Runaway Reaction: Adiabatic Temperature Rise and Phi Factor

Adiabatic temperature rise of a reacting mass, the maximum temperature it can reach, and the correction of a test-cell result to plant scale by the phi factor.

Method: Crowl and Louvar; Chemical Process Safety: Fundamentals with Applications; ...

Input parameters

Unit system: SI

Parameter	Value	Unit
Heat of reaction (released, per kg of reactant)	1,500.0	kJ/kg
Mass fraction of reactant in the mixture	30.000	%
Specific heat of the mixture	2.5000	kJ/(kg·K)
Starting temperature	60.000	°C
Sample mass in the test cell	0.010000	kg
Test cell mass	0.008000	kg
Test cell specific heat	0.46000	kJ/(kg·K)
Temperature rise measured in the test	120.00	K

Calculated results

Parameter	Value	Unit
Adiabatic temperature rise	180.00	K
Maximum temperature after full conversion	240.00	°C
Phi factor of the test	1.1472	
Test result corrected to plant scale	137.66	K

Notes for this case

- Adiabatic: no heat loss and full conversion of the limiting reactant. Large plant reactors have a phi factor of about 1.1 or less; a test with a high phi factor understates the plant's temperature rise.
- A screening estimate for training and early design, not a hazard or risk study.
- A temperature rise above about 50 K is commonly treated as a high severity runaway.

Formula and method

$$\Delta T_{ad} = \frac{(-\Delta H_r)x}{C_p}, \quad T_{max} = T_0 + \Delta T_{ad}, \quad \phi = 1 + \frac{m_c C_{p,c}}{m_s C_p}$$

Variables

$-\Delta H_r$	Heat of reaction (released, per kg of reactant)	J/kg
x	Mass fraction of reactant in the mixture	-
C_p	Specific heat of the mixture	J/(kg·K)
T_0	Starting temperature	K
m_s	Sample mass in the test cell	kg
m_c	Test cell mass	kg
$C_{p,c}$	Test cell specific heat	J/(kg·K)
ΔT_{meas}	Temperature rise measured in the test	K
ΔT_{ad}	Adiabatic temperature rise	K
T_{max}	Maximum temperature after full conversion	K

ϕ	Phi factor of the test	-
$\phi\Delta T_{meas}$	Test result corrected to plant scale	K

Method and standards

Adiabatic heat balance and the phi factor.

Assumptions and limits

- Adiabatic; full conversion.

References

- Crowl and Louvar
- Chemical Process Safety: Fundamentals with Applications
- 2nd ed. (Prentice Hall, 2002)
- ch. 8
- eq. 8-1 (phi factor) and adiabatic heat balance

Report details

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

This calculator online

https://calc.firecad.com/chemical/process-safety/runaway-adiabatic-temperature-rise

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