Heat Confinement

Module 4

ENG 431: Safety Chemical Processes

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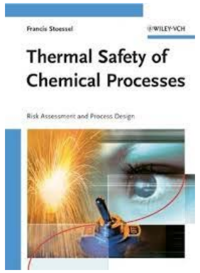
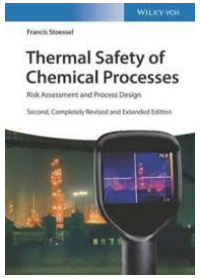
Heat Accumulation

- Introduction
- Mechanism of heat transfer
  - Stirred systems: forced convection
  - Solid systems, viscous liquids: conduction
  - Low viscosity liquids: natural convection
- Analysis procedure
- Practical examples

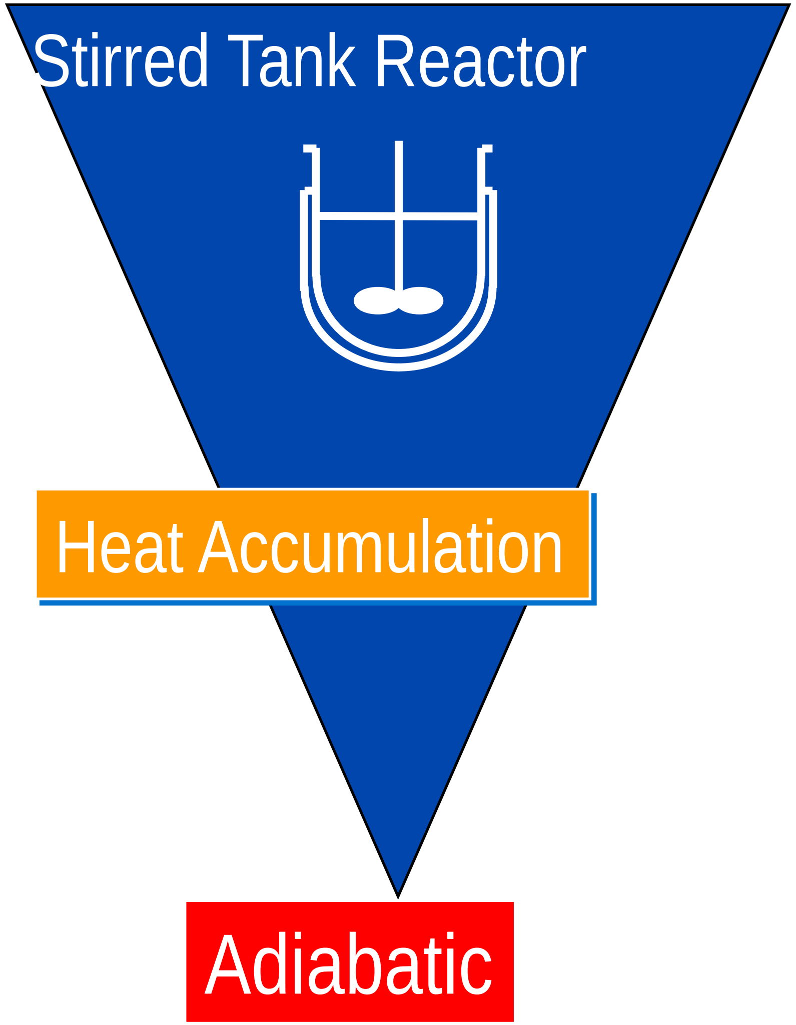


Chapter 13



Chapter 12

How realistic are adiabatic conditions?



Heat accumulation

Heat accumulation situations: effect of mass

- Decomposition of a reaction mass. ΔT_{ad} 200°C, c'p: 1.7 kJ/kg.K, Ea: 100 kJ/mol
- Reaction mass is in different containers (different sizes)

Heat release rate (W/kg)	Temperature at beginning of storage (°C)	Adiabatic	Mass			
			0.5 kg	50 kg	5000 kg	
10	129					ΔT [°C]
						Released after [h]
1	100					ΔT [°C]
						Released after [h]
0.1	75					ΔT [°C]
						Released after [h]
0.01	53					ΔT [°C]
						Released after [h]

Heat removal

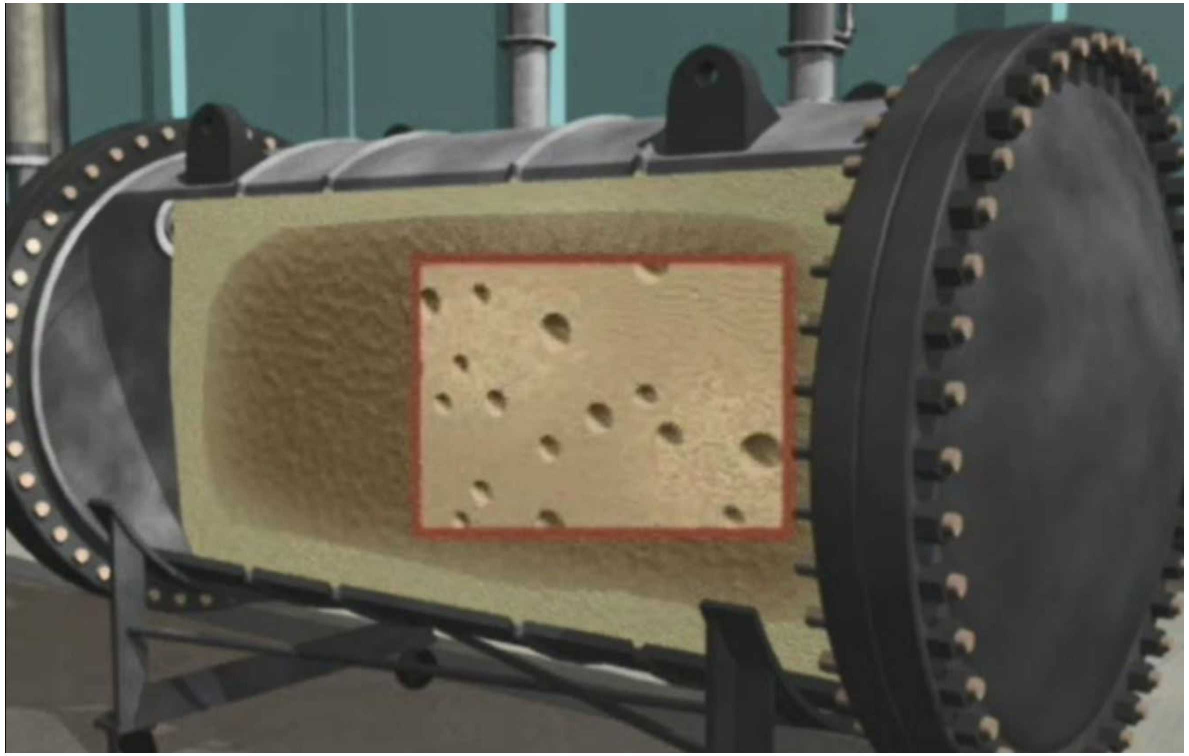
- Agitated vessel: Main resistance to heat transfer is located at the wall

- Unstirred non-insulated storage tank containing liquid: main resistance to heat transfer is located outside of the wall (natural convection in the liquid)

- Storage silo containing a solid: main resistance to heat transfer in the solid (conduction)

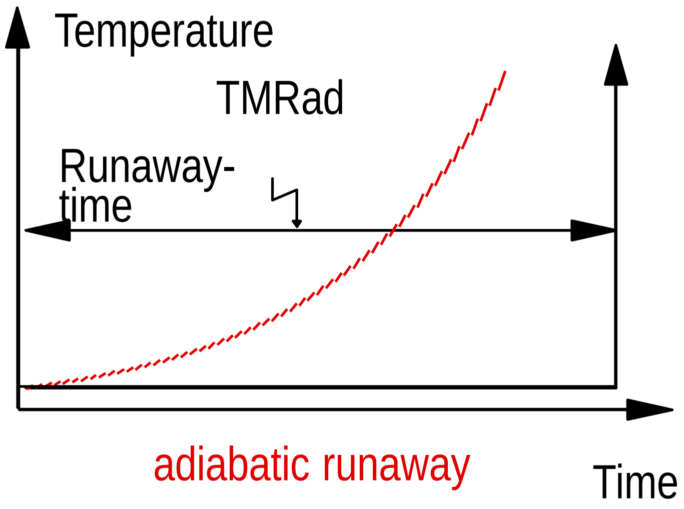
Heat Accumulation in Industrial Context

- Hot discharge
- Heating chambers
- Storage
- Transport
- Inadvertent shut down
- Heated pipes



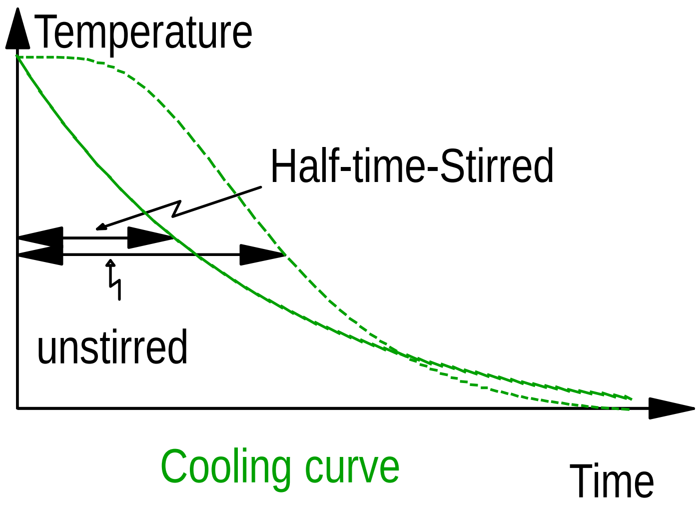
Heat balance using time scales

Heat production



adiabatic runaway

Heat removal



Cooling curve

Thermal Explosion if: Heat production > Heat removal

Adiabatic Runaway-time < Cooling time

Heat Accumulation

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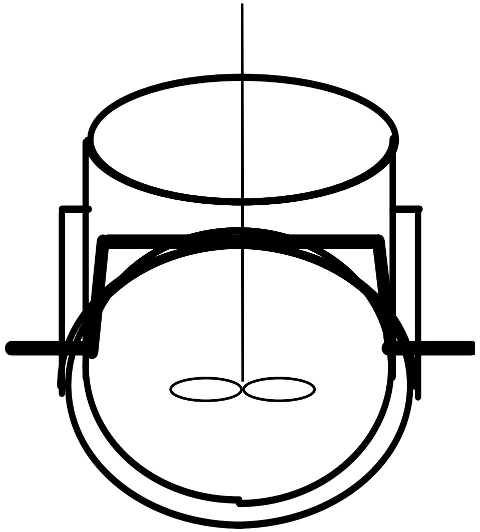
Agitated System

- Semenov
- Newtonian cooling

$$q_{ex} = U \cdot A \cdot (T - T_C)$$



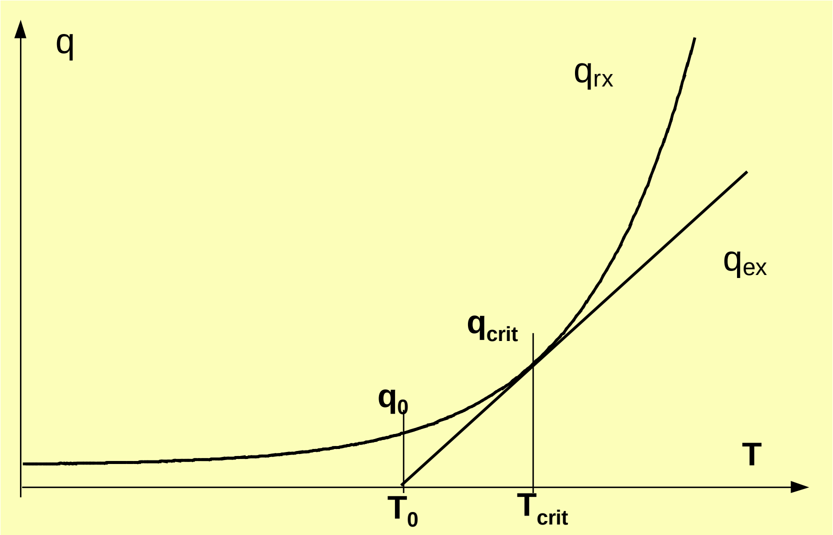
U : *Overal heat transfer coefficient* $[W\ m^{-2}\ K^{-1}]$

A : *Heat exchange area* $[m^2]$

T : *Temperature reacting medium* $[°C, K]$

T_C : *Temperature cooling medium* $[°C, K]$

Heat Balance



$$q_{rx} = q_{ex} = Q_{rx}.\rho \cdot V \cdot k_0 \cdot \exp\left[\frac{-E}{RT_{crit}}\right] = U \cdot A \cdot \left(T_{crit} - T_0\right)$$

$$\frac{dq_{rx}}{dT} = Q_{rx}.\rho \cdot V \cdot k_0 \cdot \frac{E}{RT_{crit}^2} \cdot \exp\left[\frac{-E}{RT_{crit}}\right] = \frac{dq_{ex}}{dT} = U \cdot A$$

Heat Balance

Solves both equation if $\Delta T_{crit} = T_{crit} - T_0 = \frac{RT_{crit}^2}{E} \approx \frac{RT_0^2}{E}$

$$Q_{rx}.\rho \cdot V \cdot k_0 \cdot \exp\left[\frac{-E}{R}\left(\frac{1}{T_{crit}} - \frac{1}{T_0}\right)\right] = U \cdot A \cdot \Delta T_{crit} \quad \text{since} \quad q_{crit} = q_0 \cdot \exp\left[\frac{-E}{R}\left(\frac{1}{T_{crit}} - \frac{1}{T_0}\right)\right]$$

$$\frac{-E}{R}\left(\frac{1}{T_{crit}} - \frac{1}{T_0}\right) \approx \frac{-E}{RT_{crit}^2}(T_{crit} - T_0) = 1 \quad \text{since} \quad \Delta T_{crit} = \frac{RT_0^2}{E}$$

$$k_0 \cdot e \cdot \Delta T_{ad} = \frac{U \cdot A}{\rho \cdot V \cdot c_p'} \cdot \frac{RT_0^2}{E}$$

$$\frac{1}{k_0 \cdot \Delta T_{ad}} \cdot \frac{RT_0^2}{E} = TMR_{ad}$$

$$t_{1/2} = \ln(2) \cdot \tau$$

$$\tau = \frac{\rho \cdot V \cdot c_p'}{U \cdot A}$$

$$\boxed{TMR_{ad} = \frac{e}{\ln(2)} \cdot t_{1/2} = 3.92 \cdot t_{1/2}}$$

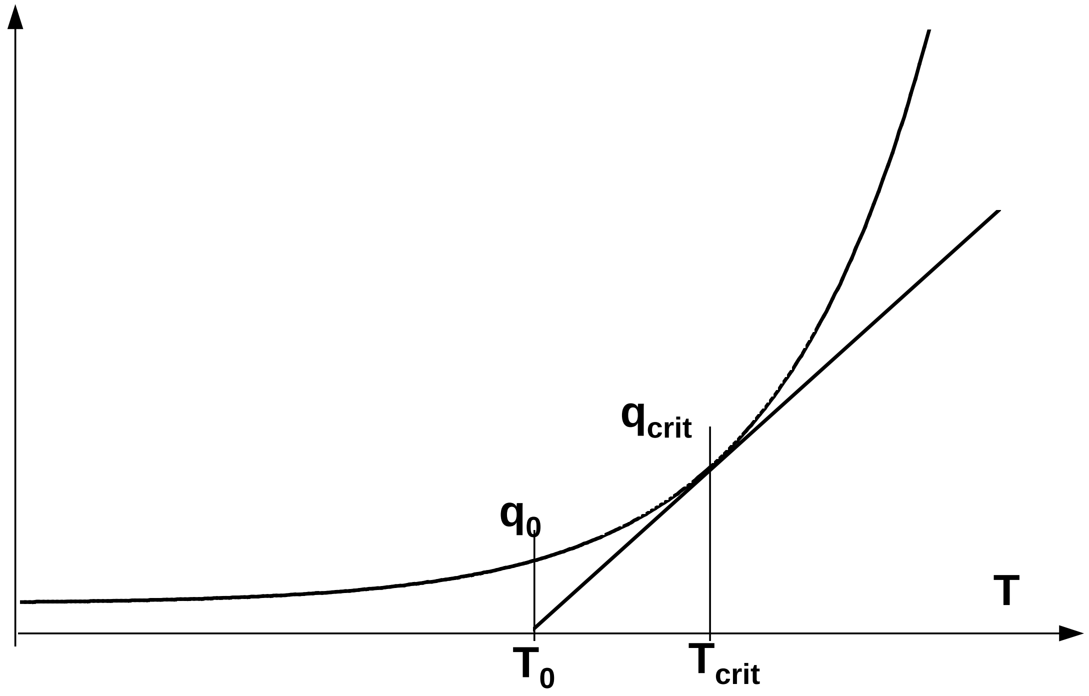
Agitated System

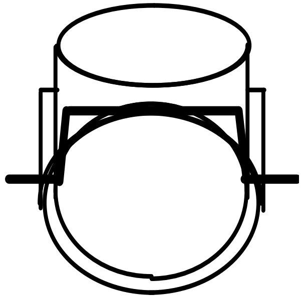
- Semenov

$$TMR_{ad} > 3.92 \cdot t_{1/2}$$

$$\tau = \frac{\rho \cdot V \cdot c'_p}{U \cdot A}$$

$$t_{1/2} = \ln(2) \cdot \tau$$





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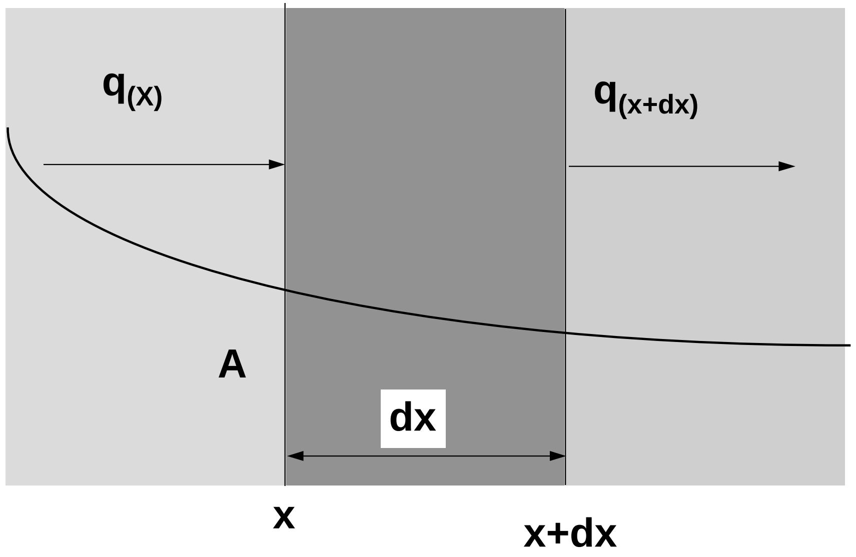
Heat Conduction in a Solid



$$\vec{q} = -\lambda \vec{\nabla} T$$

Thermal conductivity: λ [W/(K·m)]

$$\frac{\partial^2 T}{\partial x^2} = \frac{\rho \cdot c_p'}{\lambda} \frac{\partial T}{\partial t} = \frac{1}{a} \frac{\partial T}{\partial t}$$

Thermal diffusivity: a [m²/s] $$a = \frac{\lambda}{\rho \cdot c_p'} = \frac{\text{heat conducted}}{\text{heat stored}}$$

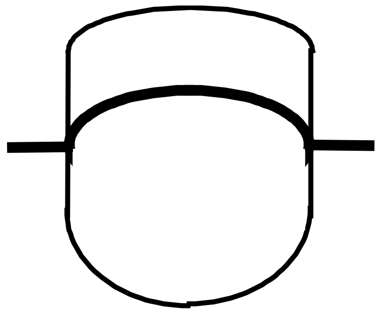
Systems with Temperature Profile

Frank-Kamenetskii

$T_0 = T_{ambiant}$

$x = r_0 \Rightarrow T = T_0$ Conditions at the wall

$x = 0 \Rightarrow \frac{\partial T}{\partial x} = 0$ Conditions at the center



$\theta = \frac{E \cdot (T - T_0)}{RT_0^{\ 2}}$ $z = \frac{x}{r_0}$ Change of variables

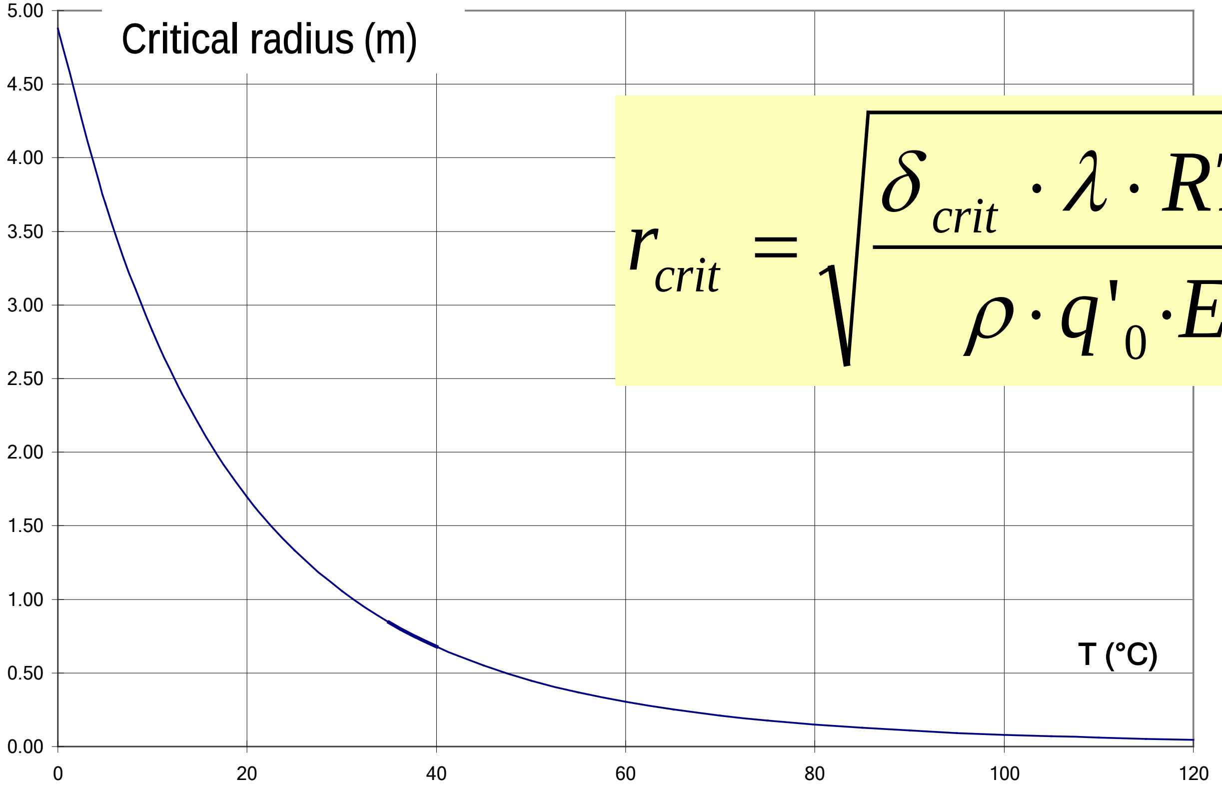
$\nabla_z^{\ 2}\theta = -\delta \cdot \exp(\theta)$ Conduction equation

$\delta = \frac{\rho_0 \cdot q'_0}{\lambda} \cdot \frac{E}{RT_0^{\ 2}} \cdot r_0^{\ 2}$ Solution

$$r_{crit} = \sqrt{\frac{\delta_{crit} \cdot \lambda \cdot RT_0^{\ 2}}{\rho \cdot q'_0 \cdot E}}$$

r: critical radius [m]
λ: Thermal conductivity [W/(K·m)]
δ_{crit}: form factor

Critical Radius



$$r_{crit} = \sqrt{\frac{\delta_{crit} \cdot \lambda \cdot RT_0^{\,2}}{\rho \cdot q'_0 \cdot E}}$$

Form Factor Frank-Kamenetskii criterion

- Slab $\delta_{crit} = 0.88$
- Infinite Cylinder $\delta_{crit} = 2.0$
- Sphere $\delta_{crit} = 3.32$

- Cylinder h = 3 r $\delta_{crit} = 2.37$
- Cube $\delta_{crit} = 2.5$

Systems with Temperature Profiles

Time Scale

- Sphere $$TMR_{ad} > \frac{0.3 \cdot r^2}{a}$$
- Cylinder $$TMR_{ad} > \frac{0.5 \cdot r^2}{a}$$
- Slab $$TMR_{ad} > \frac{1.14 \cdot r^2}{a}$$

Conduction in solid and transfer at wall

Thomas Model

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{a}\frac{\partial T}{\partial t}$$

$$z = \frac{x}{r_0} \quad \text{and} \quad \theta = \frac{\mathrm{E}\left(\mathrm{T}-\mathrm{T}_0\right)}{RT_0^{\;2}}$$

Wall $\quad \lambda \dfrac{dT}{dx} + h \cdot \left(T_s - T_0\right) = 0 \quad \text{à } x = r_0$

$$\frac{d\theta}{dz} + Bi \cdot \theta_S = 0 \quad \text{at} \quad z = 1$$

Center $\quad \dfrac{dT}{dx} = 0 \quad \text{à} \quad x = 0$

$$Bi = \frac{h \cdot r_0}{\lambda}$$

Variable exchange

Conduction in solid and transfer at wall

Zero order reaction

$$\nabla_z^{2}\theta = \frac{d^2\theta}{dz^2} + \frac{k}{z}\frac{d\theta}{dz} = \frac{d\theta}{d\tau} - \delta \exp\theta$$

$$\tau = \frac{at}{r_0^{2}} \qquad a = \frac{\lambda}{\rho \cdot Cp'}$$

Reaction characteristics

$$\delta = \frac{\rho_0 \cdot q'_0}{\lambda} \cdot \frac{E}{RT_0^{2}} \cdot r_0^{2}$$

Heat transfer

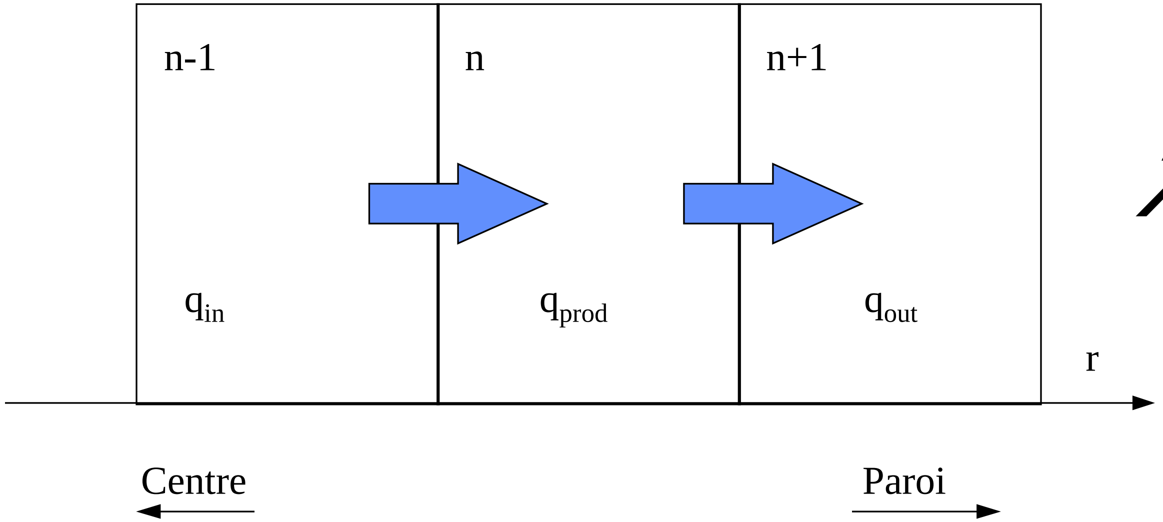
$$\delta_{crit} = \frac{1+k}{e \cdot \left(\frac{1}{\beta_\infty} - \frac{1}{Bi} \right)}$$

Slab:	$k = 0$	$\beta_\infty = 2.39$
Cylinder:	$k = 1$	$\beta_\infty = 2.72$
Sphere:	$k = 2$	$\beta_\infty = 3.01$

$$Bi = \frac{h \cdot r_0}{\lambda}$$

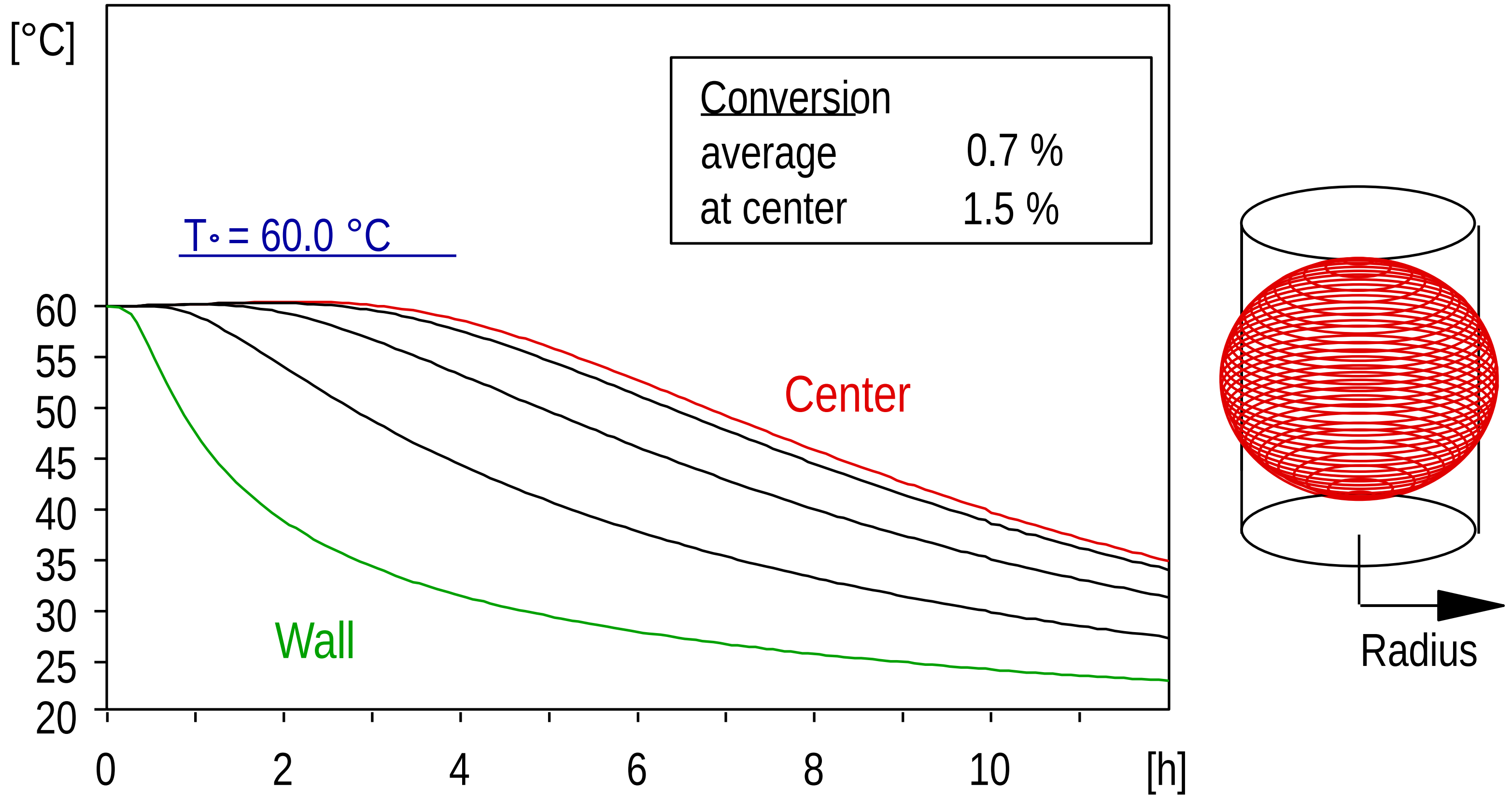
δ from Thomas model ≠ δ from Frank-Kamenetskii model

Finite elements

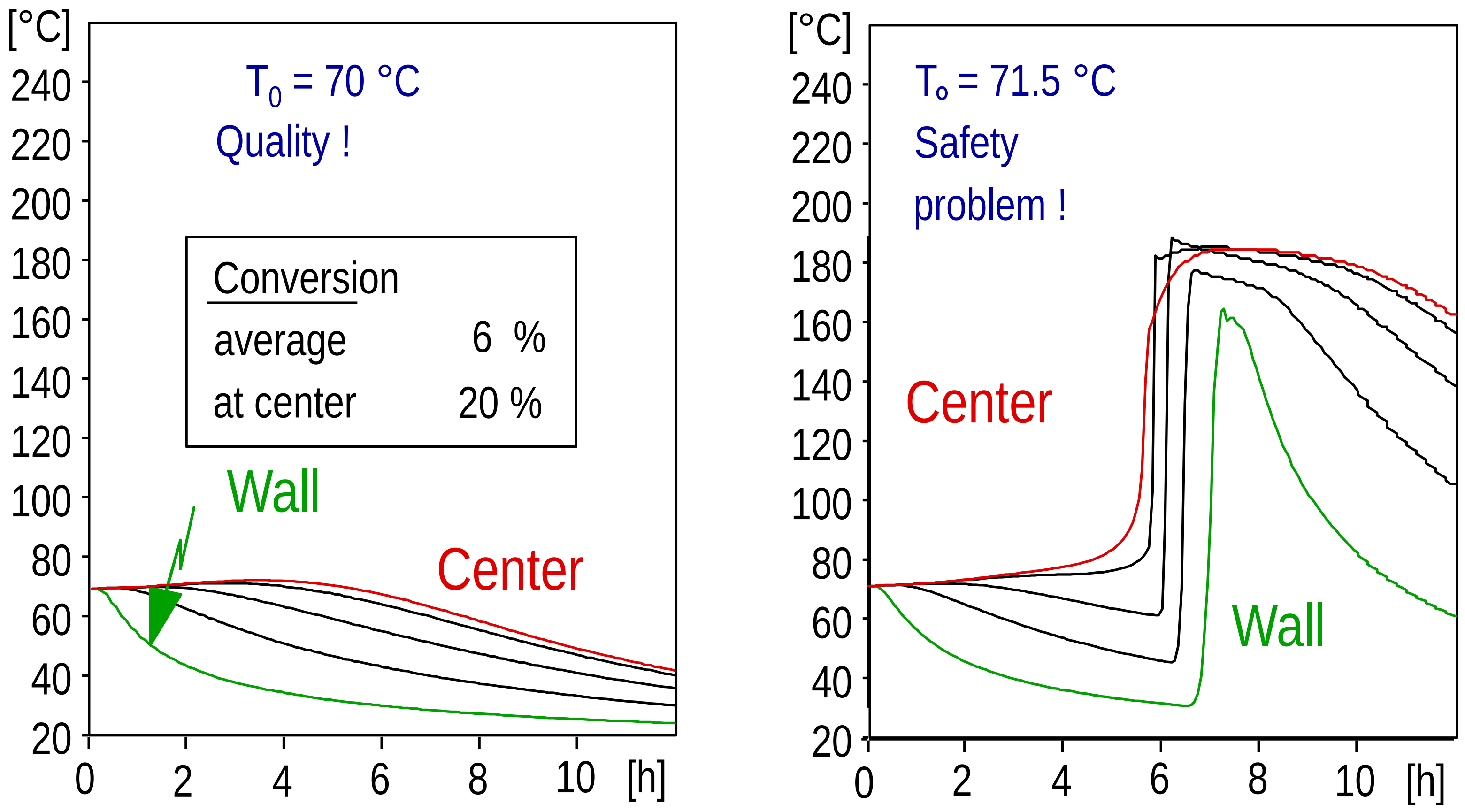


$$\lambda \frac{\partial^2 T}{\partial x^2} = q_{rx}$$

Heat accumulation: hot discharge into a drum



Heat accumulation



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Natural Convection

$$Nu = C^{te} \cdot Ra^{m}$$

with: $Nu = \dfrac{hL}{\lambda}$

and: $Ra = \dfrac{g \cdot \beta \cdot L^{3} \cdot \rho^{2} \cdot Cp' \cdot \Delta T}{\mu \cdot \lambda} = Gr \cdot \mathrm{Pr}$

Turbulent flow : Ra > 10^9	Nu=0,13 $Ra^{1/3}$
Intermediate flow : 10^4< Ra < 10^9	Nu = 0,59 $Ra^{1/4}$
Laminar flow : Ra < 10^4	Nu = 1,36 $Ra^{1/6}$

Turbulent flow: likely to have natural convection.

Otherwise, safe not rely on natural convection

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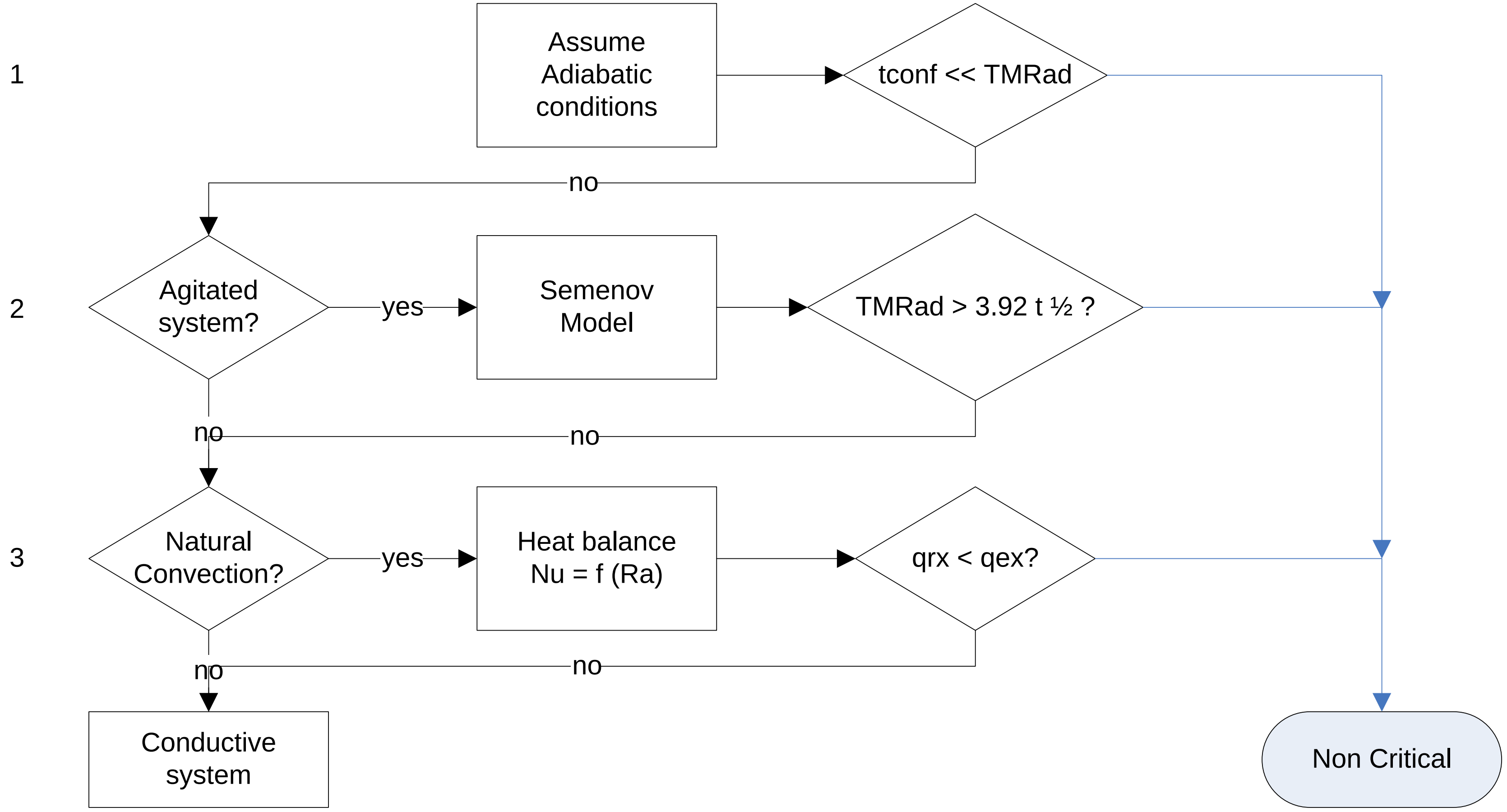
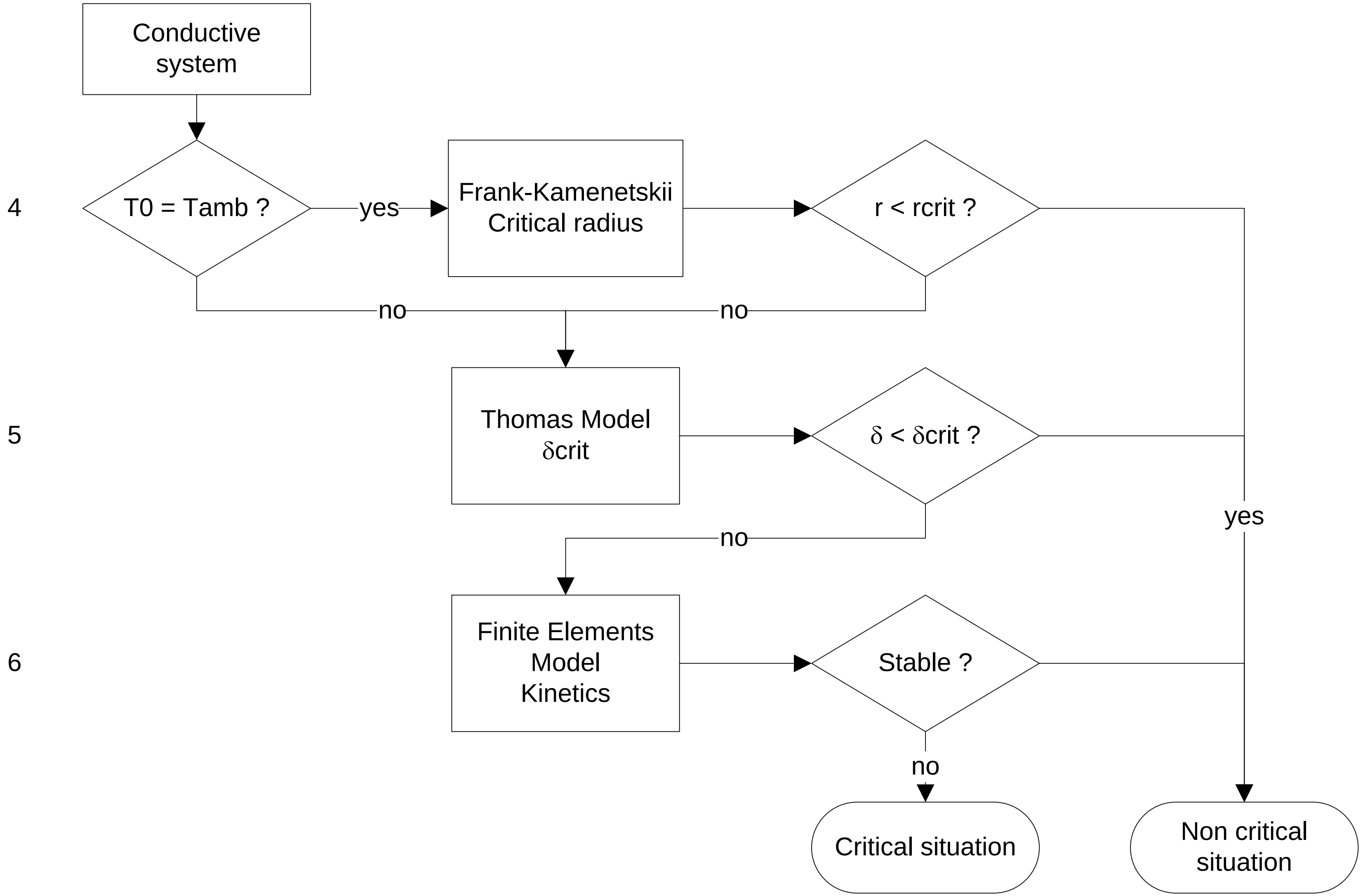
Decision tree (Part 1)



Decision tree (Part 2)



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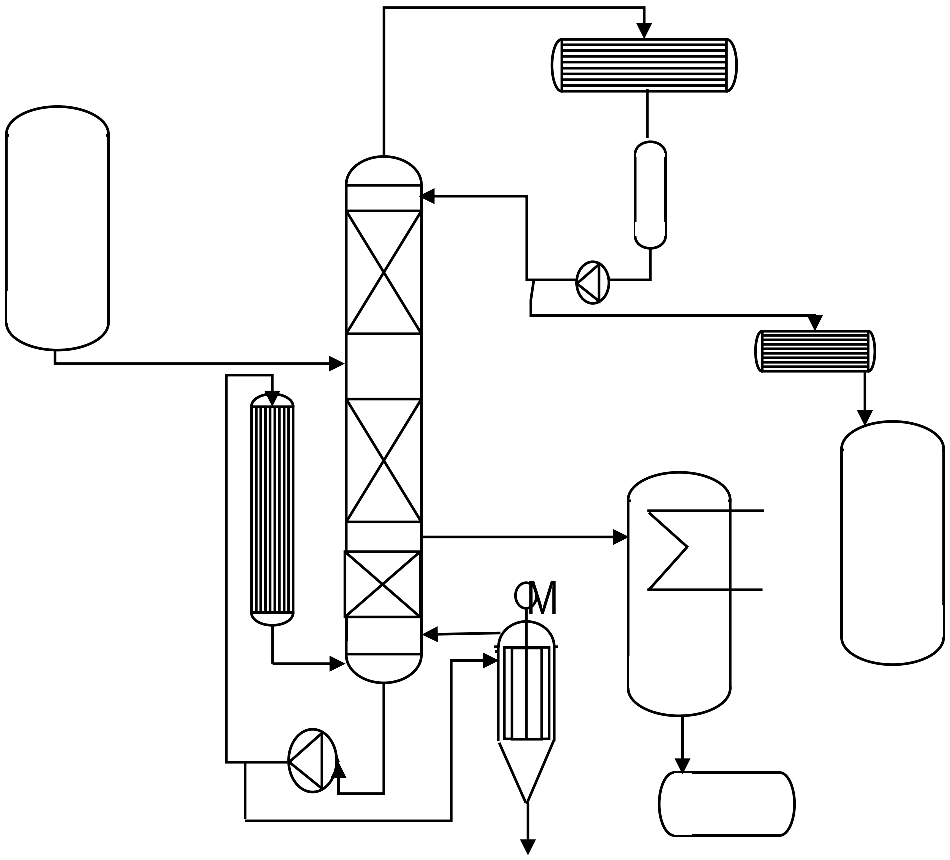
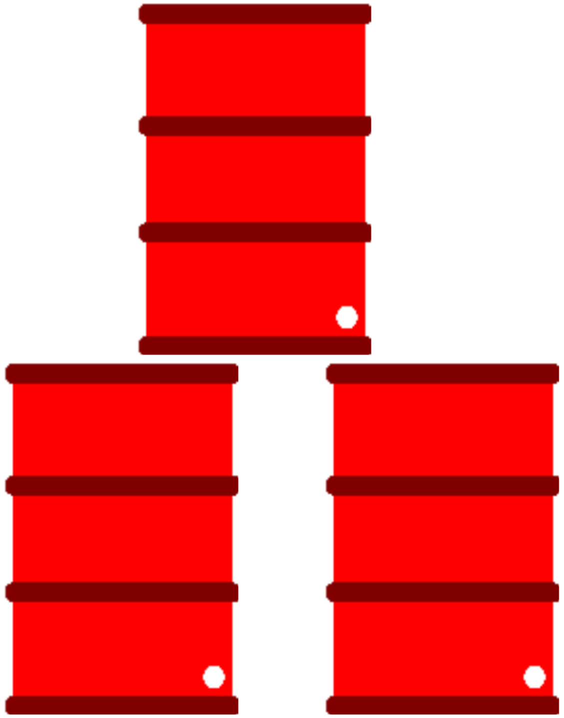
Where may Heat Accumulation Occur ?



Equipment:

- Distillation residue
- Isolated equipment
- Continous processes
  at shut down

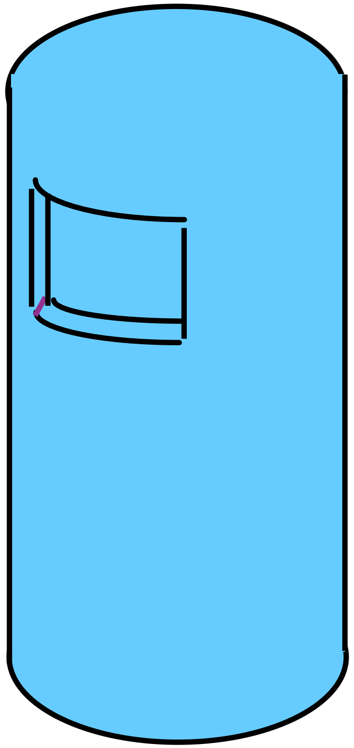
Where may Heat Accumulation Occur ?



- Storage
- Hot discharge
- Discharge after thermal stress (Drying, Milling, Blending, Formulation)

Monitor Temperature at Center !

Where may Heat Accumulation Occur ?

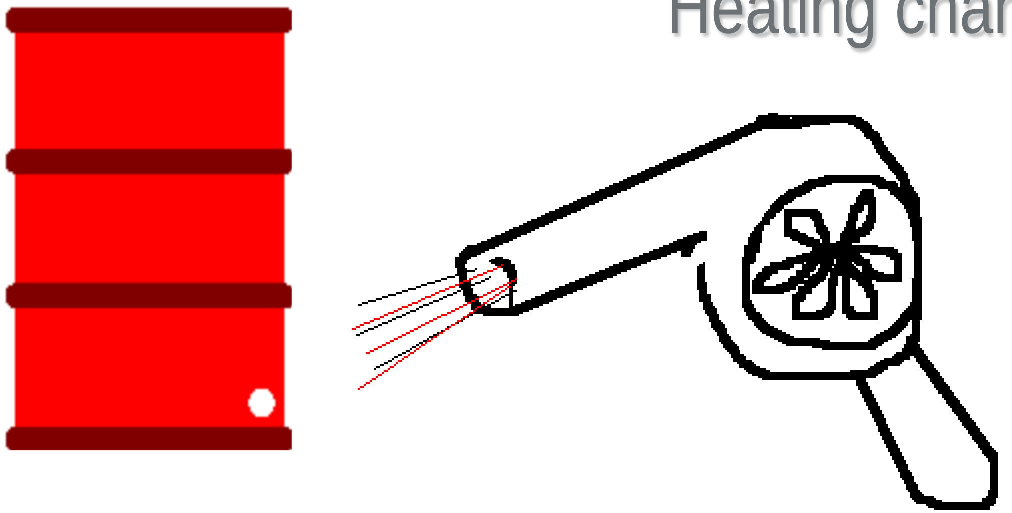


- Tanks with reactive contents
- Insulated storage tanks
- Changes in thermal insulation

Monitor Temperatur at center !

Where may Heat Accumulation Occur ?

Melting in hot air
Heating chamber



Monitor Temperature at Center of bulk !

Where may Heat Accumulation Occur ?

Transport