Adiabatic Temperature Rise of a Reactor

Adiabatic temperature rise of a liquid-phase reaction from heat of reaction, feed concentration, conversion, density and specific heat, with the outlet temperature.

Method: Energy balance ΔT_ad = (−ΔH_r) C_A0 X/(ρ c_p) (Fogler; Stoessel, Thermal Safety of Chemical Processes)

Input parameters

Unit system: SI

Parameter	Value	Unit
Heat of reaction (negative: exothermic)	-80.000	kJ/mol
Feed concentration of the key reactant	2.0000	mol/L
Conversion	90.000	%
Mixture density	950.00	kg/m³
Mixture specific heat	2.4000	kJ/(kg·K)
Feed temperature	50.000	°C

Calculated results

Parameter	Value	Unit
Adiabatic temperature rise	63.158	K
Outlet temperature (adiabatic)	113.16	°C
Rise at full conversion	70.175	K

Notes for this case

- A large adiabatic rise means a cooling failure could run away: check it against the decomposition temperature.
- Screening energy balance only (no heat of mixing, vaporisation or decomposition): not a basis for relief sizing.

Formula and method

$$\Delta T_{ad} = \frac{(-\Delta H_r) C_{A0} X}{\rho c_p}$$

Variables

ΔH_r	Heat of reaction (negative: exothermic)	J/mol
C_{A0}	Feed concentration of the key reactant	mol/m³
X	Conversion	-
ρ	Mixture density	kg/m³
c_p	Mixture specific heat	J/(kg·K)
T_0	Feed temperature	K
ΔT_{ad}	Adiabatic temperature rise	K
T	Outlet temperature (adiabatic)	K
$\Delta T_{ad,100}$	Rise at full conversion	K

Method and standards

Energy balance.

Assumptions and limits

- Constant properties, no heat loss.
- Screening energy balance: no heat of mixing, no vaporisation or vapour pressure, no decomposition onset. Not a design basis for relief sizing (use calorimetry data and a recognised relief method).
- An endothermic reaction (ΔH_r > 0) gives a fall; a fall that would take the mixture below 0 K is rejected.

References

• Energy balance ΔT_ad = (−ΔH_r) C_A0 X/(ρ c_p) (Fogler; Stoessel, Thermal Safety of Chemical Processes)

Report details

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Release checks	2 reference cases of this calculator, computed independently, are checked on every release

Results are for engineering estimation. Verify critical designs against the referenced standards and your own data.

This calculator online

https://calc.firecad.com/chemical/reactors/adiabatic-temperature-rise

Open this case on calc.firecad.com →

Reopens the calculator with the inputs of this report.