
Thermal Stability Predictions for Inherently Safe Process Design

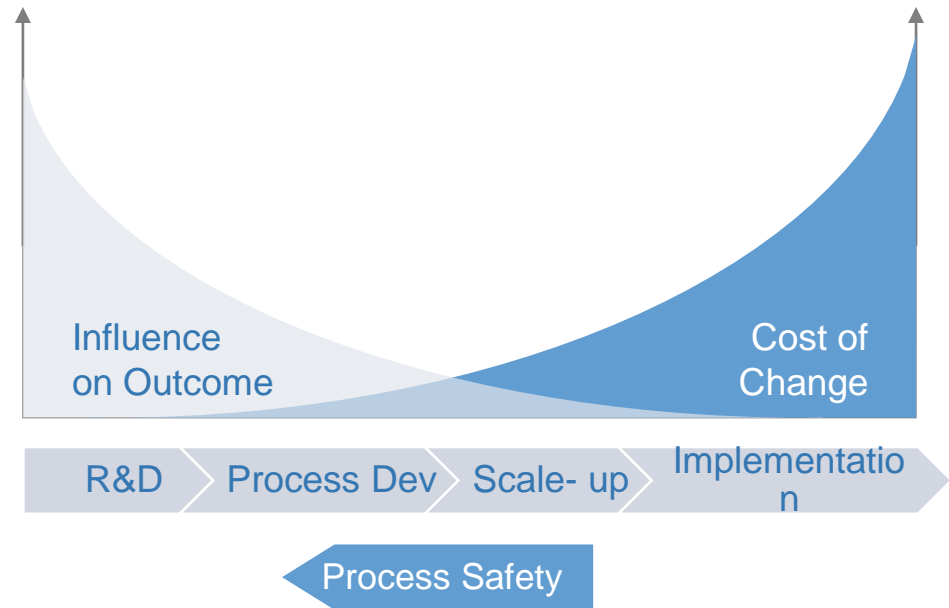
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Simulations

- Anticipation
- Greater influence
- Savings
 - Time
 - Material
 - Financial



Inherent Safety

“Reduce the hazards rather than managing the risks”

- Minimize the quantities of hazardous materials handled
- Substitute a hazardous compound for a less hazardous one
- Moderate the potential effects of residual risks
- Simplify the system and avoid additional equipment or features

(Kletz 2003; CCPS 2009)



Time Factor

Motivations and Objectives



- Benefits of simulations
- Inherent safety
- Complement to design and analysis



Predictive Simulations

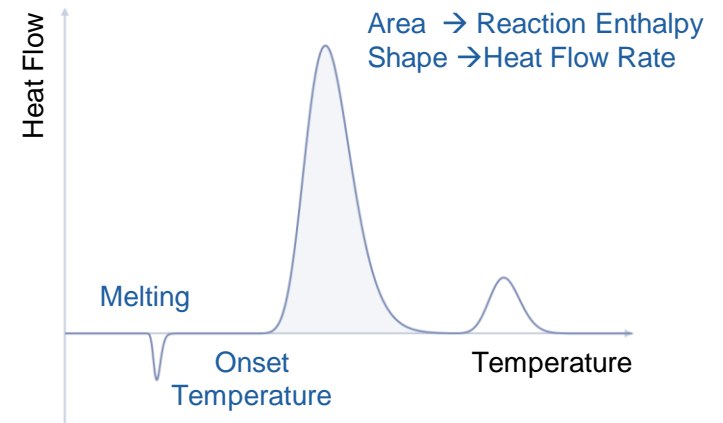
- Forecasting physical-chemical properties
- Potential use in design, analysis, screening
- Improve testing strategy

Risk Assessment

Thermal Risk

- Can this chemical decompose?
- In which temperature range?
- How much heat is released?
- At which rate?

➤ Differential Scanning Calorimetry



Motivations and Objectives



Predictive Simulations

- Forecasting physical-chemical properties
 - Potential use in design, analysis, screening
 - Improve testing strategy
-
- Time/material consuming experiments
 - Unavailable compounds
 - Requiring minimal information feed

Molecular-Based Simulations Methods

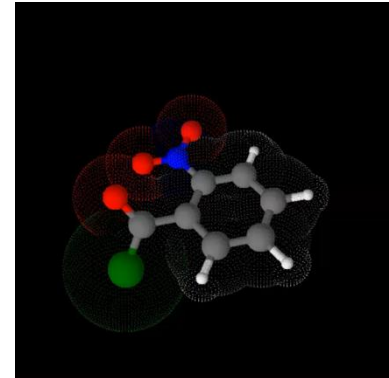


Process Safety

QSPR

Structural aspects covered:

- Constitution
- Topology
- Geometry
- Electronic
- Quantum derived



Molecular-Based Simulations Methods



Process Safety

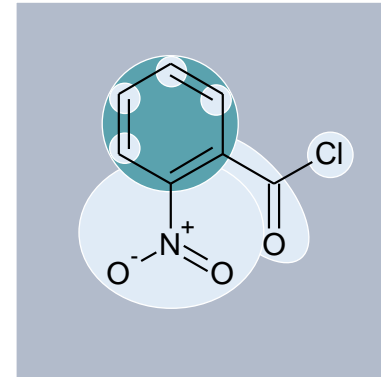
GCM

Functional Groups

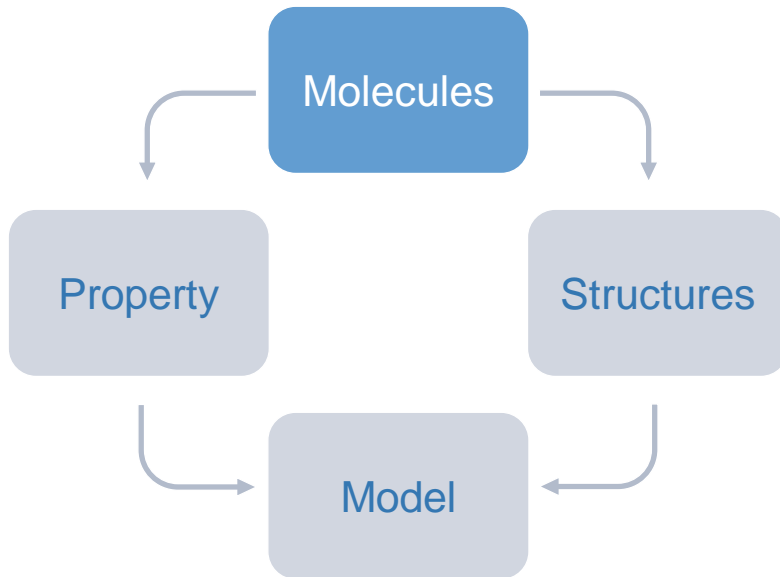
- Several levels

Various Frameworks

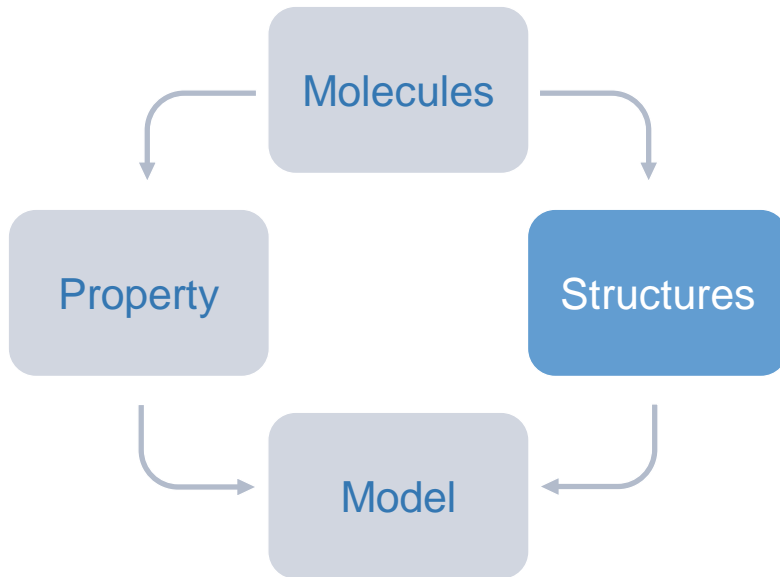
- Marrero-Gani



Modeling Procedure

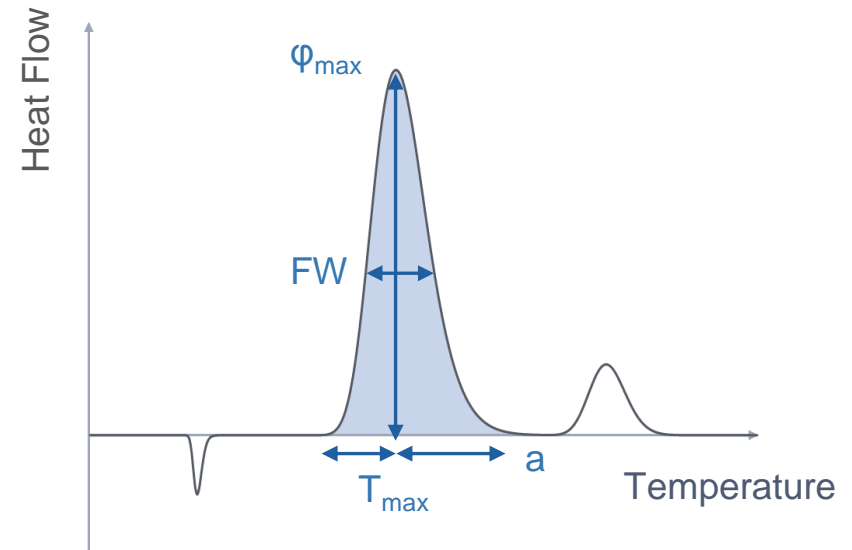
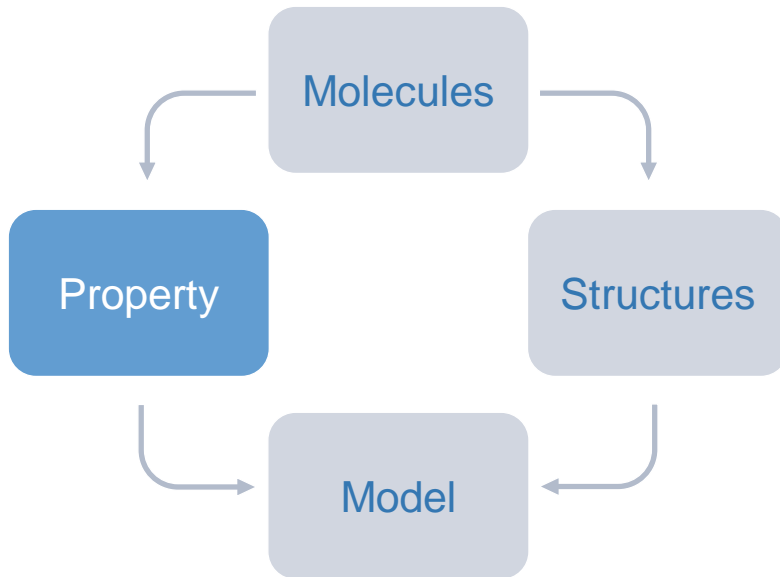


Modeling Procedure

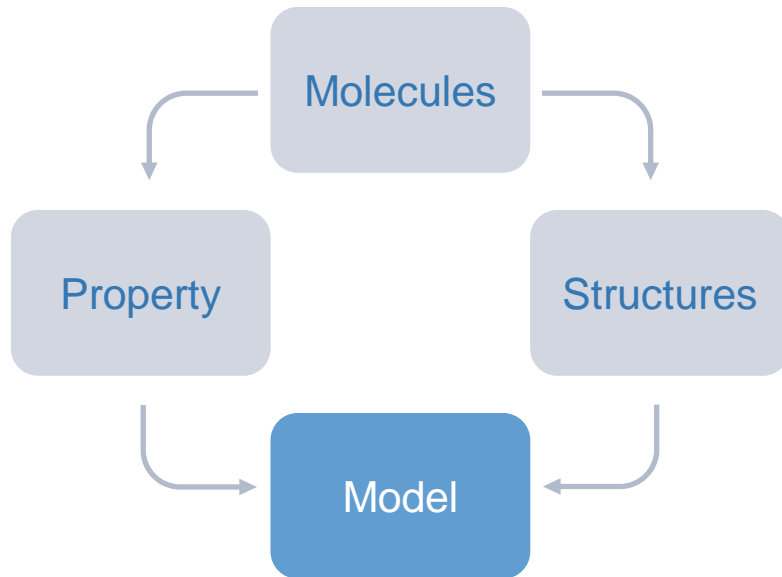


- Generate Structure
- Represent in selected framework
- Compute descriptors / groups

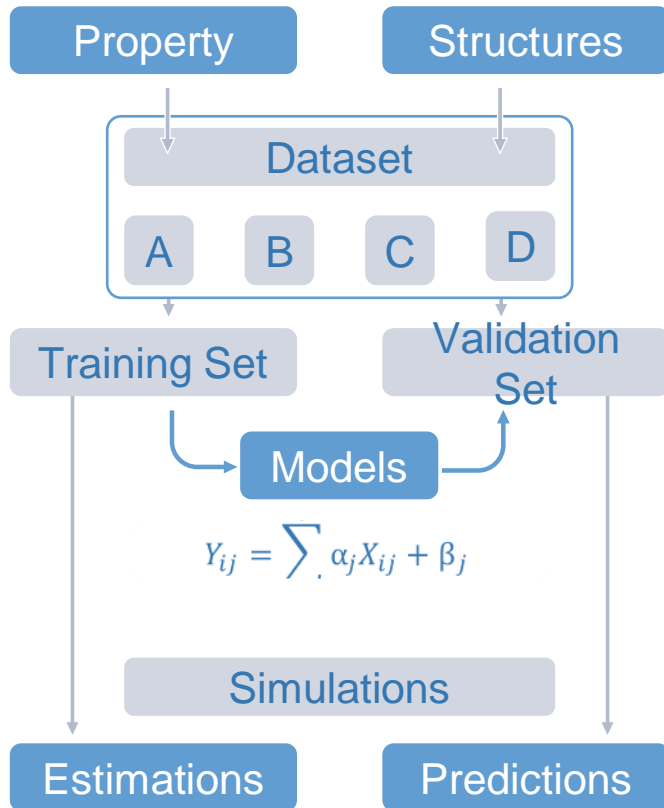
Modeling Procedure



Modeling Procedure

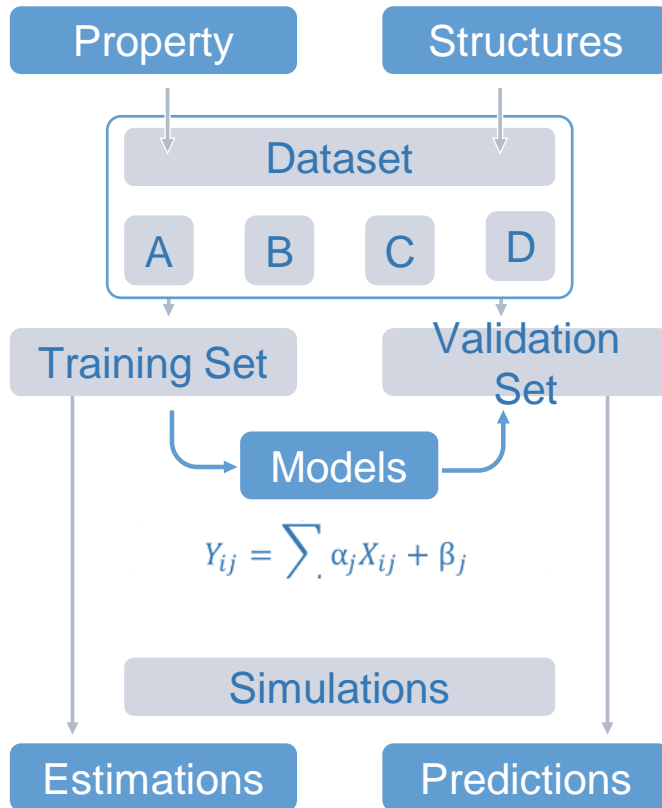


Modeling Procedure



- Training - Validation
- Linear regressions
- Local subsets

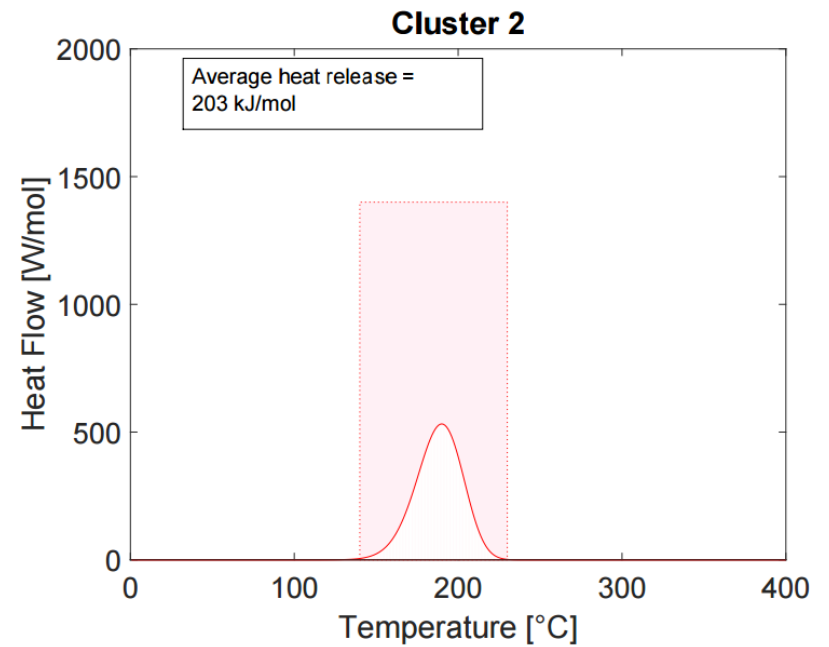
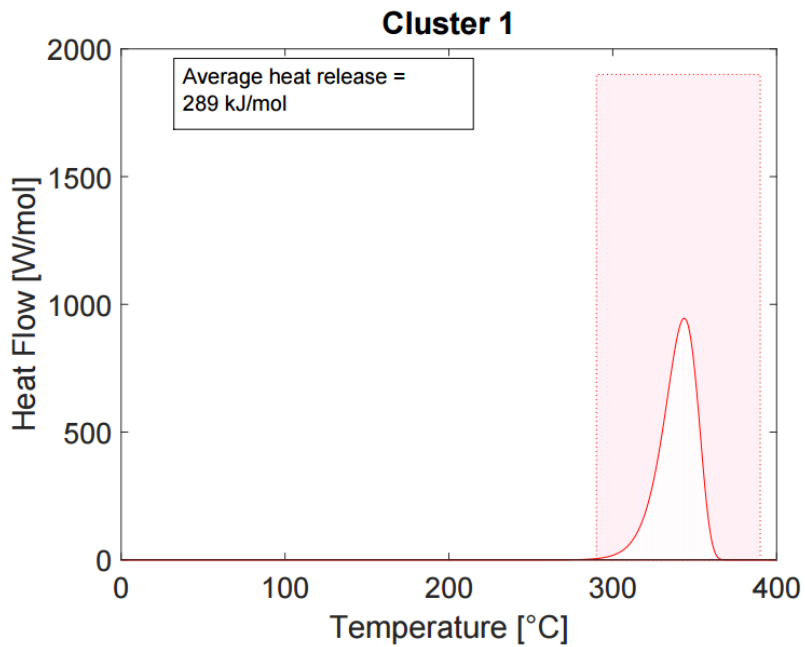
Modeling Procedure



- Cluster Assignment
- Local Regressions
- Primary Risk Assessment

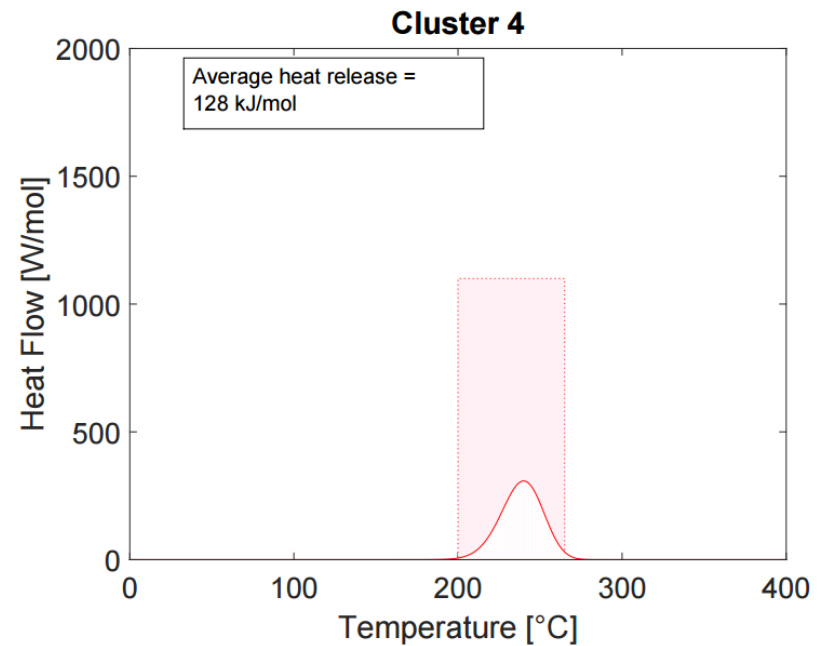
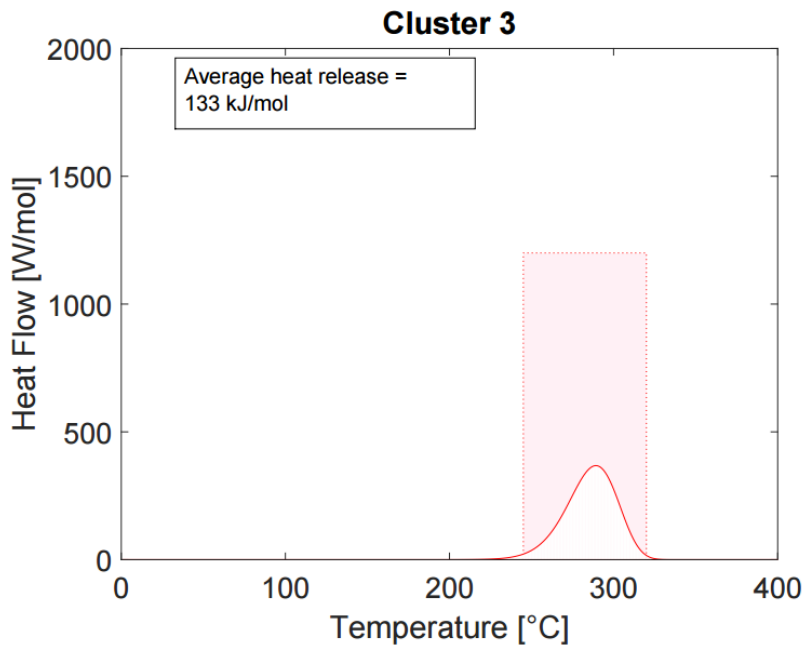
Results: Classification

- DSC Image processing
- 7 clusters



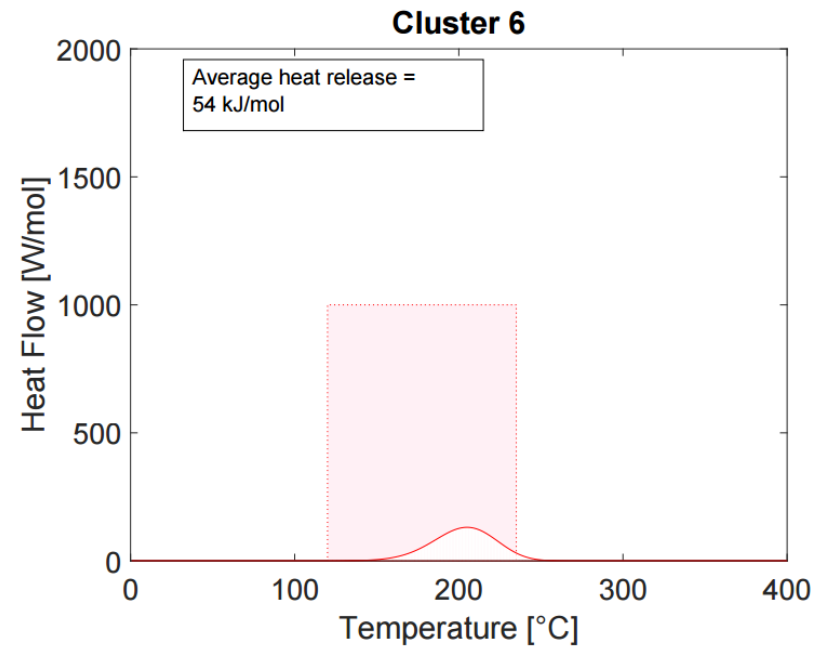
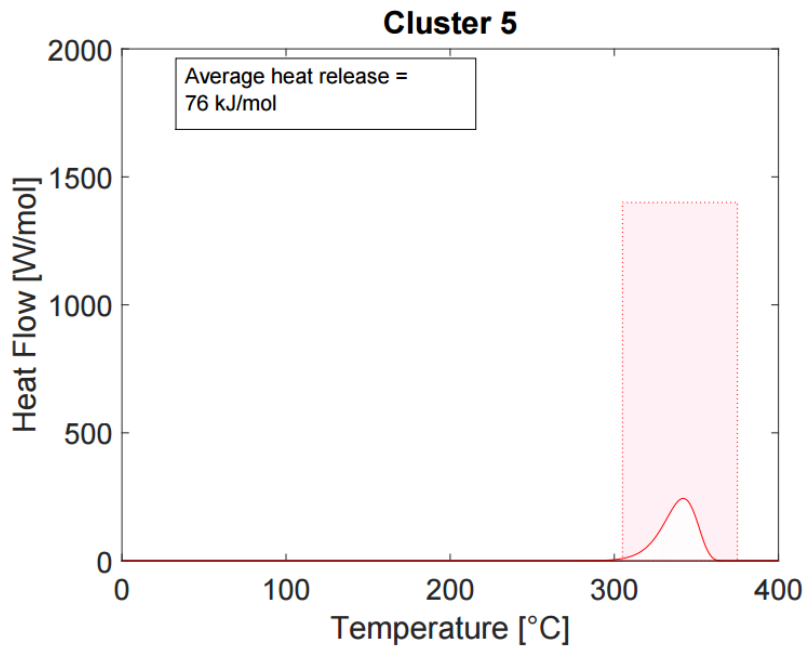
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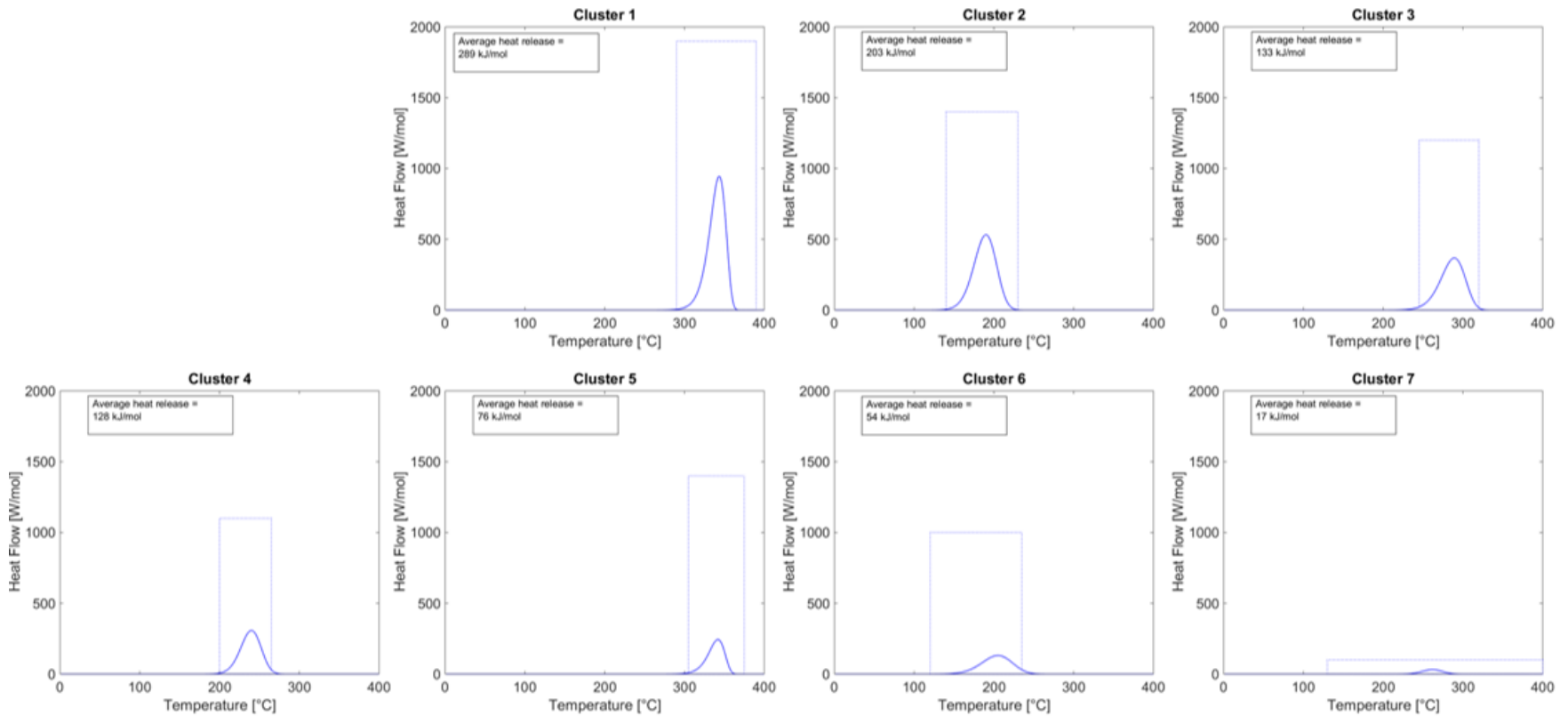
Results: Classification

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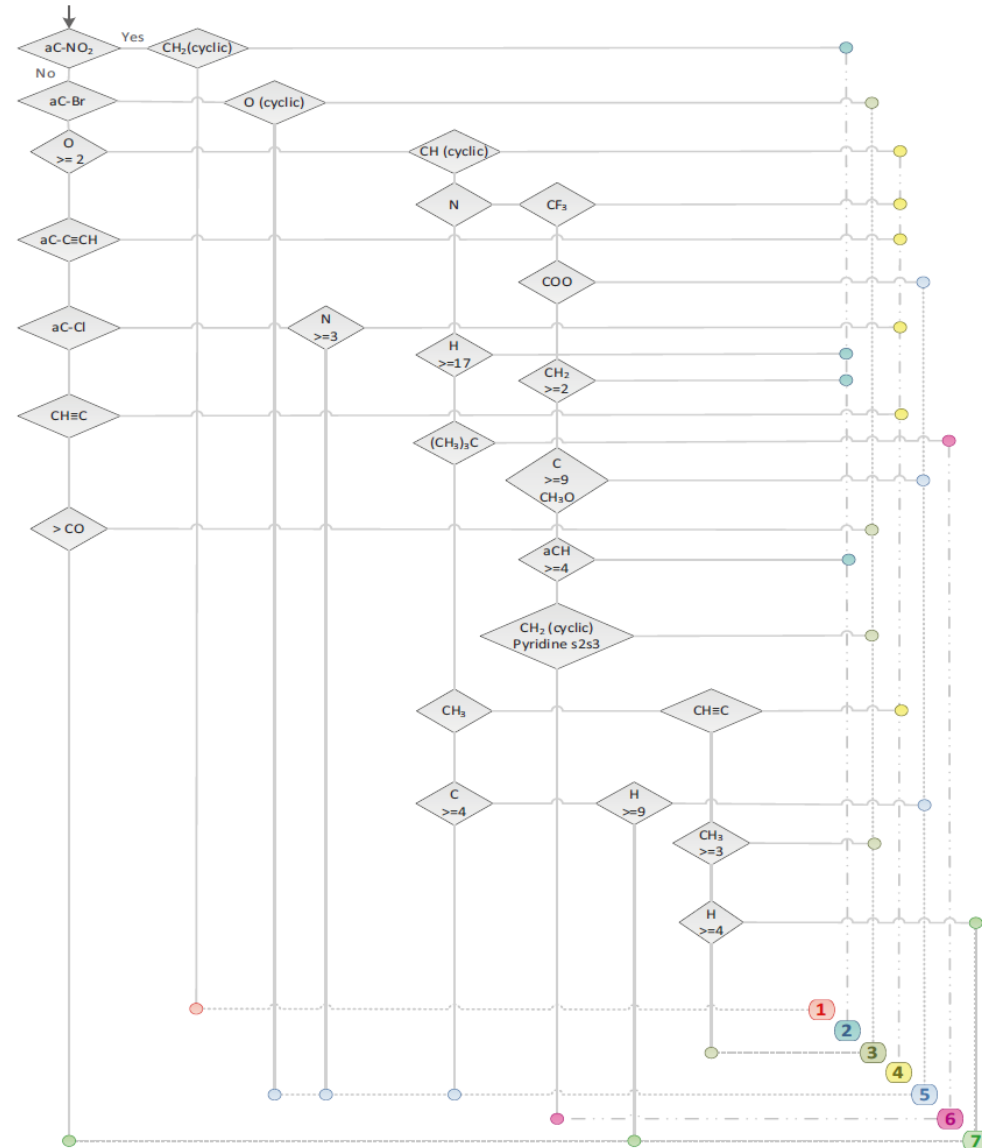
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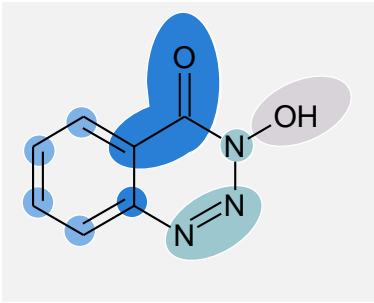
Results: Classification

- DSC Image processing
- 7 clusters
- GCM (GC+)



Results: Example

3-Hydroxy-1,2,3-benzotriazin-4(3H)-one:

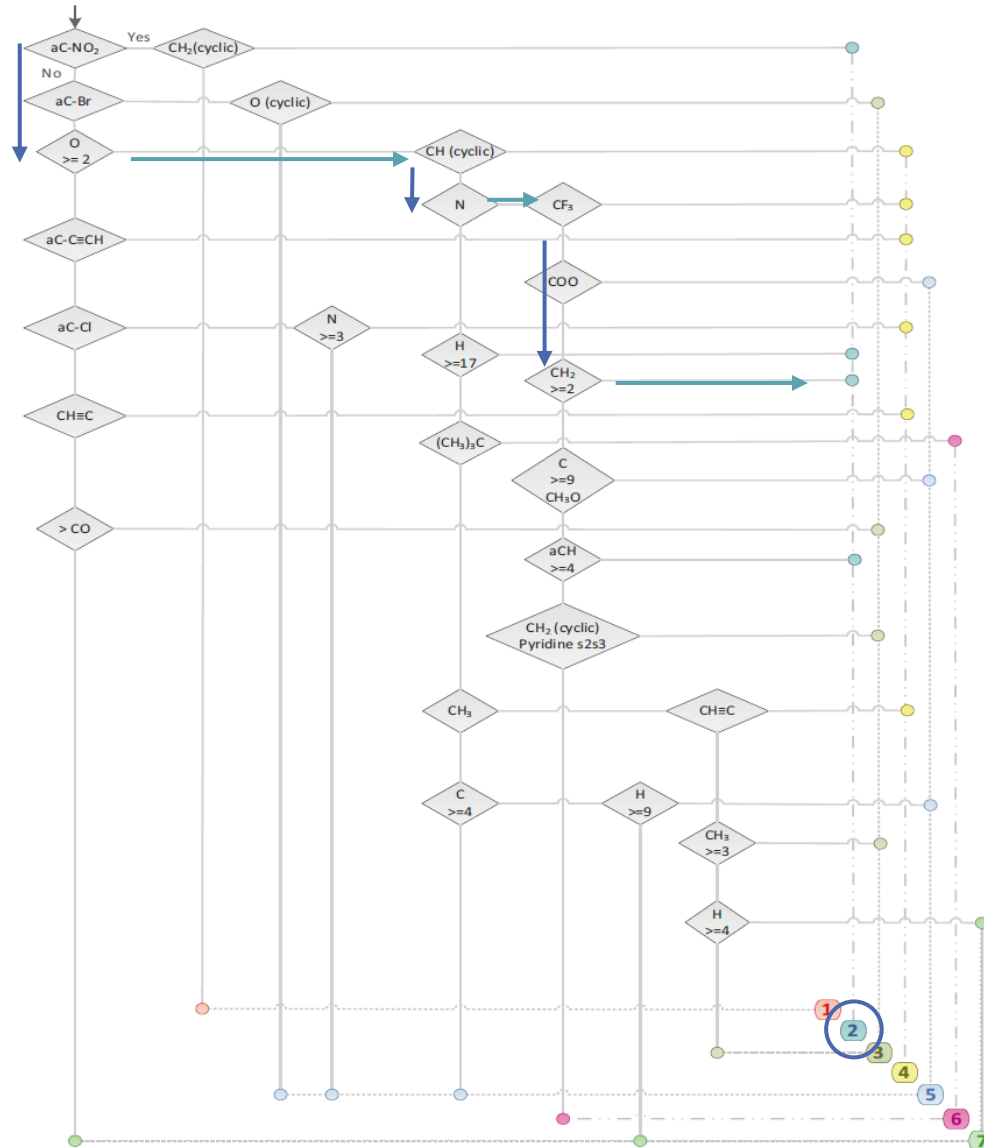


1st order:

- 4 aCH
- 2 aC fused w/ cyclic
- 1 OH
- 1 N (cyclic)
- 1 CO (cyclic)
- 1 N= N

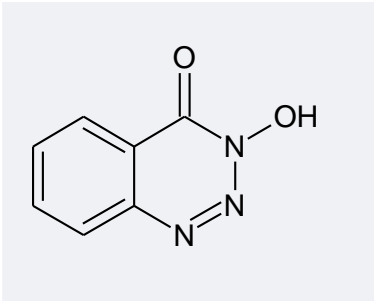
3rd order

- aC-CO (cyclic)

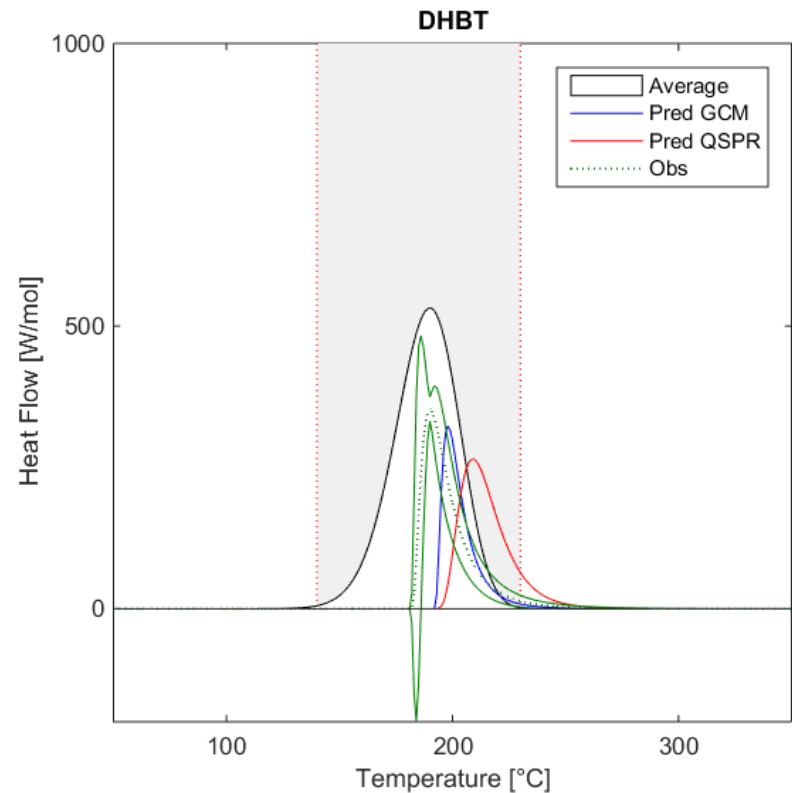


Results: Example

3-Hydroxy-1,2,3-benzotriazin-4(3H)-one:

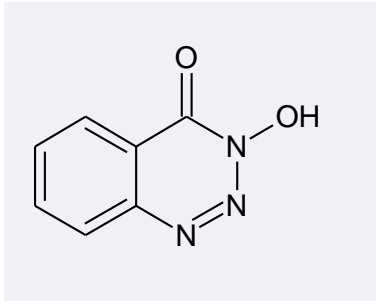


- Cluster Average
- Regressions



Results: Example

3-Hydroxy-1,2,3-benzotriazin-4(3H)-one:



- Cluster Average
- Regressions
- Primary Risk Assessment

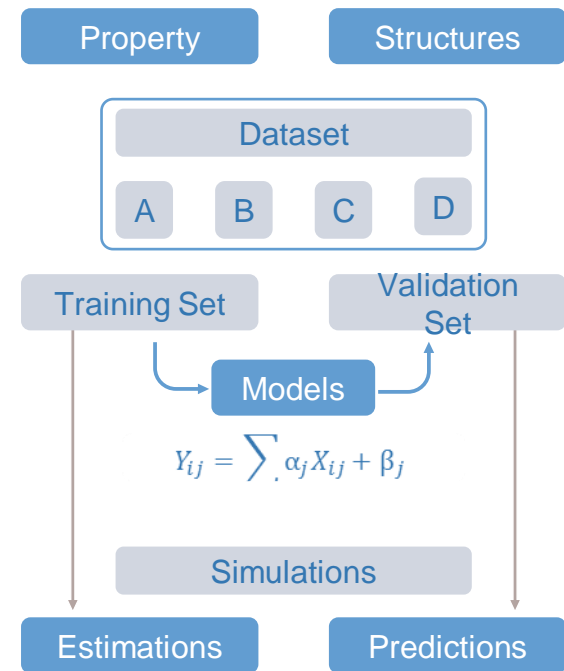
NN: Azo & Tetrazoles

2: Cluster 2

Severity	High $\Delta H_r > 800$ J/g		NN	2
	Medium $\Delta H_r < 800$ J/g			
	Low $\Delta H_r < 100$ J/g			
		$TD_{24} > 200^\circ\text{C}$ Low	$TD_{24} < 200^\circ\text{C}$ Medium	$TD_{24} < 150^\circ\text{C}$ High
Probability of occurrence				

Conclusions

- Methodology successful and adaptive
- Global models
 - Regression: limited performances
 - Classification: efficient
- Local models:
 - Regression: higher performances
 - Systematic repartitions
- Early Application



Applications

- Estimation of Missing Data
- Screening Tool
 - Test & evaluate several alternatives
 - Identify the most/least hazardous ones
- Process Design
 - Minimal intrinsic hazard
 - Inherently Safer Design
- Future Applications
 - Kinetic Parameters Estimation
 - Criticality Classification



Not a replacement for
experimental testing
and proper
characterization !

Acknowledgments



Process Safety



This project is supported by the
Swiss Commission for Technology and Innovation
(project n°:14711.1 PFIW-IW)

AKTS

Advanced Kinetic and Thermal Analysis Software

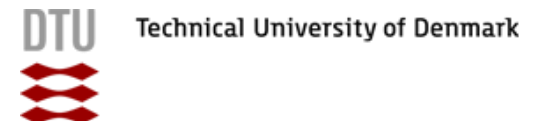


Novartis Pharma
Safety Laboratory



CAPEC

Computer Aided Process Engineering Center



Thank you for your attention