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# Temperature and Pressure Effects Formulas

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## List of 9 Temperature and Pressure Effects Formulas

### Temperature and Pressure Effects ↗

#### 1) Adiabatic Heat of Equilibrium Conversion ↗

$$fx \Delta H_{r1} = \left( -\frac{\left( C' \cdot \Delta T \right) + \left( \left( C'' - C' \right) \cdot \Delta T \right) \cdot X_A}{X_A} \right)$$

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ex

$$-886.666667 \text{ J/mol} = \left( -\frac{(7.98 \text{ J/(kg*K)} \cdot 50 \text{ K}) + ((14.63 \text{ J/(kg*K)} - 7.98 \text{ J/(kg*K)}) \cdot 50 \text{ K}) \cdot 0.72}{0.72} \right)$$

#### 2) Equilibrium Conversion of Reaction at Final Temperature ↗

$$fx K_2 = K_1 \cdot \exp \left( - \left( \frac{\Delta H_r}{[R]} \right) \cdot \left( \frac{1}{T_2} - \frac{1}{T_1} \right) \right)$$

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$$ex 0.62993 = 0.6 \cdot \exp \left( - \left( \frac{-955 \text{ J/mol}}{[R]} \right) \cdot \left( \frac{1}{368 \text{ K}} - \frac{1}{436 \text{ K}} \right) \right)$$

#### 3) Equilibrium Conversion of Reaction at Initial Temperature ↗

$$fx K_1 = \frac{K_2}{\exp \left( - \left( \frac{\Delta H_r}{[R]} \right) \cdot \left( \frac{1}{T_2} - \frac{1}{T_1} \right) \right)}$$

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$$ex 0.600067 = \frac{0.63}{\exp \left( - \left( \frac{-955 \text{ J/mol}}{[R]} \right) \cdot \left( \frac{1}{368 \text{ K}} - \frac{1}{436 \text{ K}} \right) \right)}$$

#### 4) Final Temperature for Equilibrium Conversion ↗

$$fx T_2 = \frac{-(\Delta H_r) \cdot T_1}{\left( T_1 \cdot \ln \left( \frac{K_2}{K_1} \right) \cdot [R] \right) + (-(\Delta H_r))}$$

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$$ex 367.8693 \text{ K} = \frac{-(-955 \text{ J/mol}) \cdot 436 \text{ K}}{(436 \text{ K} \cdot \ln \left( \frac{0.63}{0.6} \right) \cdot [R]) + (-(-955 \text{ J/mol}))}$$



## 5) Heat of Reaction at Equilibrium Conversion ↗

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$$fx \Delta H_r = \left( -\frac{\ln\left(\frac{K_2}{K_1}\right) \cdot [R]}{\frac{1}{T_2} - \frac{1}{T_1}} \right)$$

$$ex -957.17613 \text{ J/mol} = \left( -\frac{\ln\left(\frac{0.63}{0.6}\right) \cdot [R]}{\frac{1}{368\text{K}} - \frac{1}{436\text{K}}} \right)$$

## 6) Initial Temperature for Equilibrium Conversion ↗

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$$fx T_1 = \frac{-(\Delta H_r) \cdot T_2}{-(\Delta H_r) - \left( \ln\left(\frac{K_2}{K_1}\right) \cdot [R] \cdot T_2 \right)}$$

$$ex 436.1837 \text{ K} = \frac{-(-955 \text{ J/mol}) \cdot 368 \text{ K}}{-(-955 \text{ J/mol}) - \left( \ln\left(\frac{0.63}{0.6}\right) \cdot [R] \cdot 368 \text{ K} \right)}$$

## 7) Non Adiabatic Heat of Equilibrium Conversion ↗

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$$fx Q = (X_A \cdot \Delta H_{r2}) + (C' \cdot \Delta T)$$

$$ex 1908.12 \text{ J/mol} = (0.72 \cdot 2096 \text{ J/mol}) + (7.98 \text{ J/(kg*K)} \cdot 50 \text{ K})$$

## 8) Reactant Conversion at Adiabatic Conditions ↗

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$$fx X_A = \frac{C' \cdot \Delta T}{-\Delta H_{r1} - (C'' - C') \cdot \Delta T}$$

$$ex 0.722172 = \frac{7.98 \text{ J/(kg*K)} \cdot 50 \text{ K}}{-885 \text{ J/mol} - (14.63 \text{ J/(kg*K)} - 7.98 \text{ J/(kg*K)}) \cdot 50 \text{ K}}$$

## 9) Reactant Conversion at Non Adiabatic Conditions ↗

[Open Calculator ↗](#)

$$fx X_A = \frac{(C' \cdot \Delta T) - Q}{-\Delta H_{r2}}$$

$$ex 0.718511 = \frac{(7.98 \text{ J/(kg*K)} \cdot 50 \text{ K}) - 1905 \text{ J/mol}}{-2096 \text{ J/mol}}$$



## Variables Used

- $\Delta T$  Change in Temperature (*Kelvin*)
- $C'$  Mean Specific Heat of Unreacted Stream (*Joule per Kilogram per K*)
- $C''$  Mean Specific Heat of Product Stream (*Joule per Kilogram per K*)
- $K_1$  Thermodynamic Constant at Initial Temperature
- $K_2$  Thermodynamic Constant at Final Temperature
- $Q$  Total Heat (*Joule Per Mole*)
- $T_1$  Initial Temperature for Equilibrium Conversion (*Kelvin*)
- $T_2$  Final Temperature for Equilibrium Conversion (*Kelvin*)
- $X_A$  Reactant Conversion
- $\Delta H_r$  Heat of Reaction per Mole (*Joule Per Mole*)
- $\Delta H_{r1}$  Heat of Reaction at Initial Temperature (*Joule Per Mole*)
- $\Delta H_{r2}$  Heat of Reaction per Mole at Temperature T2 (*Joule Per Mole*)



## Constants, Functions, Measurements used

- **Constant:** **[R]**, 8.31446261815324 Joule / Kelvin \* Mole  
*Universal gas constant*
- **Function:** **exp**, **exp(Number)**  
*Exponential function*
- **Function:** **ln**, **ln(Number)**  
*Natural logarithm function (base e)*
- **Measurement:** **Temperature** in Kelvin (K)  
*Temperature Unit Conversion* ↗
- **Measurement:** **Temperature Difference** in Kelvin (K)  
*Temperature Difference Unit Conversion* ↗
- **Measurement:** **Specific Heat Capacity** in Joule per Kilogram per K (J/(kg\*K))  
*Specific Heat Capacity Unit Conversion* ↗
- **Measurement:** **Energy Per Mole** in Joule Per Mole (J/mol)  
*Energy Per Mole Unit Conversion* ↗



## Check other formula lists

- [Design for Single Reactions Formulas](#) ↗
- [Ideal Reactors for a Single Reaction Formulas](#) ↗
- [Interpretation of Batch Reactor Data Formulas](#) ↗
- [Introduction to Reactor Design Formulas](#) ↗
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