Learnings from reactor explosion:

Catalyst reactivity learnings for energy transition processes

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Catalyst/adsorbent: inert “facilitator” or reactant?

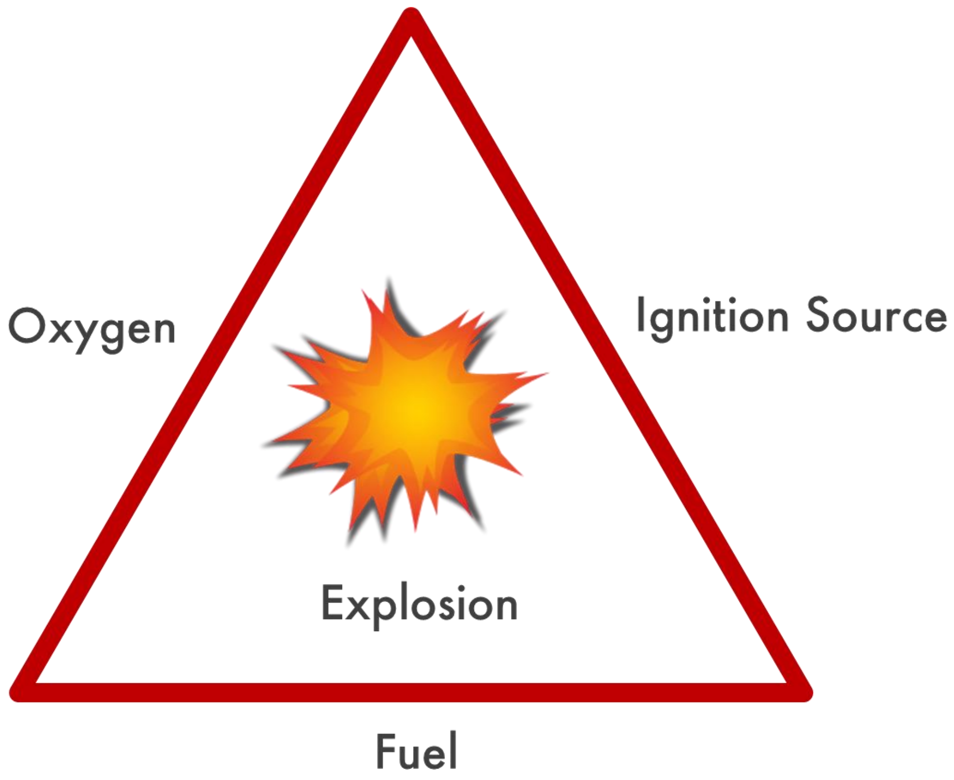
Do you understand exactly what reactions happen during start-up?

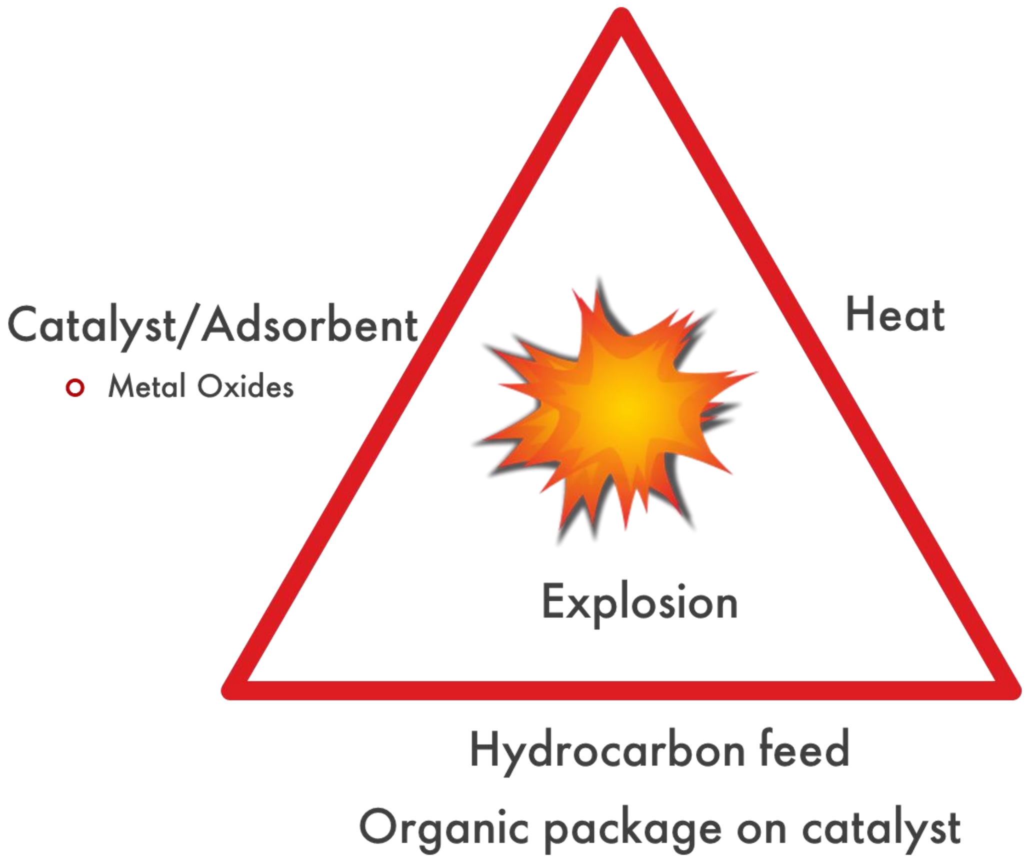
Explosion – main catalyst learnings

- Tons of latent oxygen present in reactor

- Latent (reactive) oxygen from catalysts can react exothermally with a hydrocarbon
  - Exothermic reaction: Hydrocarbon + copper chromite catalyst → gas

- Crucial to review the reactive hazards in both transient and steady state operations


Oxygen
Ignition Source
Explosion
Fuel


Catalyst/Adsorbent
Metal Oxides
Heat
Explosion
Hydrocarbon feed
Organic package on catalyst

Catalyst/adsorbent: inert “facilitator” or reactant?

Could other systems have similar phenomena?

Shell’s approach for improved focus on risks during transient phases of start-ups with catalysts and adsorbents:

Catalyst Safety Assessment (CSA)

CSA screening tool

- Gibbs energy and Enthalpy:
  $M_xO_y + HC \rightarrow M + CO_2 + H_2O$
- Flow regime:
  liquid full/trickle phase/gas phase
- Metal oxide loading
- Calculation of maximum P and T
  if all metal oxides are converted

Medium/High risk systems

- Negative ΔG & ΔH_r
- Liquid full
- Trickle phase > 5% Metal oxides

Calorimetric experiments are considered

Experimental facilities @ Shell ETCA, the Netherlands

Processing biofeeds to make fuels

Stability certain bio-oils

	Without catalyst
Exotherms	320-390°C
Start exobar	320-350°C

Data given are indicative for certain triglycerides

Avoid hot spots in stagnant parts of the feed pre-heat train!

Effect catalysts on reactivity bio-oils

	Without catalyst	With catalyst
Exotherms	320-390^{o}C	220-300^{o}C
Start exobar	320-350^{o}C	220-360^{o}C

Data given are indicative for certain triglycerides

- Catalysts lower the reactivity temperature
- Consider a non-reactive start-up feed

Heat of Adsorption

Heat of ethylene adsorption

Large exotherm (40 to 650°C) in Guard bed methane feed section of an ethylene oxide unit

1. Upset upstream column → large amount of ethylene in methane
2. Ethylene adsorbs on guard bed → Moderate Temperature increase
3. $CuO + H_2 \rightarrow Cu + H_2O$ → Moderate Temperature increase
4. Local hotspots cause ethylene polymerisation → Large Temperature increase

Heat of ethylene adsorption

	Adsorbent
Current	$CuO/Cu(OH)_2/CuCO_3$ on activated carbon
Potential new	CuO/ZnO on aluminium oxide

Heat of ethylene adsorption

	Adsorbent	Heat of ethylene adsorption
Current	$CuO/Cu(OH)_2/CuCO_3$ on activated carbon	$-60\ J/g_{cat}$
Potential new	CuO/ZnO on aluminium oxide	$-5\ J/g_{cat}$

Heat of ethylene adsorption

	Adsorbent	Heat of ethylene adsorption	Ethylene polymerisation start temperature
Current	$CuO/Cu(OH)_2/CuCO_3$ on activated carbon	-60 J/g_{cat}	260°C
Potential new	CuO/ZnO on aluminium oxide	-5 J/g_{cat}	260°C

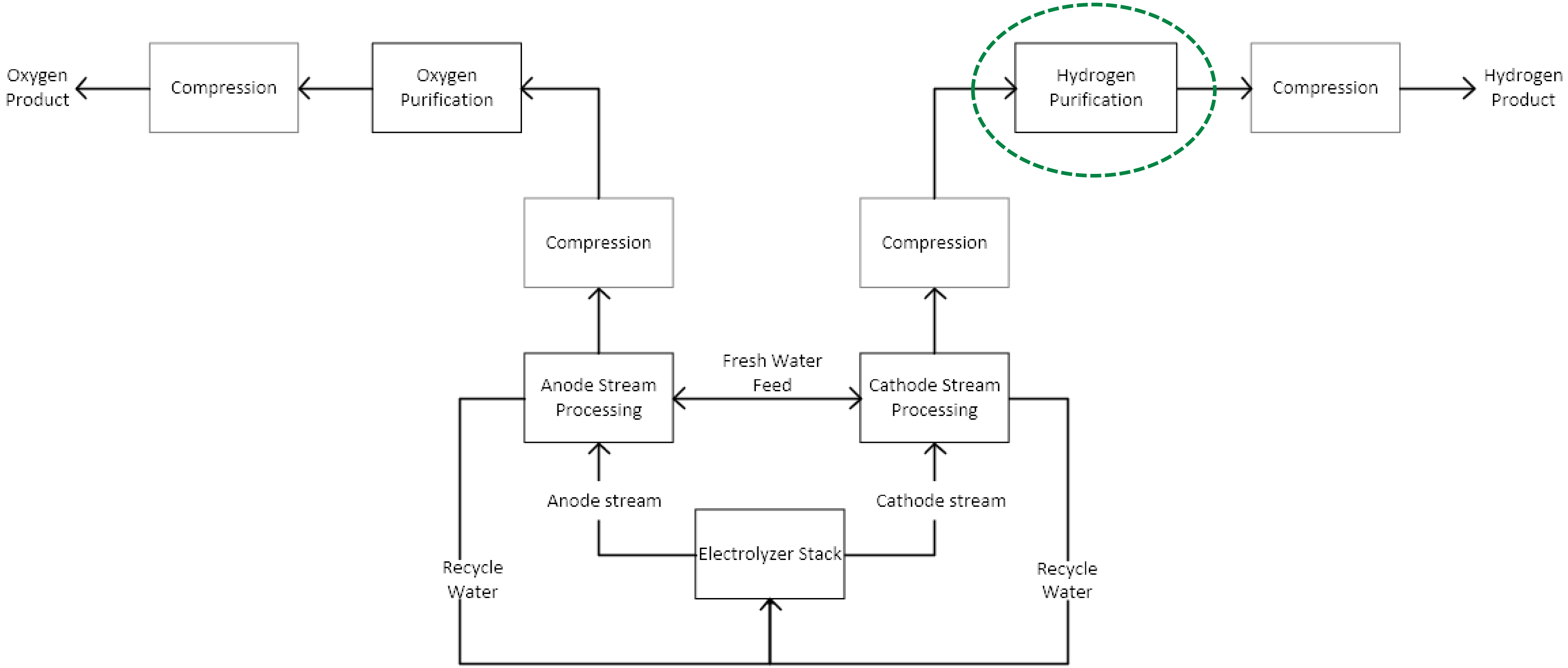
Heat of adsorption - learning

Taking into account Adsorption heat could make your process more robust

Transient modelling

Deoxygenation of H_2 from electrolysers

Schematic Green H_2 plant

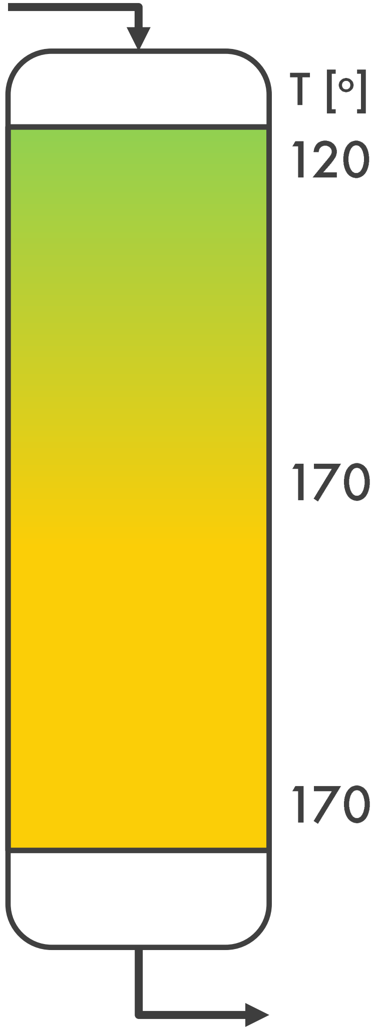


Some key challenges in designing deoxo units

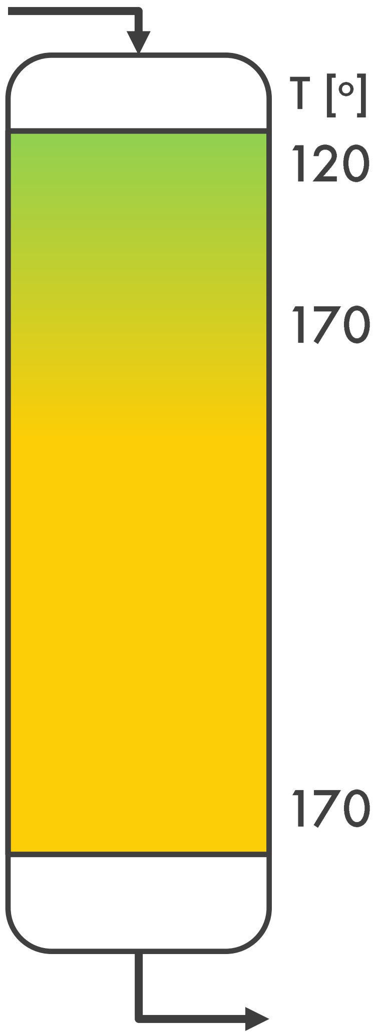
- Intermittent operation 0-100%
  - No wind → No power/electron → No production
- Change in flow and O_2 conc. (low to high) within minutes
- Exothermic reaction $H_2 + ½ O_2 → H_2O$
  - 17°C ΔT per 1000 ppmv of O_2

Potential for large Temperature fluctuations/waves

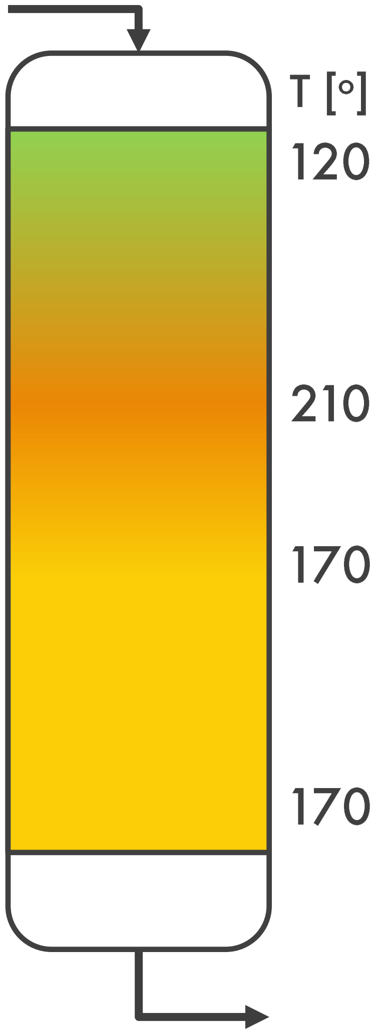
Case: Normal flow, 3000 ppm O_2



Case: 30% turn-down, 3000 ppm O_2



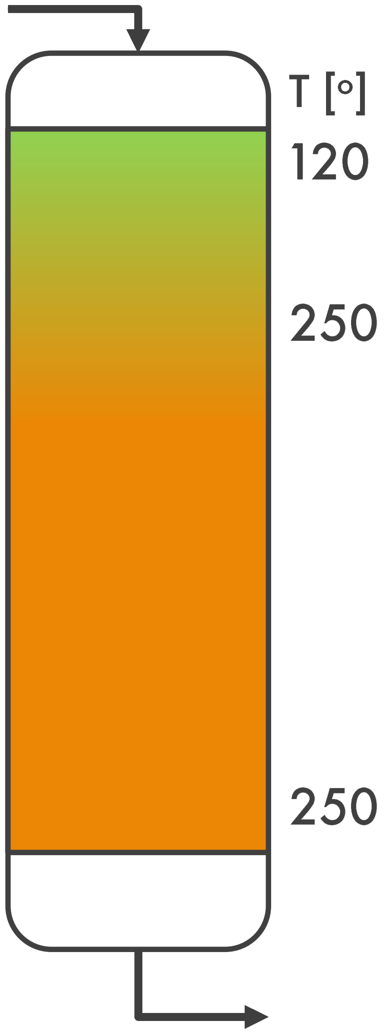
Case: from 30% turn-down to normal flow, 3000 ppm O_2



Info based on done rule of thumbs from [1]

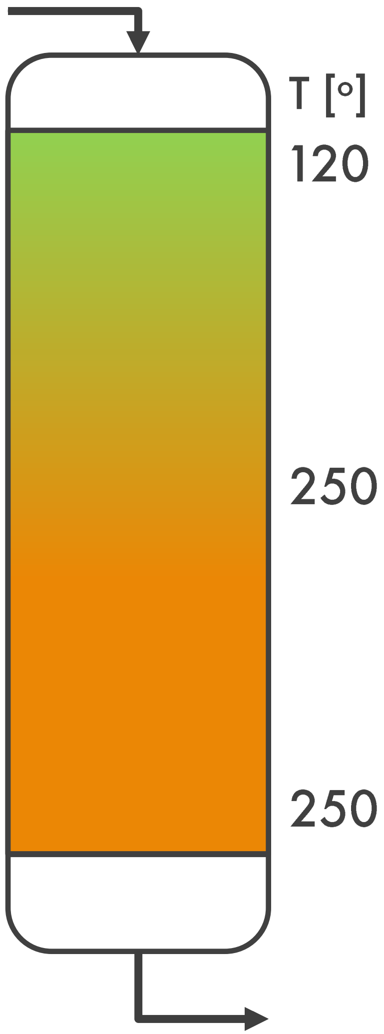
[1] Wrong-Way Behavior of Packed-Bed Reactors: II. Impact of Thermal Dispersion, V. Pinjala, Y. C. Chen, and D. Luss, AIChE Journal October 1988 Vol. 34, No. 10., https://doi.org/10.1002/aic.690341010

Case: from 30% turn-down 7000 ppm O_2 to normal flow 7000 ppm



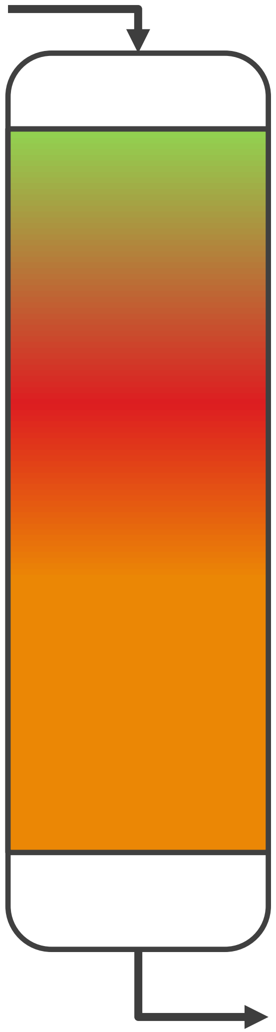
Phase	Flow	O_2 [ppmv]
1	30%	7000

Case: from 30% turn-down 7000 ppm O_2 to normal flow 7000 ppm



Phase	Flow	O_2 [ppmv]
1	30%	7000
T1	100%	7000
T2	100%	7000
2	100%	7000

Case: from 30% turn-down 7000 ppm O_2 to normal flow 7000 ppm



Phase	Flow	O_2 [ppmv]
1	30%	7000
T1	100%	7000

High temperature

- Effect on catalyst?
- Can be issue for downstream equipment

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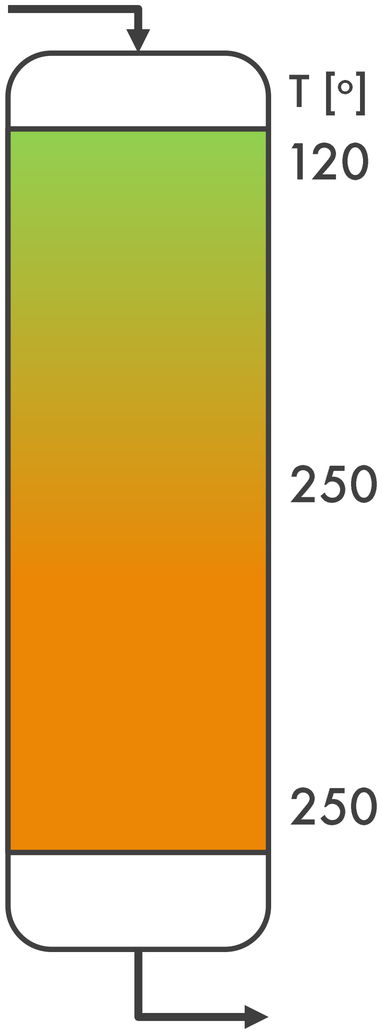

Phase	Flow	O_2 [ppmv]
1	30%	7000
T1	100%	7000
T2	100%	7000
2	100%	7000

Transient modelling - learnings

- Be aware of wrong way behaviour
- Heat effects can add up, causing temperatures above the adiabatic temperature rise

Summary

Summary

Catalyst/adsorbent can be a reactant!

- Focus on transient conditions for catalysts/adsorbents
  - Start-up is crucial:
    Catalyst in reactive state + transient operating conditions → increased risk
  - Metal oxides can be oxidizing agents for hydrocarbons

- Think transient!
  - Exothermicity of bio-oils
  - Heat of adsorption
  - Transient modelling: temporary high temperature

Summary

Shell's Catalyst Safety Assessment

is a process that helps

make catalyst/adsorbent start-ups safer.

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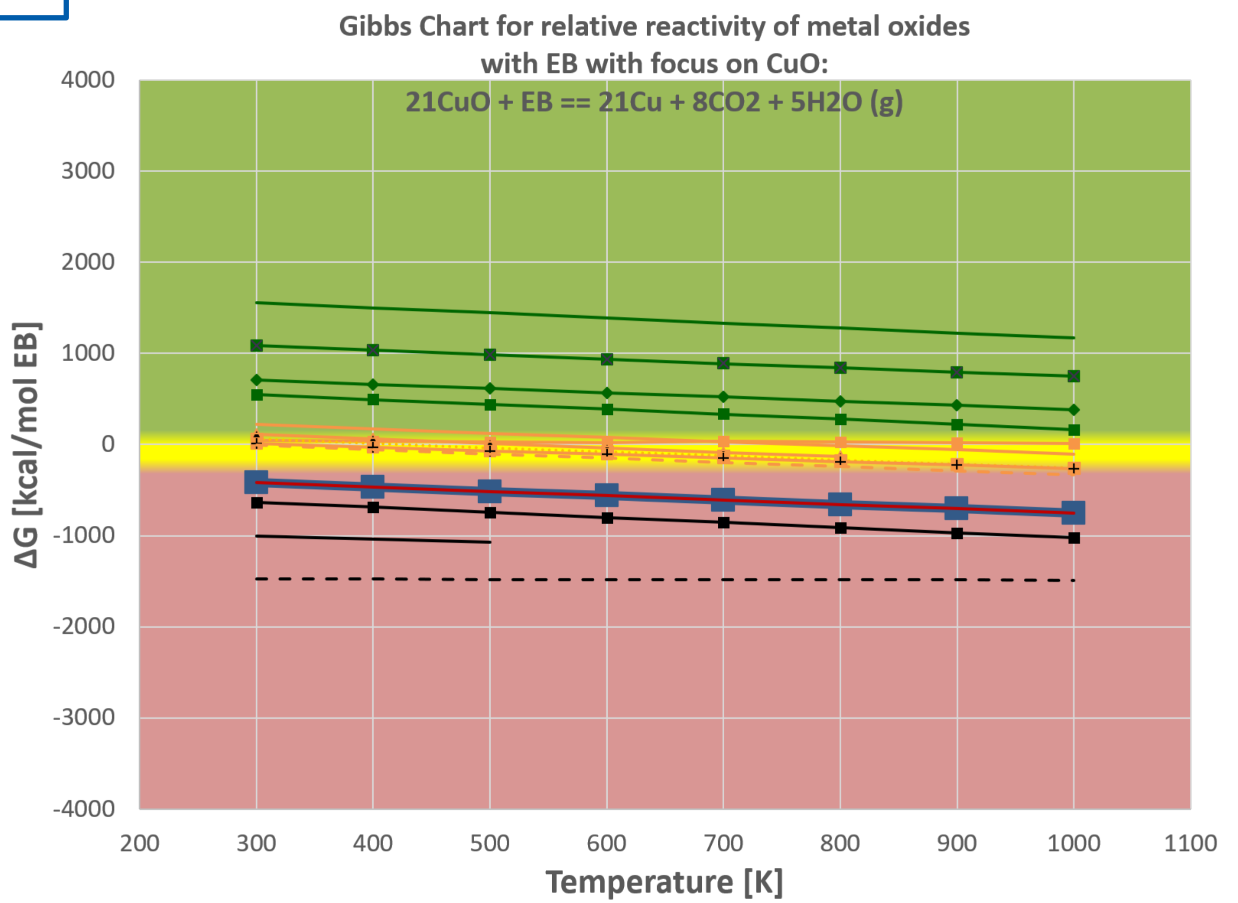
Back-up slides

Gibbs plot

Pick Metal oxide and hydrocarbon

Input: Choose Metal oxide and Hydrocarbon	
Focus Metal oxide	CuO
Hydrocarbon	EB

$$M_xO_y + C_kH_lO_m \rightarrow M + CO_2 + H_2O\ (g)$$



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