APPENDIX A
TOOLS FROM THE CALCULUS
Mainly For Properties & Constraints

1. *Partial derivatives* - in thermo, what's held constant is explicit: for $z(x,y)$ use $\left(\frac{\partial z}{\partial x}\right)_y$

When see partial derivative, know on what function & derivatives depend $\Rightarrow$ $z(x,y)$, *e.g.*, for $H(T,P) \Rightarrow C_p(T,P) = \left(\frac{\partial H}{\partial T}\right)_P$

Geometric interpretation (p. A-2)

2. *Total Differential* - Function changes as independent variables change

$$dz = \left(\frac{\partial z}{\partial x}\right)_y dx + \left(\frac{\partial z}{\partial y}\right)_x dy$$

3. *Implicit Function Theorem* - Reformulation of equation $y = f(x)$ gives operations

$\Rightarrow F(x,y) = 0 \qquad dF = 0 \qquad y = y(F,x)$

$\Rightarrow$ **Triple Product Rule** $\left(\frac{\partial y}{\partial x}\right)_F = -\frac{\left(\frac{\partial F}{\partial x}\right)_y}{\left(\frac{\partial F}{\partial y}\right)_x}$ **or**

$$\left(\frac{\partial y}{\partial x}\right)_F \left(\frac{\partial F}{\partial y}\right)_x \left(\frac{\partial x}{\partial F}\right)_y = -1$$

4. *Exact Differentials* - Differentials of form

$$M(x,y)dx + N(x,y)dy = 0$$

Are exact [there exists $u(x,y)$] to give

$M = \left(\frac{\partial u}{\partial x}\right)_y$ **&** $N = \left(\frac{\partial u}{\partial y}\right)_x$ **whenever** $\left(\frac{\partial M}{\partial x}\right)_y = \left(\frac{\partial N}{\partial x}\right)_y$

5. *Integrating Factors* - Inexact differentials may be made into exact differentials
Example for single variable, *x*

$$\frac{dy}{dx} + yP(x) = Q(x)$$

Can find function $F(x) = \exp\{\int P(x)dx\}$ so that $u(x,y) = yF(x)$ exists; solution is

$$u(x,y) = \int F(x)\,Q(x)\,dx + Const.$$

or $y = [\int F(x)\,Q(x)\,dx + Const.]/F(x)$

6. *Legendre Transformations* - Change independent variables via mapping

$$z(x,y) \rightarrow z(x,w)$$

7. *Euler's Theorem* - Manipulating "homogeneous functions"

$$f(\lambda x, \lambda y) = \lambda^n f(x,y) \Rightarrow x\left(\frac{\partial f}{\partial x}\right)_y + y\left(\frac{\partial f}{\partial y}\right)_x = nf(x,y)$$

In Thermodynamics $\lambda = N$ & $n = 1$

8. *Gibbs-Duhem Equation* - discussed elsewhere

9. *Mean Value Theorem* for integration, averaging

10. *Taylor's Series* for continuous & differentiable functions:
Example: single variable *x*, in range *a*, *b*

$$f(b) = f(a) + (b-a)\left(\frac{df}{dx}\right)_{x=a} + \frac{(b-a)^2}{2!}\left(\frac{d^2f}{dx^2}\right)_{x=a} + \ldots$$

11. *Leibnitz Rule* for Differentiating Integrals

$$F(x) = \int_{a(x)}^{b(x)} f(x,z)dz$$

$$\Rightarrow \quad \frac{dF}{dx} = f(x,b)\frac{db}{dx} - f(x,a)\frac{da}{dx} + \int_{a(x)}^{b(x)} \frac{df}{dx}(x,z)dz$$

12. *L'Hospital's Rule* - Values of "divergent" ratios (*e.g.*, $\frac{0}{0}$, $\frac{\infty}{\infty}$) $\qquad \lim_{x \to x_o} \frac{f(x)}{g(x)} = \frac{\left(\frac{\partial f}{\partial x}\right)_{x=x_o}}{\left(\frac{\partial g}{\partial x}\right)_{x=x_o}}$

APPENDIX B
LINEAR ALGEBRA
Mainly for Reactions

Matrices
Operations
Addition & Multiplication
Determinants
Linear Independence
Systems of Linear Equations
Quadratic Forms