Chemical Hazard Assessments (CHA)

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Maastricht, 13th December 2023

Add value.
Inspire trust.

Accidents due to chemical runaways

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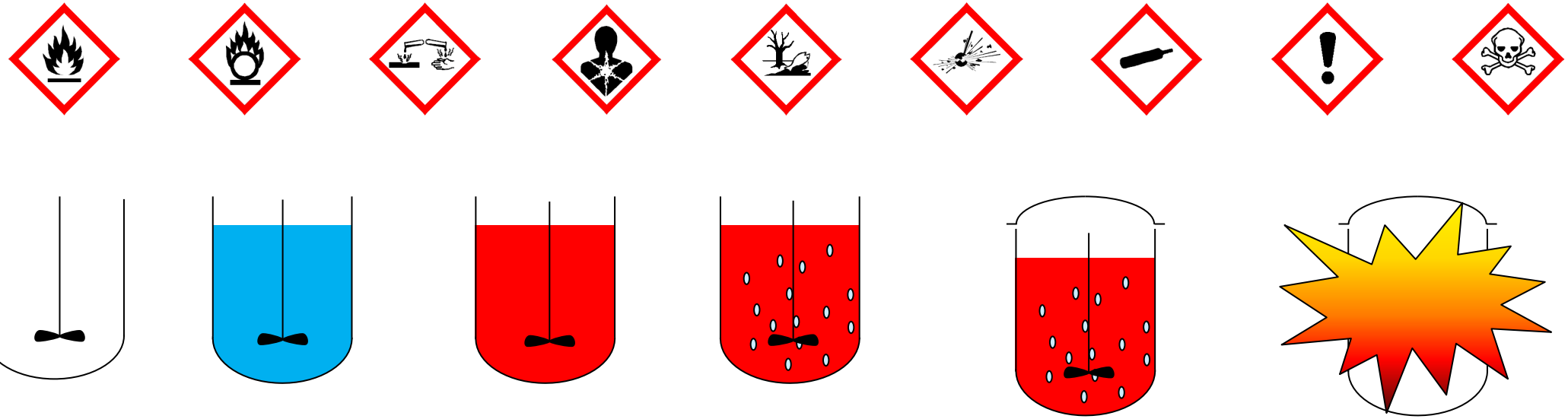
Extracts from the CSB video

https://www.youtube.com/watch?v=C561PCq5E1g

Assessed hazards

- Assess systematically chemical hazards



Goals of a CHA

1. Collection of data on the chemical process
   - Properties
   - Interactions
   - Reactivity
     - Intended and unintended reactions (synthesis, and decomposition/secondary reactions)
2. Interpretation of data:
   - Defining safe conditions & consequences of deviations

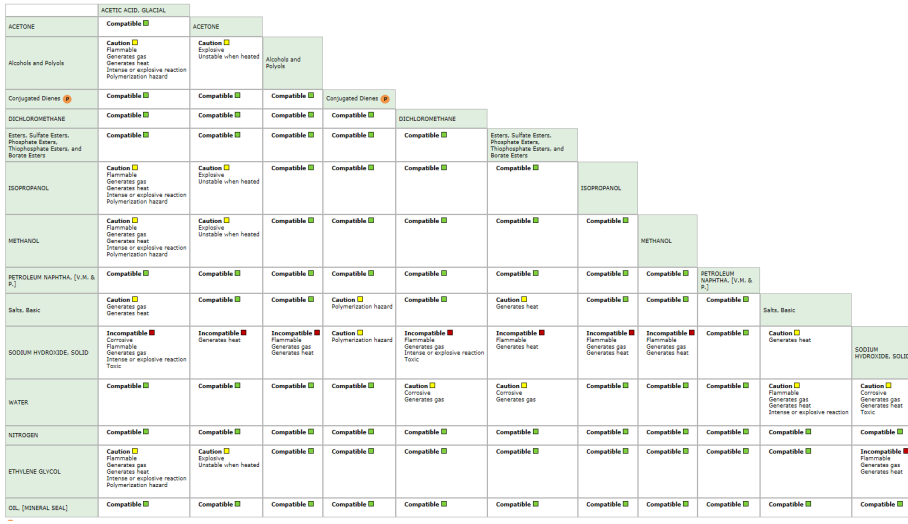
3.1 Physical properties data

Substances (Raw material, Pro Intermediates, ...)
Content
CAS number
Molar Mass
Aggregate state by 20°C and 1 (solid/liquid/gaseous)
Aggregate state occurring in th (solid/liquid/gaseous))
Melting point
Boiling point
Density at 20°C
Vapor pressure at 20°C
Vapor pressure at 100°C
Relative vapor density (air =1)
Thermal conductivity

na: not applicable

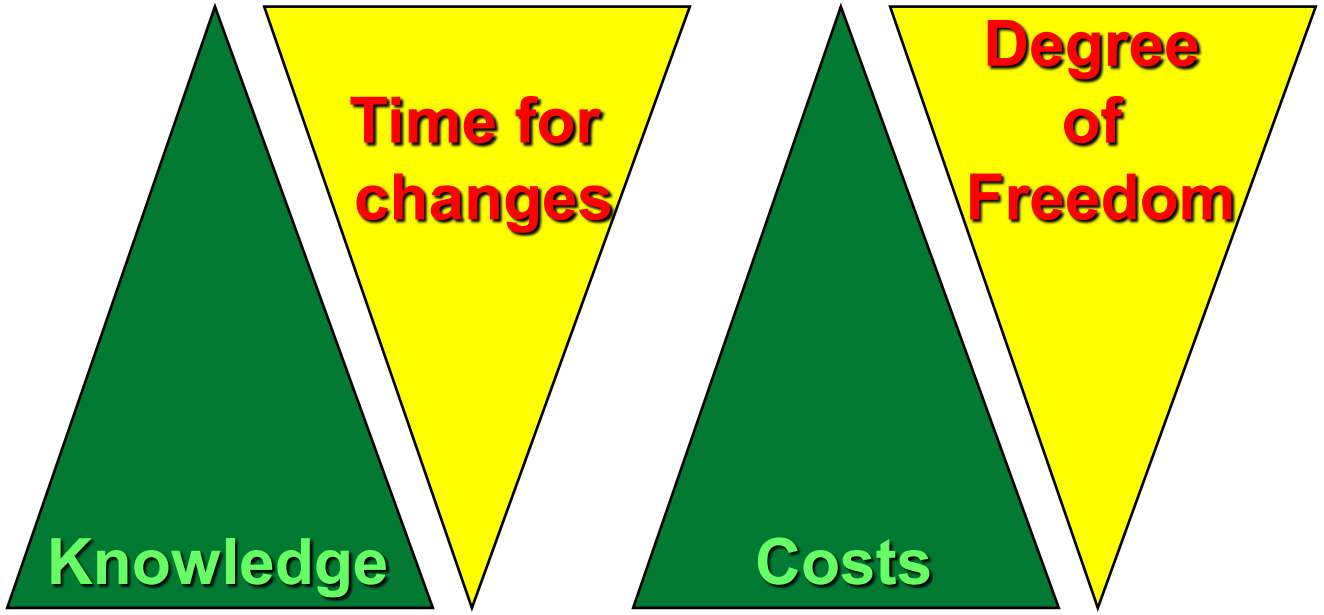
3.2 Thermal stability data

Substances (Raw material, Products, Intermediates, ...)		
Nr (reactivity) according to NFPA 704 [1]		
Dangerous Goods (Class 1.1 to 1.6 / 4.1 to 4.3)		
Self-Accelerating Decomposition Temperature (SADT) (Applicable for storage and transport)	[°C]	
Safe storage temperature	[°C]	
Substance stabilized?	[Y/N]	
No of SILAB report		
Other information source		
T_{onset} DSC High Pressure Crucible	[°C]	
Heat of decomposition (report exotherm with "-" and endotherm with "+")	[kJ/kg]	
Autocatalytic decomposition	[Y/N]	
Decomposition gas	[l/kg]	
Decomposition gas combustible?	[Y/N]	
Explosibility (Class 1.1 to 1.6)		
Friction	[Y/N]	
Impact	[Y/N]	
Koenen Test	[Y/N]	
Oxidation		
T_{onset} Grewer (for combustible powders)	[°C]	
$T_{critical}$ (400mL basket) (for combustible powders)	[°C]	
T_{onset} DSC High Pressure Oxygen	[°C]	

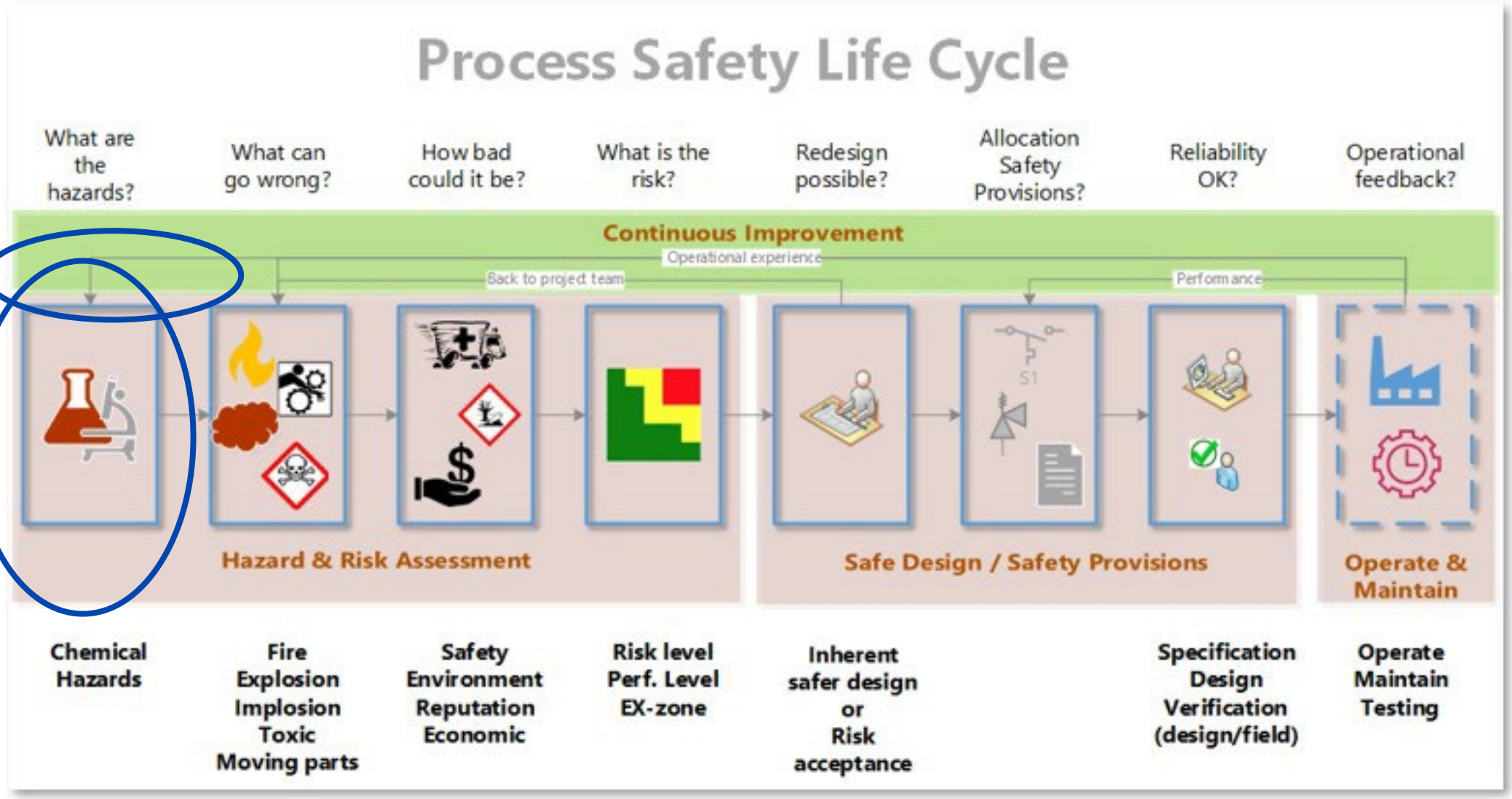


Ideal time point for a CHA

- Discovery, Innovation
- Feasibility Study
- Laboratory Study
- Study in Pilot Plant
- Engineering
- Building and Start Up
- Process Working
- Process Death



Ideal time point for a CHA



Example

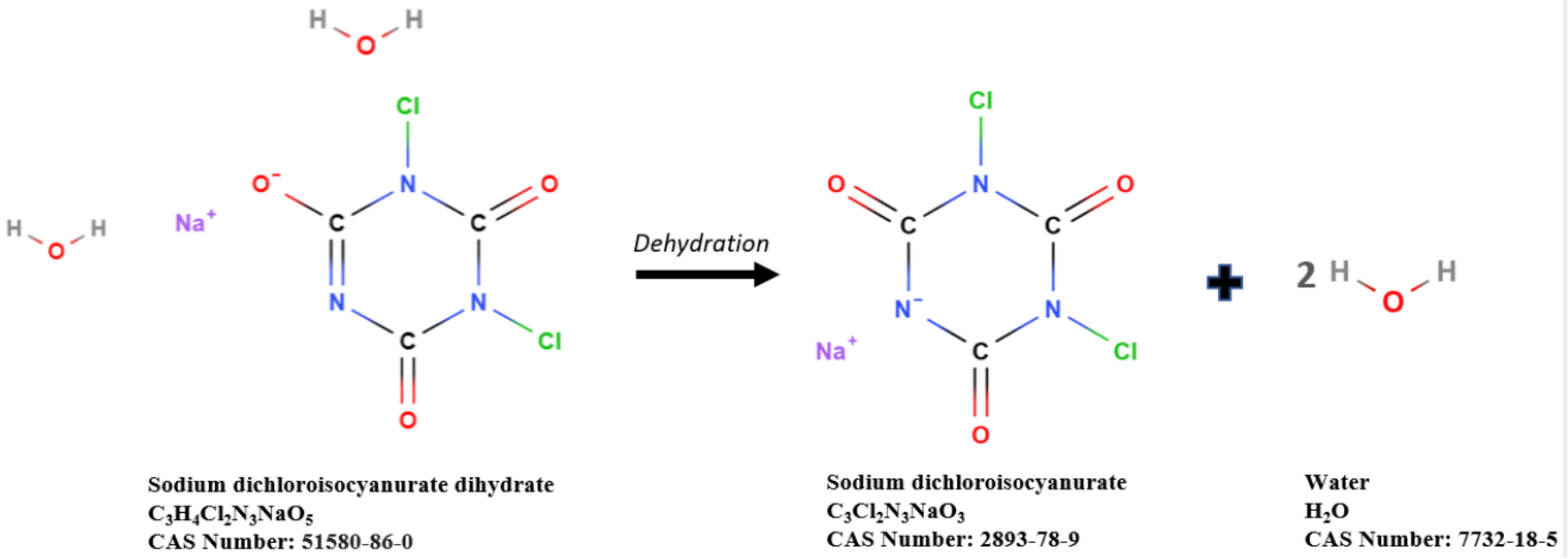
Process Information

Sodium dichloroisocyanurate dihydrate → (NaDCC dihydrate)

Drying @ 120°C

Anhydrous sodium dichloroisocyanurate → (NaDCC)

Water ↓



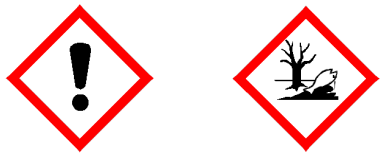
Sodium dichloroisocyanurate dihydrate
$C_3H_4Cl_2N_3NaO_5$
CAS Number: 51580-86-0

Sodium dichloroisocyanurate
$C_3Cl_2N_3NaO_3$
CAS Number: 2893-78-9

Water
H_2O
CAS Number: 7732-18-5

Example

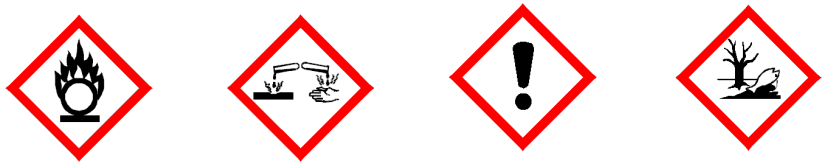
NaDCC dihydrate



EUH031: contact with acids liberates toxic gas

Decomposition T > 240°C

NaDCC



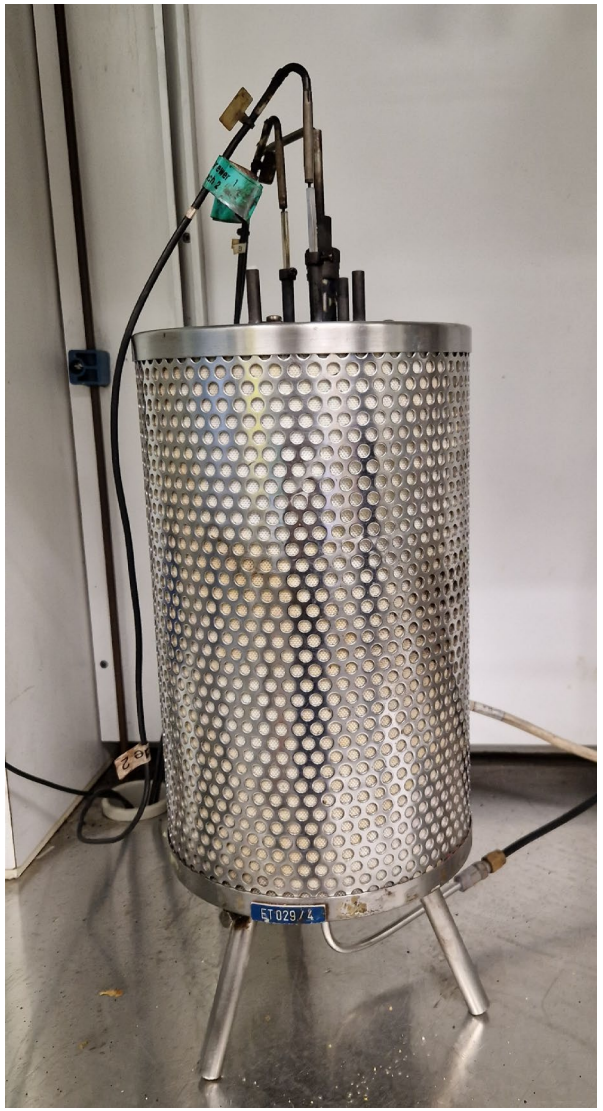
EUH031: contact with acids liberates toxic gas

Decomposition T 240°C – 250°C

Data from Gestis (https://gestis-database.dguv.de/)

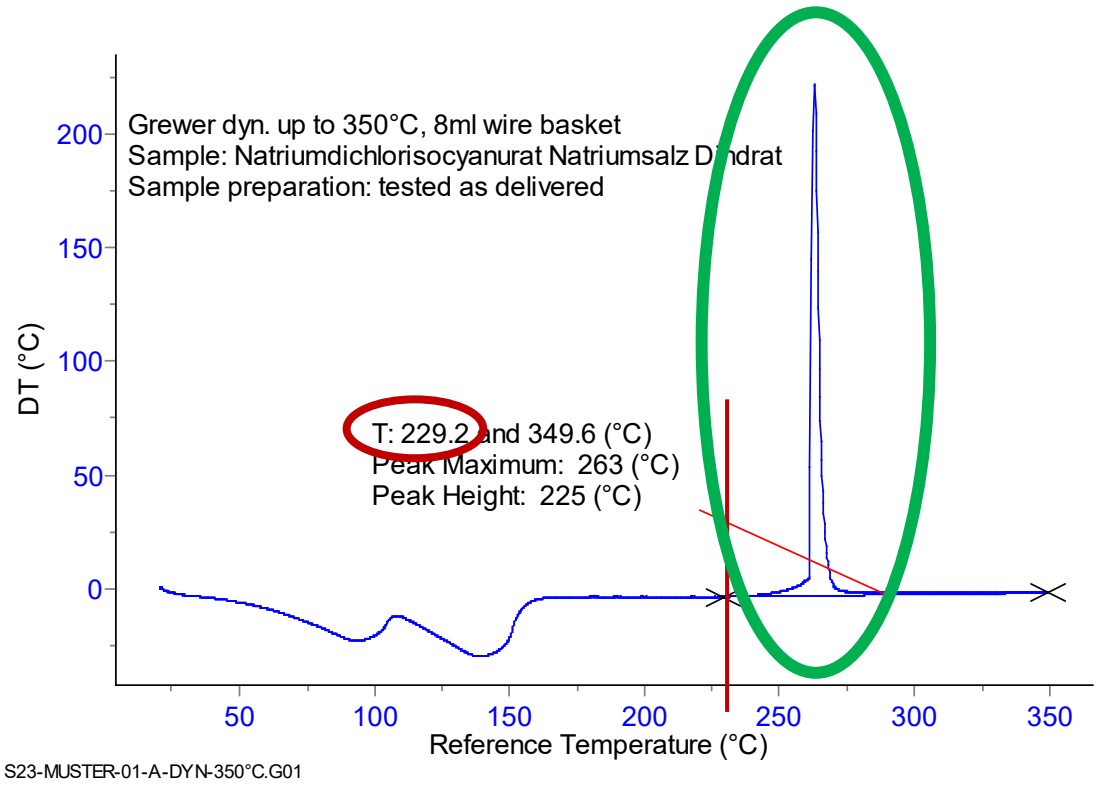
Example

- Grewer measurement

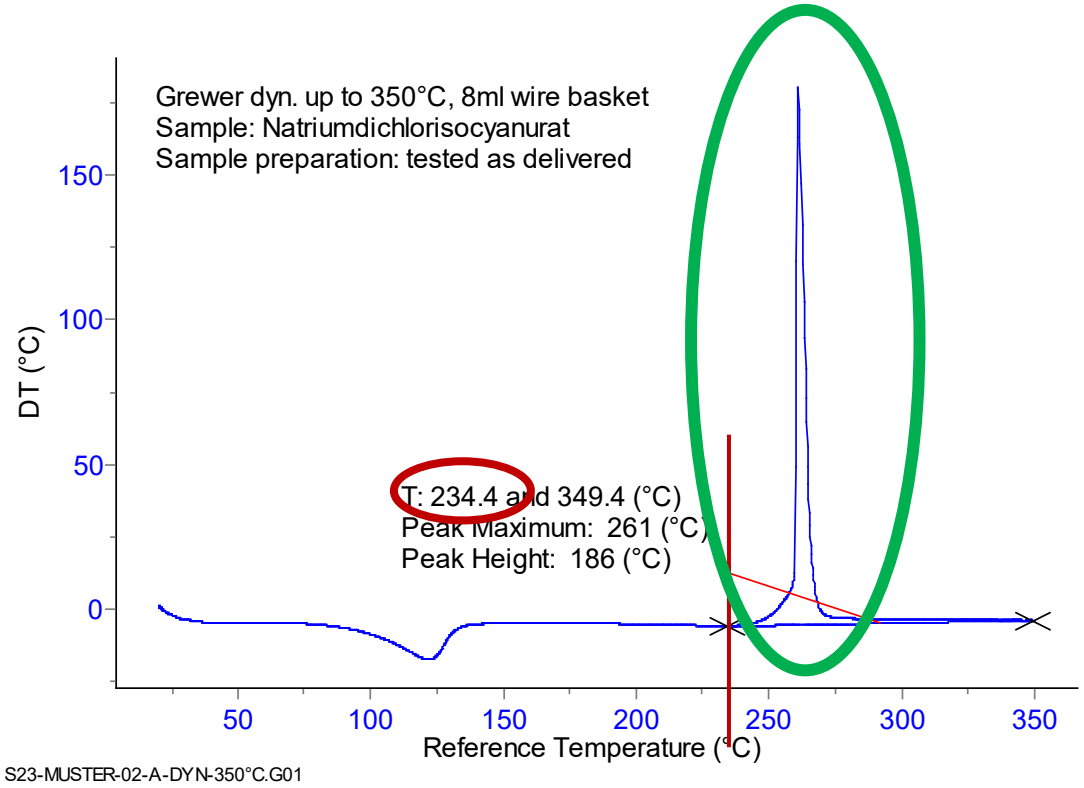


Example

- NaDCC dihydrate Grewer



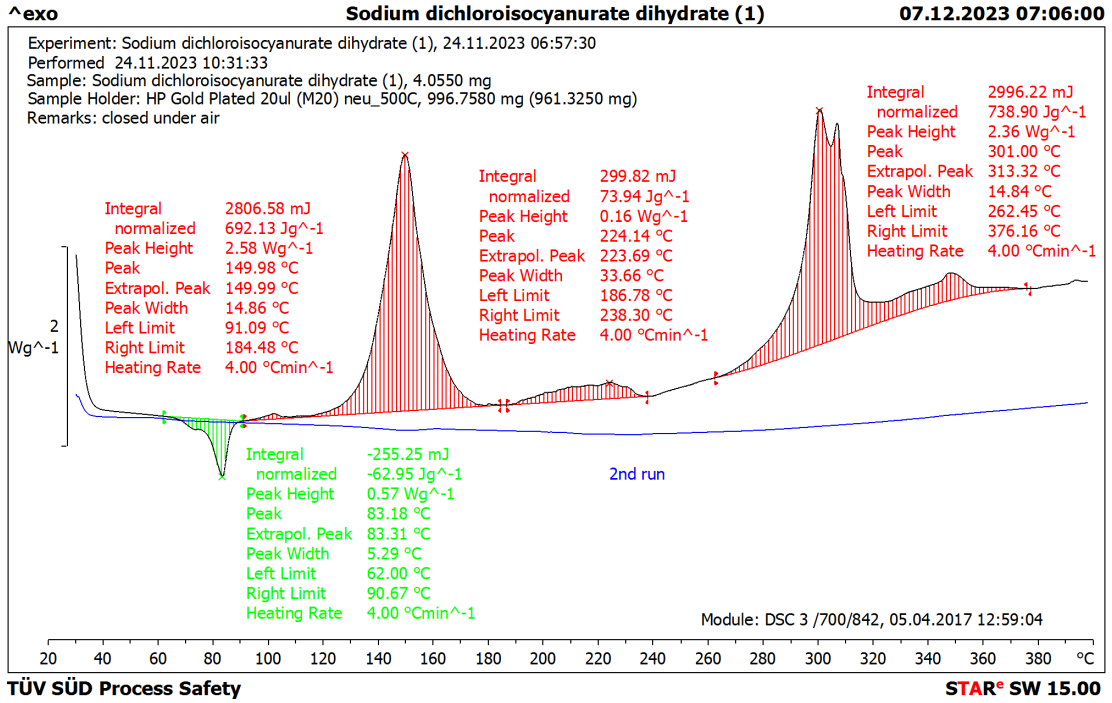
- NaDCC Grewer



Confirm decomposition temperature ranges mentioned in Gestis (or other MSDS)

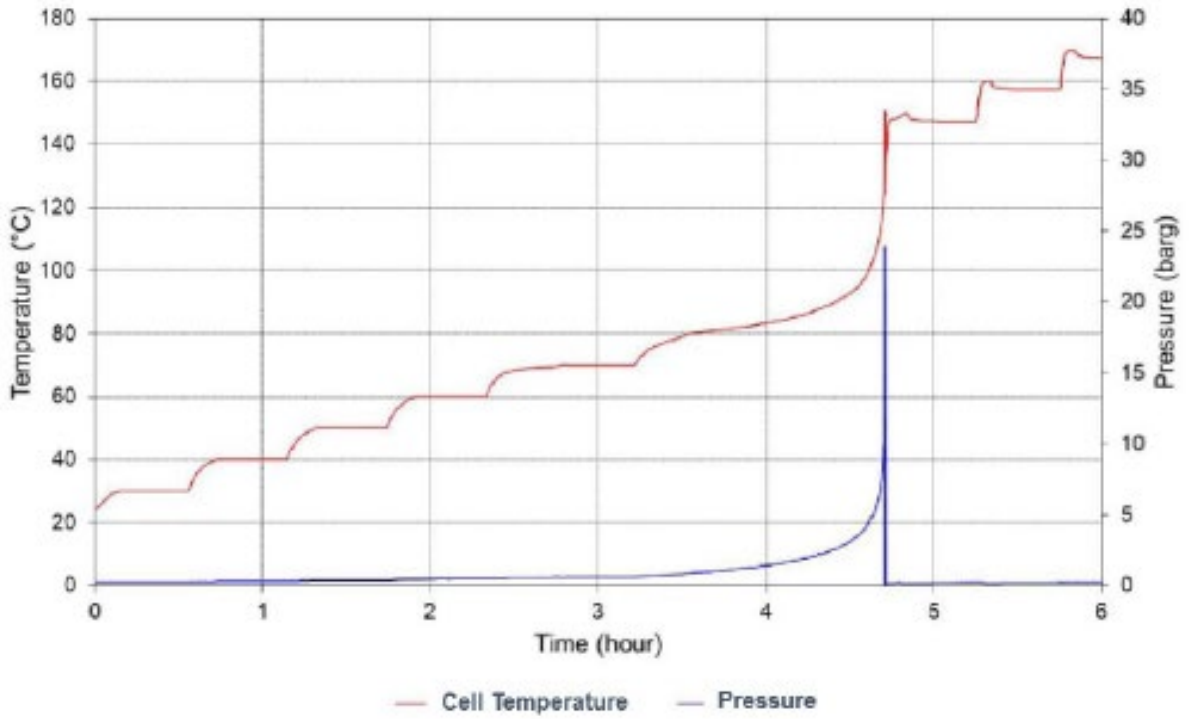
Example

- NaDCC dihydrate DSC



- Total of 1500 kJ/kg decomposition energy
- Decomposition measured from ~90°C

- NaDCC dihydrate ARC (Heat-Wait-Search Mode)[1]

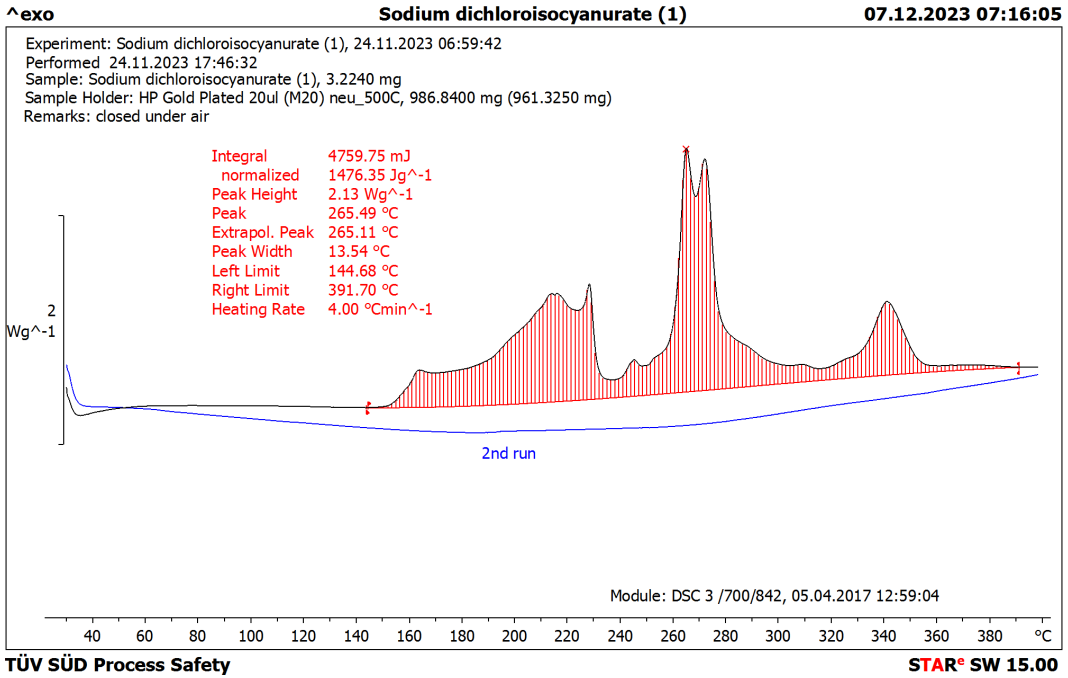


- Decomposition measured from 80°C on
- Important pressure increase

[1]Source: CSB investigation report July, 6, 2023 «Fatal Chemical Decomposition Reaction and Explosion at Optima Belle LLC»

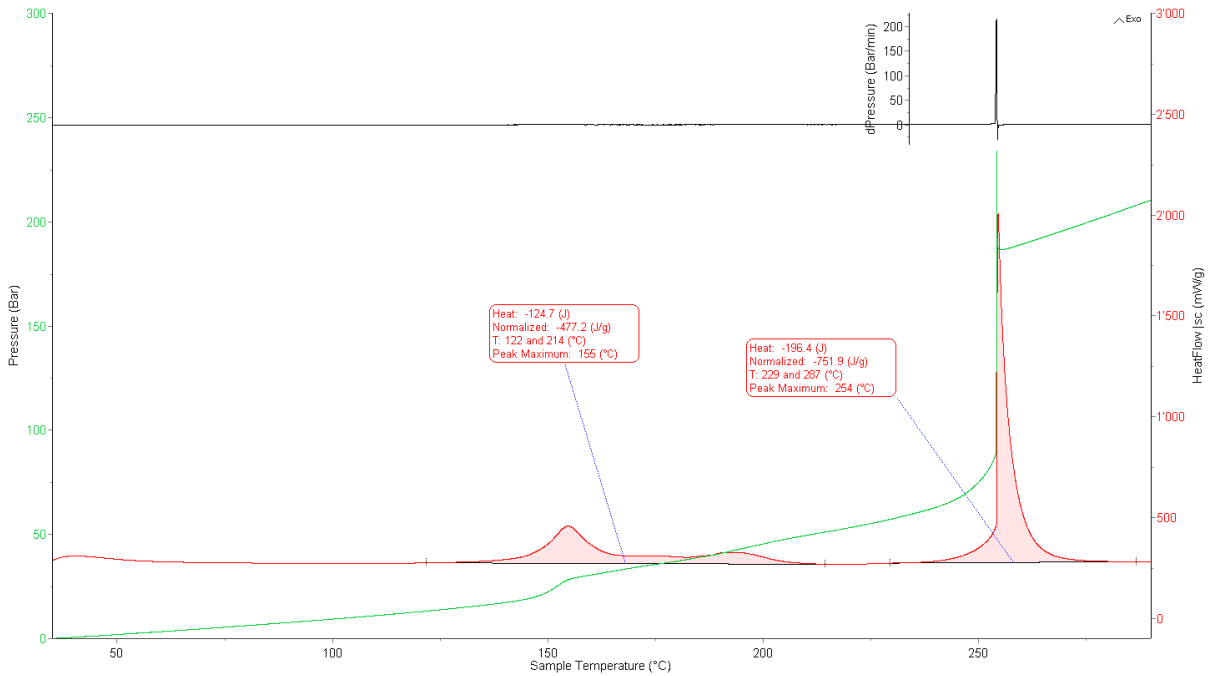
Example

- NaDCC DSC



- Total of 1480 kJ/kg decomposition energy
- Decomposition measured from ~145°C

- NaDCC C80



- High energy
- Large pressure increase

Example: Safe limits and effects

1. Assess normal process conditions
   - Severe decomposition (temperature increase > 1000°C)
   - In an open system (e.g. fluidized bed dryer) → maximum drying temperature ~ 120°C

2. Assess response of process to deviations
   - **Closed system, layers of products**:
     - decomposition with high severity (T and P) and T_{D24}~20°C (very high probability)
     - Violent gas production → pressure relief might be difficult
   - **Temperature too high**: Gas production around 100 l/kg (in open system @ 350°C)

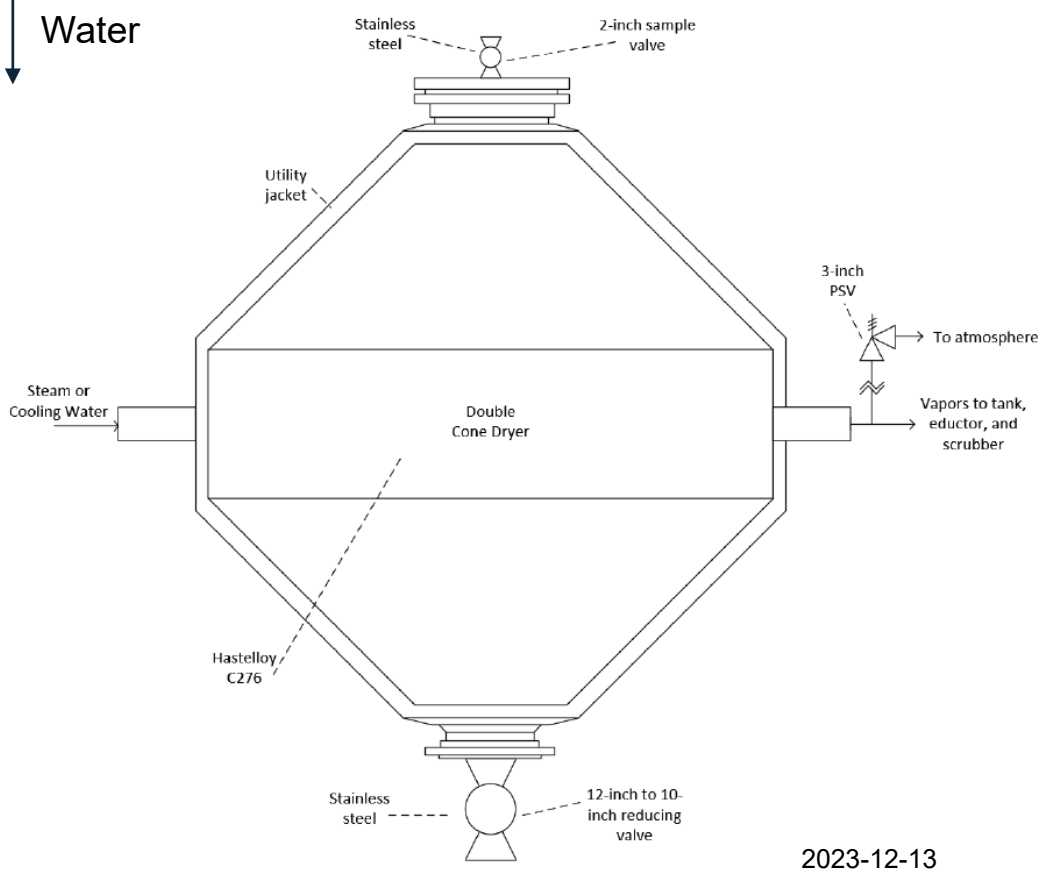
Example

Process Information

Sodium dichloroisocyanurate dihydrate (NaDCC dihydrate) → **Drying @ 120°C** → Anhydrous sodium dichloroisocyanurate (NaDCC)

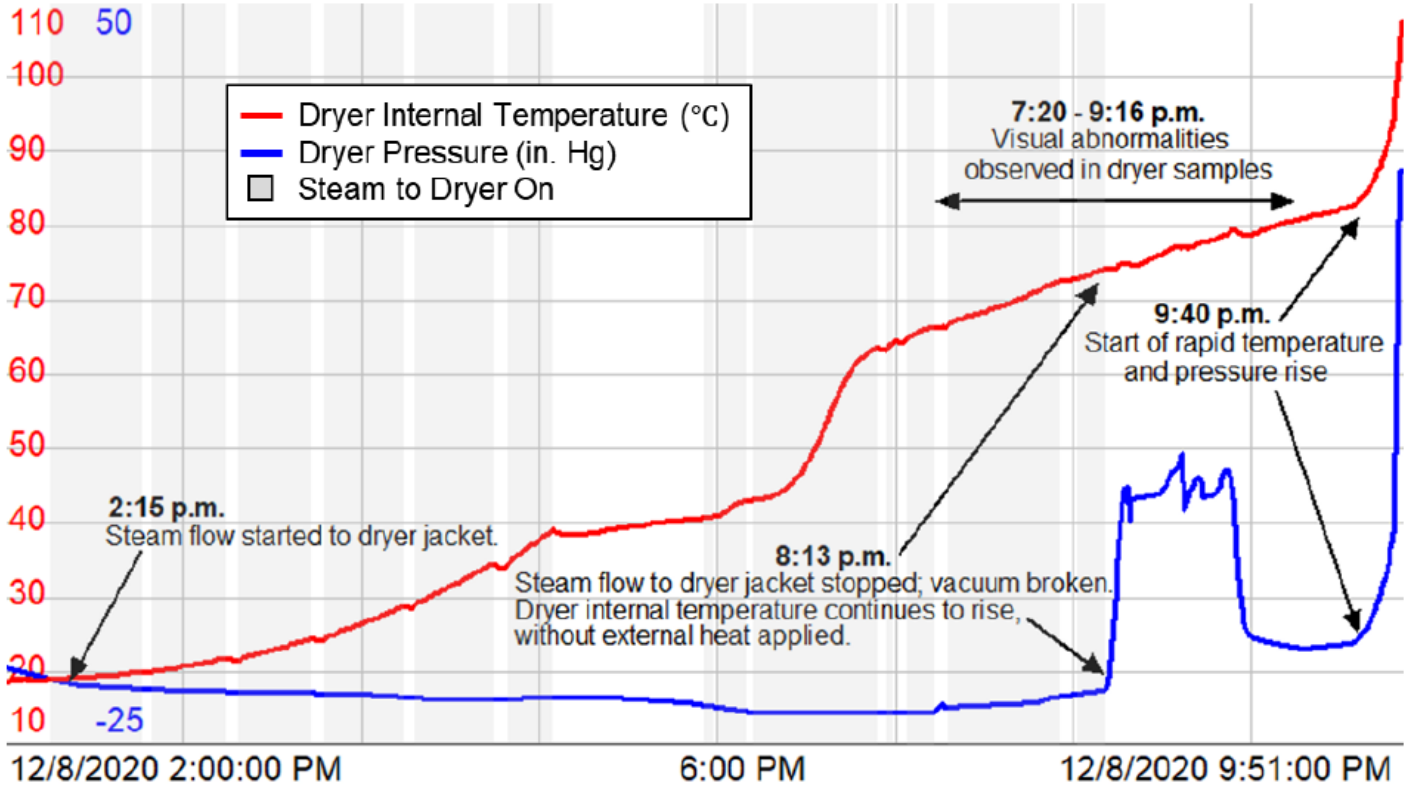
Water

- Process conditions for fluidized bed
- Company looking for third party to dry NaDCC dihydrate
- Option found: rotary double cone dryer (pressure equipment)
- Tests directly in $4m^3$



Example

Figure 2. Optima Belle's rotary double cone jacketed dryer. (Credit: Optima Belle)

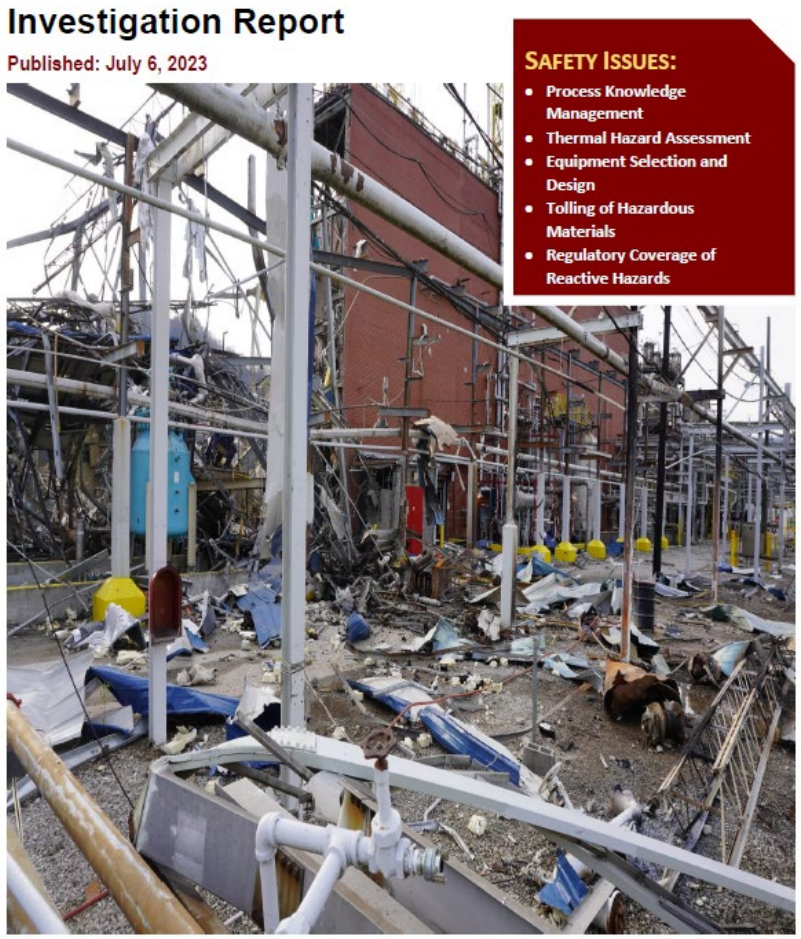


Source: CSB investigation report July, 6, 2023
«Fatal Chemical Decomposition Reaction and Explosion at Optima Belle LLC»

Example

- 8th December 2020
  - One employee fatally injured, two others respiratory irritation
  - Debris found ~ up to 800 m away from the site

Source: CSB investigation report July, 6, 2023
«Fatal Chemical Decomposition Reaction and Explosion at Optima Belle LLC»



Conclusion

- Chemical Hazard assessment …
  - … are key to define safety concept and safe limits of a process
  - … are complex and require expertise
  - … mostly installation/scale independent
  - … are key for preparation of HAZOP

EPSC will be starting a working group on chemical hazard assessments in 2024 – **Join us**

Thank you

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