inside the spectroscopic cell.

## $\mu$ -DRIFTS - Diffusive Reflectance IR-Spectroscopy

- » Cell designed for operando and iso-potential spectroscopy
- » 3x higher signal intensity compared to other DRIFTS accessories
- » Two individually controlled reaction chambers for catalyst and reference sample
- » Temperature measurement in catalyst bed
- » Minimized dead volume
- »  $T = 50 - 550\text{ }^{\circ}\text{C}$
- »  $p = 1 - 10\text{ bar}$ 
  - » Spectral range  $1000 - 5000\text{ cm}^{-1}$
  - » Heated windows to avoid condensation
  - » Software for automated operation

# $\mu$ -DRIFTS Cell

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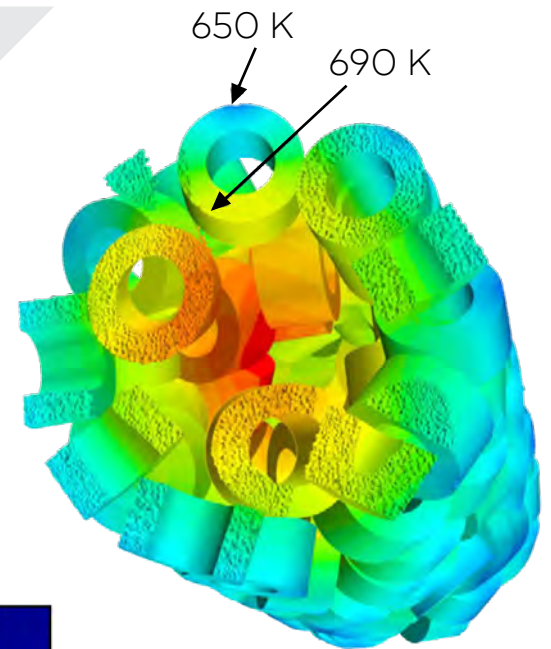
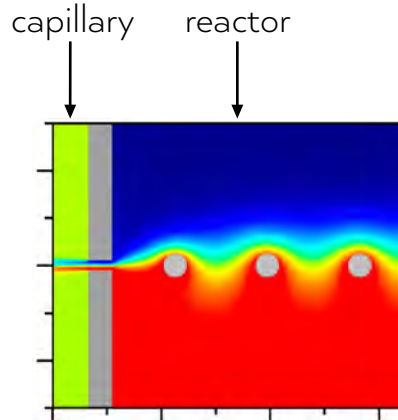


» For further information, see brochure „REACNOSTICS  $\mu$ -DRIFTS“

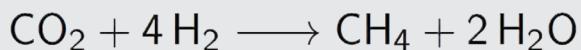
# Modelling & Data Science

## CFD simulations

- » Understanding and interpretation of experimental reactor profiles
- » Discrimination of physical and chemical effects
- » Scrutinizing the invasiveness of the sampling process







$$k = A_0 T^\beta \exp \left[ \frac{-E_a}{RT} \right]$$

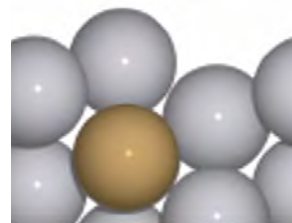
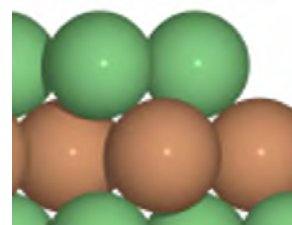
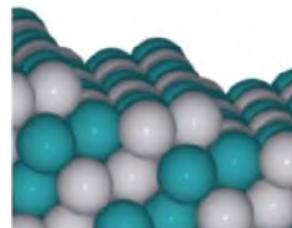
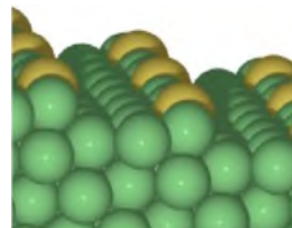
profiles  $\longrightarrow$  AI  $\longrightarrow$  kinetic parameters

### Kinetic models

- » Automatic generation of kinetic reaction models from profile data
- » Artificial intelligence (AI) optimizes model discrimination
- » AI drives data acquisition through active learning

### AI-based screening for catalysts

- » Improved performance (activity, selectivity, stability)
- » Novel materials for new processes
- » Experimental feedback loops



# Services

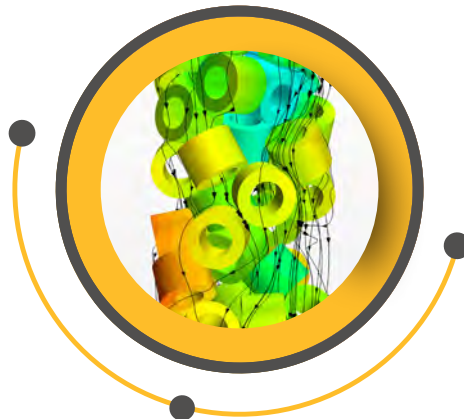
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REACNOSTICS provides reactor hardware, measurement services and modeling capabilities to help customers optimize their catalytic reactors based on knowledge. We strive to make the reactor „transparent“ by measuring and/or modeling the concentration, temperature and flow field inside the reactor and characterize the local state of the catalyst by spatially resolved spectroscopy.

## Measure



## Model



## Optimize



# Customer

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## Industry

- » Understand reactor and catalyst behavior
- » Optimize reactor design and reaction conditions
- » Increase conversion, selectivity and yield
- » Extend catalyst lifetime
- » Minimize waste and reactor downtime

## Academia

- » Spatially resolved investigation of new catalyst materials
- » Flexible profile reactors for various reaction conditions (gas-solid, liquid-solid, gas-liquid-solid)
- » Establishing structure-activity correlations by spatially resolved operando-spectroscopy

# Benefits

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[www.reacnostics.com](http://www.reacnostics.com)

REACNOSTICS specializes in catalytic reaction engineering and operando catalysis research. We offer novel measurement hardware and modeling services to enable our customers optimizing their catalytic processes, reducing costs and environmental impact while maximizing profitability.



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