Topics/ Exam

- Introduction to process safety
- Systematics; Cooling failure scenario
- Criticality classes
- Calorimetry
- Decompositions, TMRad
- Autocatalysis
- Heat confinement
- Synthesis reaction, different types of reactors
- Risk reducing measures
- Explosion, ignition sources, unit operations

Key points – Systematics, cooling failure scenario

- Assessment of thermal risk
- Heat Balance
  - Stable and Unstable working point
  - Influence of UA and Tc
- Cooling Failure Scenario
  - Graph
  - Six questions and Nomenclature
- Criteria for severity and probability assessment for thermal hazard
- Criticality classes

Key points – Calorimetry

- Study of main reaction:
  - Reaction calorimeters (RC1, CPA)
  - Data obtained: Reaction energy Q'_{rxn}, heat release rate q'_{rxn}, accumulation X_{acc} → can calculate MTSR
  - Screening possible in DSC and C80
- Study of decomposition reactions
  - Screening: DSC, C80, ARC (adiabatic)
    - Data obtained DSC and C80 from scan experiment:
      - decomposition energy, information on gas production (C80).
      - TMRad is calculated (see lecture on thermal stability)
    - Data obtained for ARC
      - TMRad and ΔTad
      - Correction for non adiabacity (Φ factor)
  - Low heat release rate (e.g. Storage)
    - TAM; isothermal measurement
    - Data obtained: decomposition energy, heat release rate
    - TMRad calculated (see lecture on thermal stability), or heat balance calculated (see lecture on heat confinement)
  - Adiabatic: VSP, Dewar
    - Data obtained: TMRad and ΔTad
    - Correction for non adiabacity (Φ factor)

Thermal safety- Decomposition reactions

- ΔTad
- TMRad
  - Hypothesis, simplifications
  - Methods to determine TMRad
  - Calculation of TMRad

Autocatalysis

- Kinetic description
- Difference to “normal” reactions
  - Behavior isothermal, adiabatic conditions
  - Why is it important to be aware that a decomposition is autocatalytic?
  - What are additional constraints when having autocatalytic decompositions?
- Steps to evaluate TMRad and drawback of the simple methods (rule of thumb, 0 order evaluation)
- Thermal history

Heat confinement

- Which situations lead to heat confinement?
- Influence of size
- Difference between adiabatic conditions, heat confinement and well cooled reactors (stirred tank reactors)
- Difference between convection and conduction situations
- Evaluation of heat balance for heat convection
  - Heat balance with stirred reactor
- Evaluation of heat balance for heat conduction
  - Heat balance for solid (Frank – Kamenetskii, Thomas model)

Reactors – synthesis reaction

- Safety criteria for reactors
- Determination of accumulation, MTSR
- Main focus for calculations on batch and semi-batch
- Advantages, disadvantages of the different reactor types
- Make recommendation based on the obtained criticality class to improve safety of the process

Risk reducing measures

- Calculating V or Pressure reached in a reactor
- Know which type of risk reducing measures are possible
- Determine whether boiling barrier is suitable. Know the four criteria:
  - Calculate amount of vapor produced
  - Calculate required cooling power of the condenser (extrapolate heat release rate to the boiling temperature)
  - Calculate vapor rate in vapor tube (below 5 m/s ok, no flooding)
  - Know which additional criteria would need to be checked (no need to be able to calculate it)
- Make recommendations

Explosion

- What conditions are required to get an explosion?
- How can explosions be avoided?
- What are typical ignition sources and how can these be avoided?
- Know the main properties which are relevant when assessing explosion hazards
- Know the different electrostatic ignition sources and which explosive mixtures they can ignite

Exercices

- All exercises are good examples for the exam
- Autocatalysis exercise: calculation with rule of thumb/ O order and then the conclusions

- Values for the parameters will be given. Estimations might be required for Ea, c'p

Exam

- 3 hours written exam on Monday 19.1.26 from 9h15 to 12h15 (CE 1 1)
- Mixture of multiple choice, “theory”, exercises (calculations)
- Max. 4.5 points for the exam + 0.5 points for presentation + 1 point for presence

- 1 A4 sheet, written on both sides (recto-verso)
- Simple, non programmable calculator