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5.60 Thermodynamics & Kinetics
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Math Review

Differentiation

$$df = \left(\frac{\partial f}{\partial x}\right)_y dx + \left(\frac{\partial f}{\partial y}\right)_x dy \quad \text{and if } z = z(x, y)$$

$$\left(\frac{\partial f}{\partial x}\right)_z = \left(\frac{\partial f}{\partial x}\right)_y + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial x}\right)_z$$

$$\left(\frac{\partial x}{\partial y}\right)_z = \frac{1}{\left(\frac{\partial y}{\partial x}\right)_z}$$

$$\left(\frac{\partial x}{\partial y}\right)_z = - \left(\frac{\partial x}{\partial z}\right)_y \left(\frac{\partial z}{\partial y}\right)_x \left(\frac{\partial y}{\partial x}\right)_z \quad \text{or} \quad \left(\frac{\partial x}{\partial y}\right)_z \left(\frac{\partial y}{\partial z}\right)_x \left(\frac{\partial z}{\partial x}\right)_y = -1$$

If $df = gdx + hdy$ is exact then $\left(\frac{\partial g}{\partial y}\right)_x = \left(\frac{\partial h}{\partial x}\right)_y$

Examples:

$$\frac{d}{dx} x^r = rx^{r-1}$$

$$\frac{d}{dx} a^{bx} = ba^{bx}$$

$$\frac{d}{dx} e^{ax^2} = 2ax e^{ax^2}$$

$$\frac{d}{dx} \ln(x) = \frac{1}{x}$$

$$\frac{d}{dx} \log_a(x) = \frac{1}{x \ln(a)}$$

Sum Rule:

$$\frac{d}{dx} (5f + 3g) = 5 \frac{df}{dx} + 3 \frac{dg}{dx} \quad f=f(x); g=g(x)$$

Product Rule:

$$\frac{d}{dx} fg = f \frac{dg}{dx} + g \frac{df}{dx}$$

Quotient Rule:

$$\frac{d}{dx} \left(\frac{f}{g} \right) = \frac{g \frac{df}{dx} - f \frac{dg}{dx}}{g^2}$$

Integration

Most common integrals:

$$\int_a^b \frac{1}{x} dx = \ln \left(\frac{b}{a} \right)$$

$$\int_a^b \frac{1}{x^2} dx = -\frac{1}{x} \Big|_a^b = \frac{1}{a} - \frac{1}{b}$$

$$\int_a^b x dx = \frac{1}{2} x^2 \Big|_a^b = \frac{1}{2} (b^2 - a^2)$$

$$\int_a^b e^{3x} dx = \frac{1}{3} e^{3x} \Big|_a^b = \left[\frac{1}{3(e^{3b} - e^{3a})} \right]$$

Quadratic Equation: solving for x

$$ax^2 + bx + c = 0$$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

→ Simplifications (kinetics, equilibrium problems)

The quadratic equation shows up in kinetics questions and equilibrium questions. Typically, it is not required to solve the quadratic equation IF X IS SMALL.

Example:

$$\frac{x^2}{(a-x)(b-x)} = d$$

If x is assumed to be small, then,

$$\frac{x^2}{(a)(b)} = d$$

If the answer is small for x, then it is ok. If x turns out to be pretty big (0.4) then use the quadratic formulae!

Taylor Expansions: when x is small (especially in kinetics questions!)

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots, \quad -\infty < x < \infty$$

$$\ln(x) = x - \frac{1}{2}x^2 + \frac{1}{3}x^3 - \frac{1}{4}x^4 + \dots \quad \text{For } x < 1$$

Partial Fractions

Example:

$$\frac{x-1}{(3x-5)(x-3)} = \frac{A}{3x-5} + \frac{B}{x-3}$$

Multiply by denominator everywhere:

$$\frac{(x-1)(3x-5)(x-3)}{(3x-5)(x-3)} = \frac{A(3x-5)(x-3)}{3x-5} + \frac{B(3x-5)(x-3)}{x-3}$$

Simplify:

$$x-1 = A(x-3) + B(3x-5)$$

Solve by setting values for x:

$$\text{Let } x=3; 2=A(0)+B(4) \rightarrow B=0.5$$

$$\text{Let } x=0; -1=A(-3)+0.5(-5) \rightarrow A=-0.5$$

Final Answer:

$$\frac{x-1}{(3x-5)(x-3)} = \frac{-0.5}{3x-5} + 0.5 \frac{1}{x-3} = \frac{-1}{2(3x-5)} + \frac{1}{2(x-3)}$$

Math Tricks:

$$\ln a - \ln b = \ln\left(\frac{a}{b}\right)$$

*when you have two equations in terms of ln, subtract the equations from each other and use the trick

Example:

$$\ln(p_1) = -\frac{3000}{T} + 13.1 \quad \ln(p_2) = -\frac{4000}{T} + 16.4 \quad \text{given } \frac{p_1}{p_2} = 1 \quad \text{**}(what point is this?)$$

To solve for T and you are given the ratio of the pressures, subtract the equations:

$$\ln(p_1) = -\frac{3000}{T} + 13.1$$

$$-\ln(p_2) = -\frac{4000}{T} + 16.4$$

$$\ln\left(\frac{p_1}{p_2}\right) = -\frac{3000}{T} + 13.1 - \left(-\frac{4000}{T} + 16.4\right)$$

$$\ln xy = \ln x + \ln y$$

$$\delta\left(\frac{1}{p}\right) = -\frac{1}{p^2} \delta p$$

$$\frac{1}{p} \delta p = \delta \ln p$$

$$e^a e^b = e^{a+b}$$