Learnings from a reactor explosion:
Towards safer start-ups of catalysts systems

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This **presentation** may contain certain forward-looking non-GAAP measures such as **cash capital expenditure** and **divestments**. We are unable to provide a reconciliation of these forward-looking Non-GAAP measures to the most comparable GAAP financial measures because certain information needed to reconcile those Non-GAAP measures to the most comparable GAAP financial measures is dependent on future events some of which are outside the control of Shell, such as oil and gas prices, interest rates and exchange rates. Moreover, estimating such GAAP measures with the required precision necessary to provide a meaningful reconciliation is extremely difficult and could not be accomplished without unreasonable effort. Non-GAAP measures in respect of future periods which cannot be reconciled to the most comparable GAAP financial measure are calculated in a manner which is consistent with the accounting policies applied in Shell plc’s consolidated financial statements.

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Catalyst/adsorbent: inert “facilitator” or reactant?

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

Explosion: root cause

- Exothermic reaction: Hydrocarbon + copper chromite catalyst → gas

$CuCr_2O_4$ or $CuCrO_3$ → Cr^{III} or Cr^{IV}

$CuCrO_4$ → Cr^{VI}

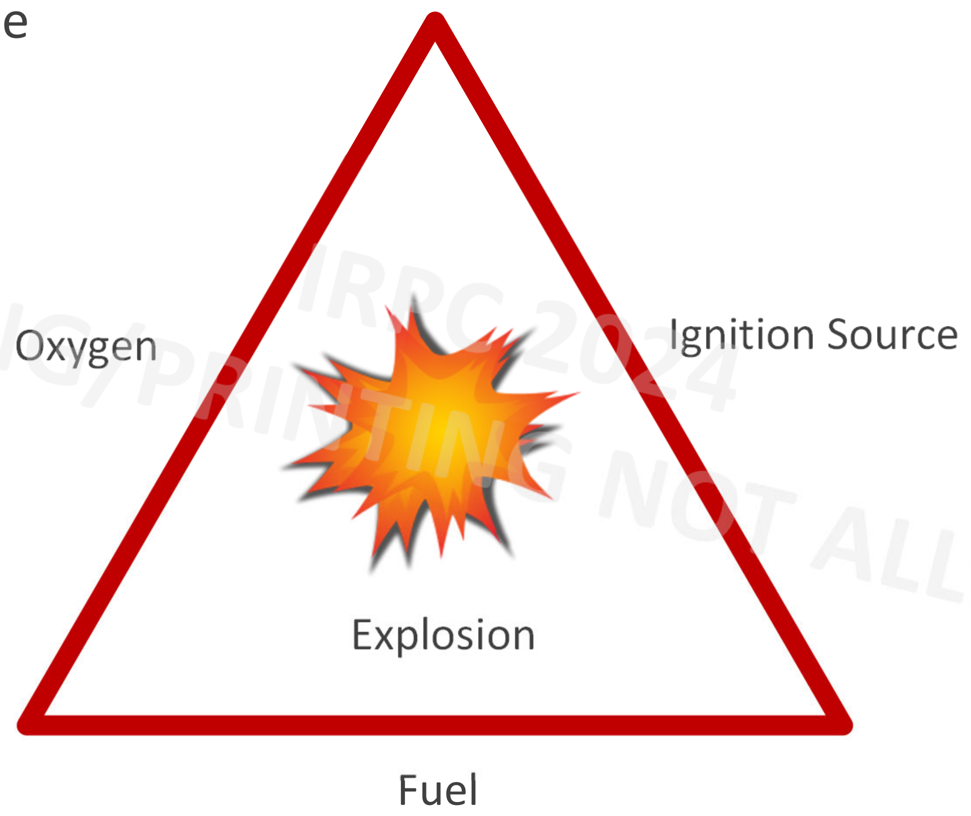
- Investigation showed:
  - Oxidic catalyst contained more copper chromate (Cr^{VI}) components
  - At 90°C (194°F): Ethyl benzene (EB) reacted with copper chromate
  - From 180°C (356°F): EB reacted with copper oxide ($Cu^{II}O$)
  - Not enough heat-sink

- Limited focus on transient conditions

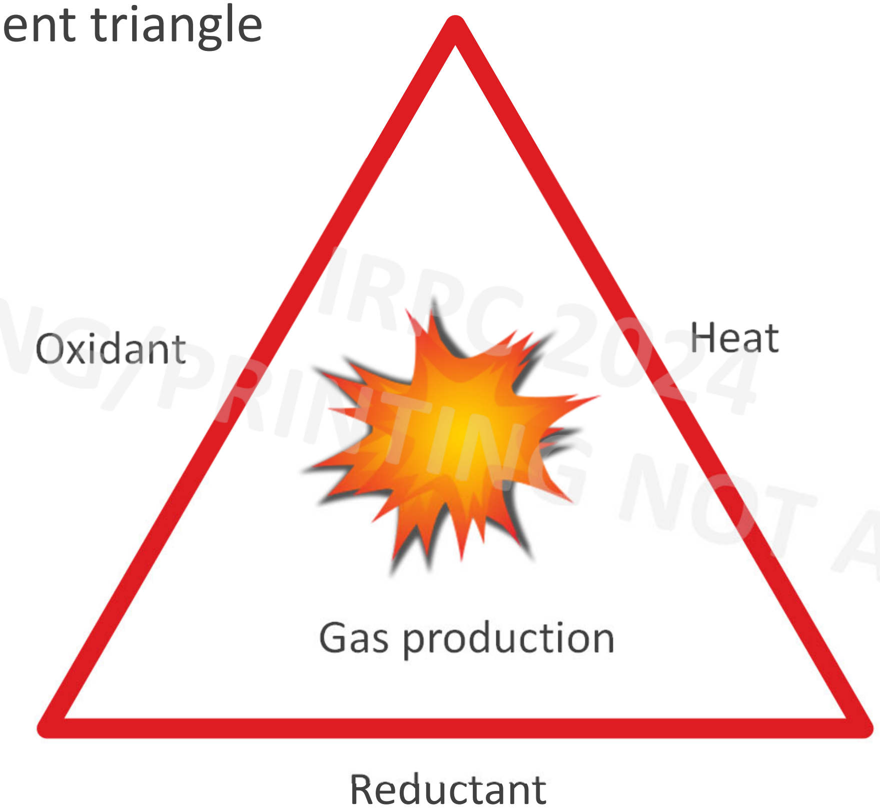
Explosion: main catalyst learnings

- Tons of latent oxygen present in reactor
- Latent (reactive) oxygen from catalysts can react exothermally with a hydrocarbon
- Crucial to review the reactive hazards in both transient and steady state operations

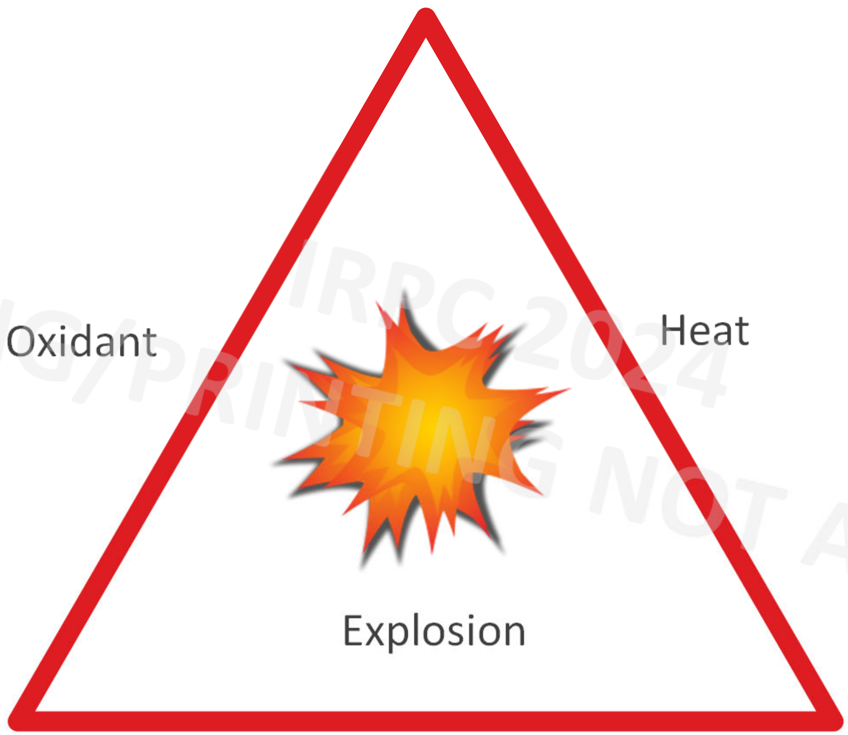
Explosion triangle



Catalyst/adsorbent triangle



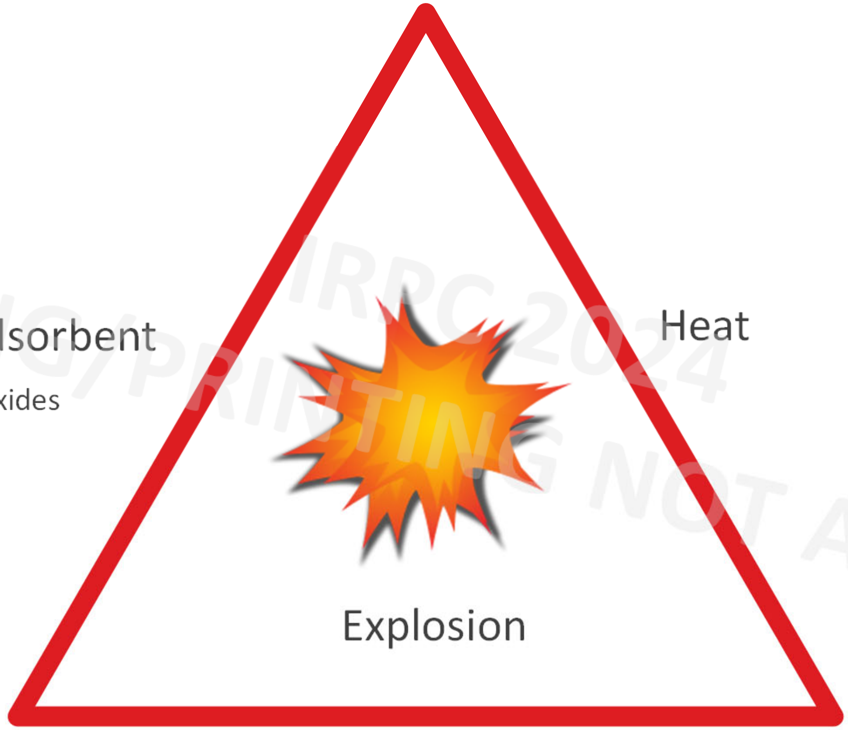
Reductant


Oxidant
Heat
Explosion
Hydrocarbon feed
Organic package on catalyst

Oxidant

Catalyst/Adsorbent

- Metal Oxides



Heat

Example:

Hydroprocessing reactor

often contains

> 10 tons of oxygen

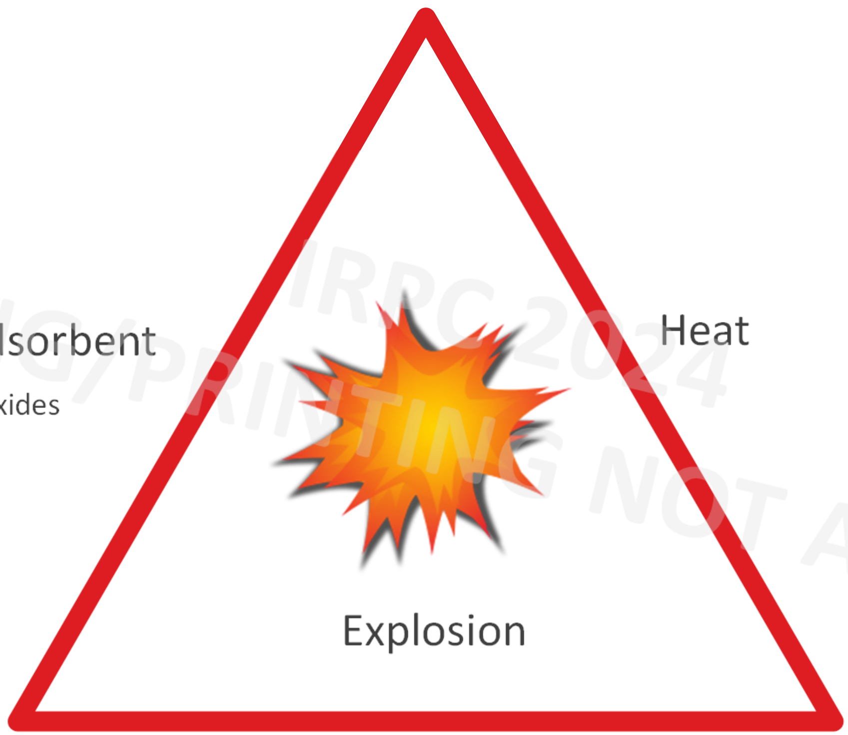
Hydrocarbon feed

Organic package on catalyst

Heat

Catalyst/Adsorbent

- Metal Oxides



Heat

Examples:

- Liquid adsorption
- H_2 chemisorption
- Sulfidation/Reduction
- Poor heat removal

  (e.g., flow maldistribution)

Hydrocarbon feed

Organic package on catalyst

Catalyst/adsorbent: inert “facilitator” or reactant?

Could other systems have similar phenomena?

Catalyst trends

Debottlenecking existing assets

Quick response to market

More activity

↓

Higher chance of more activity in all phases of start-up → Understand exactly where catalyst risks are during transient start-up phases

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

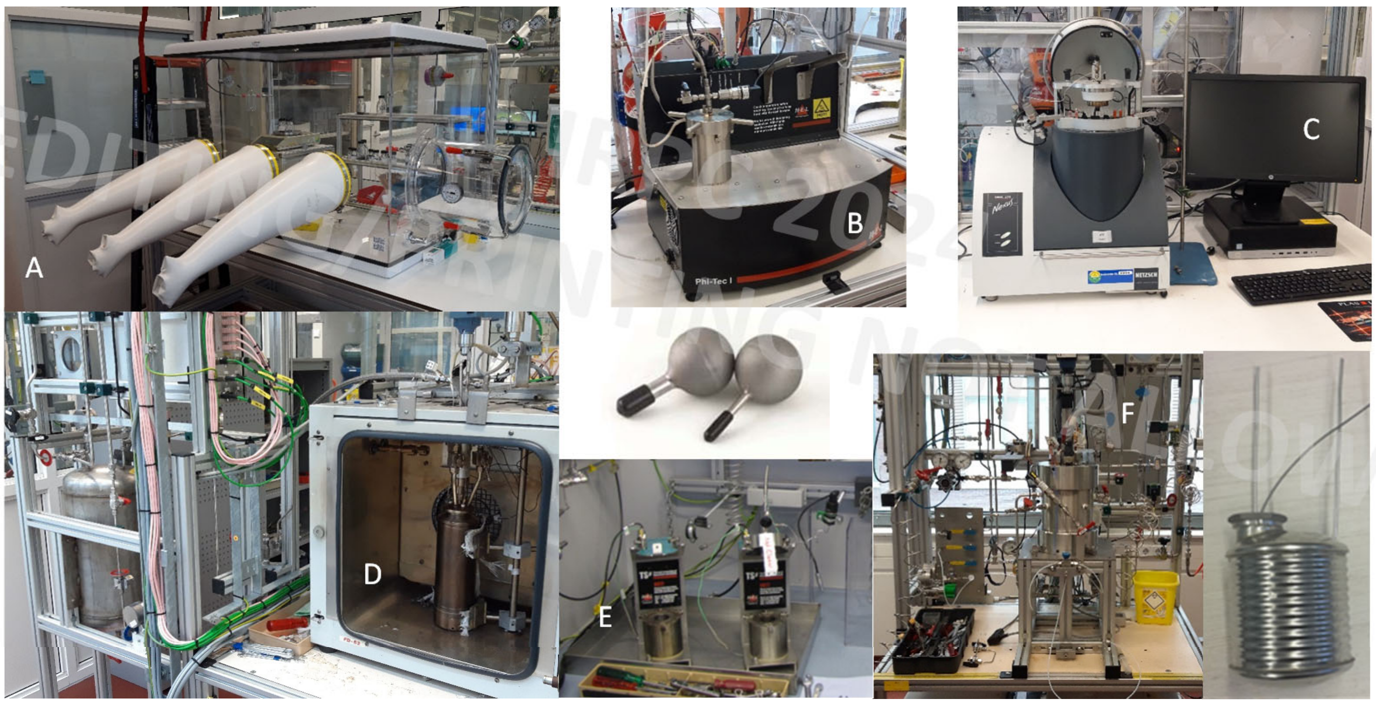
Catalyst Safety Assessment

(CSA)

CSA focus

- Behavior of catalyst/adsorbent in transient modes of operation
- Main focus: reactivity of metal oxide with hydrocarbons
- Other important aspects
  - Adsorption of gases on catalyst
  - Liquid heat of adsorption
  - Release of gases from freshly loaded catalyst
  - Enough heat sink
- Risk assessment based on Thermodynamics and/or calorimetric experiments

Experimental facilities @ Shell ETCA, the Netherlands



CSA screening tool

- Gibbs energy (ΔG) and Enthalpy (ΔH_r):

  $M_xO_y + HC \rightarrow M + CO_2 + H_2O$

- Flow regime:

  liquid full/trickle phase/gas phase

- Metal oxide loading

- Calculation of maximum P and T

  if all metal oxides are converted

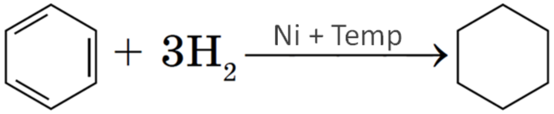
Medium/High risk systems

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

When to do a CSA?

- New catalyst/adsorbent

- New application

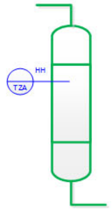


- Change in catalyst composition/production

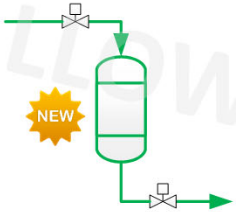
CSA outcome

Changes to start-up procedure

Unwanted reactivity of catalyst as part of catalyst selection

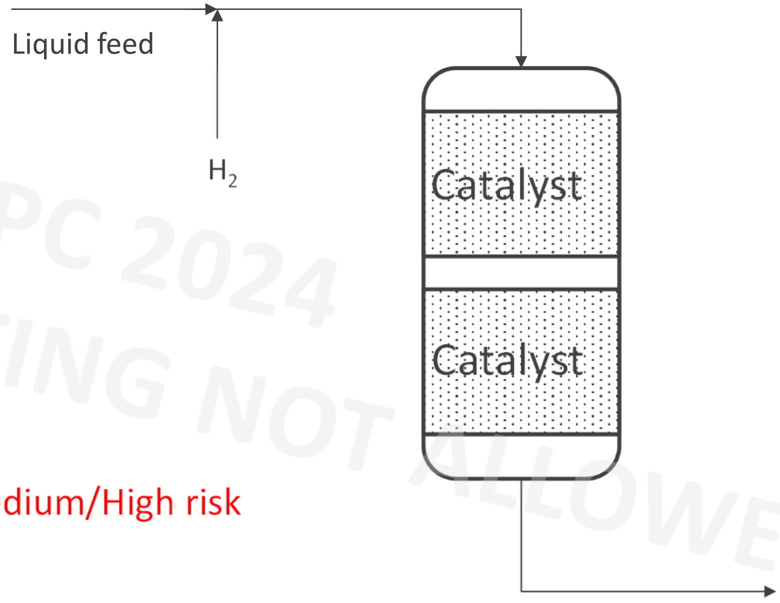


Changes to reactor safeguarding or reactor design



New blocked-in scenario found

CSA example: Nickel catalyst in hydrogenation function

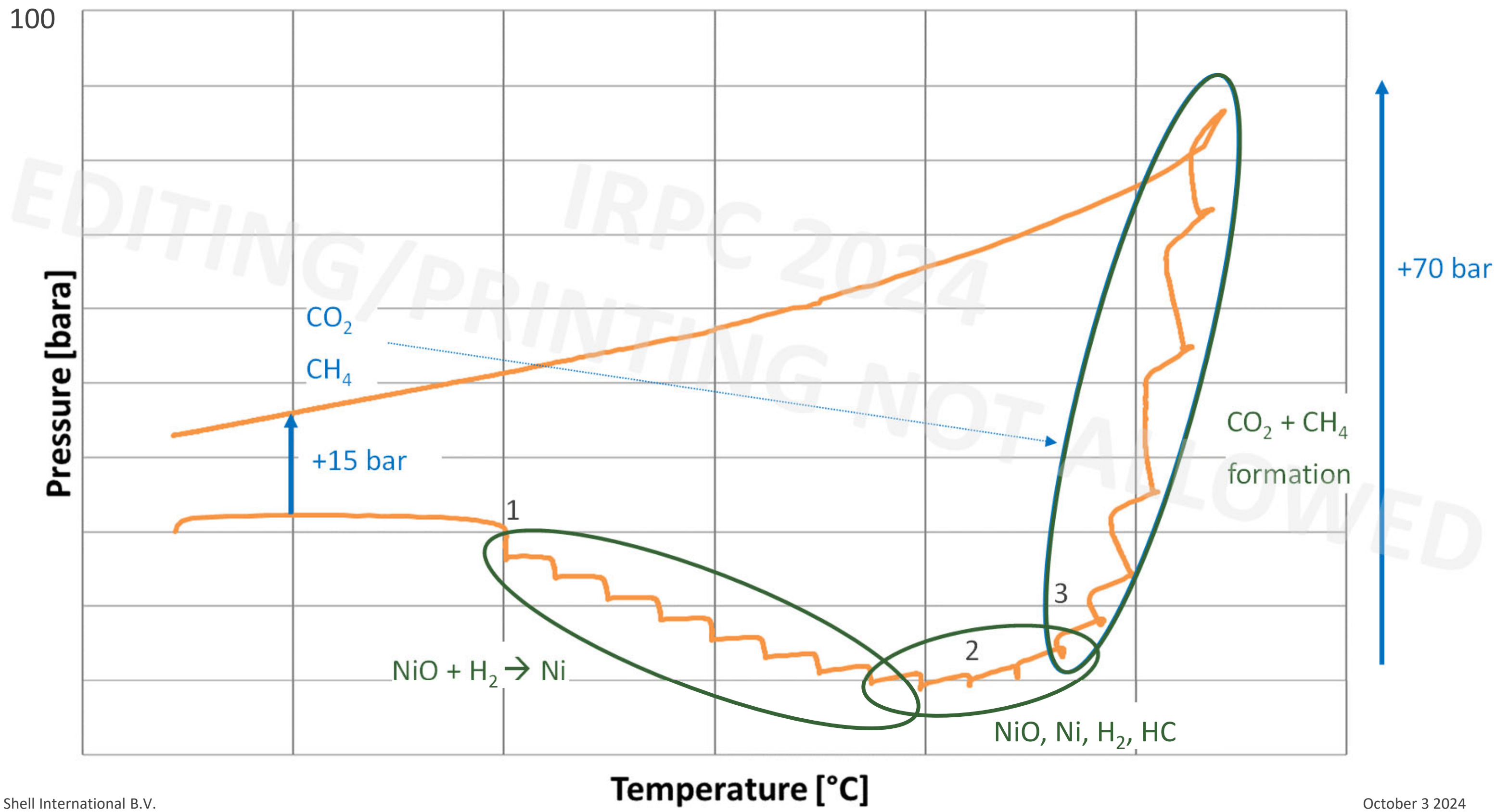


- Catalyst in reactor
  - >10% NiO on carrier
  - Trickle phase reduction

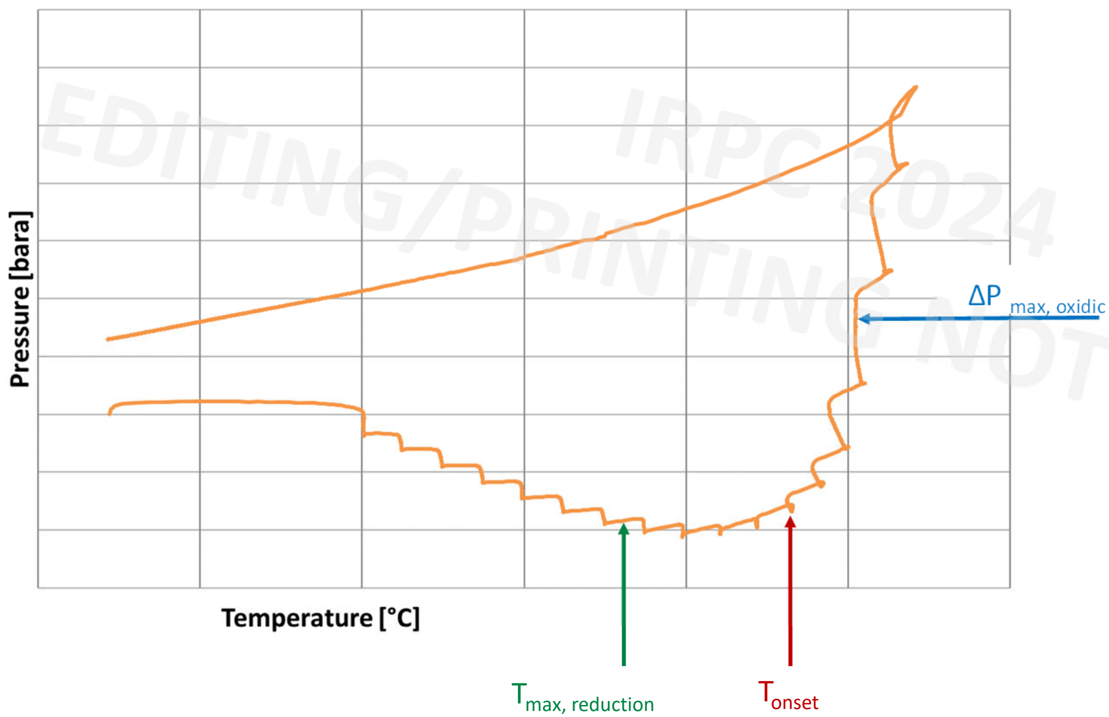
CSA assessment

- Thermodynamic results NiO + HC → Medium/High risk
  - Potential for design pressure exceedance
- Conclusion: calorimetric tests are needed

Experimental result: NiO catalyst + hydrocarbon + H_2



Experimental result: NiO catalyst + hydrocarbon + H_2



If trickle phase reduction, what is safe reduction temperature?

Shell decided

$T_{max,\ reduction} = T_{onset} - 50^{o}C$

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

- Which reactions happen at which temperature during start-up?

- Shell's Catalyst Safety Assessment is a process that helps make catalyst/adsorbent start-ups safer.

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