ChE641: Mathematical Methods in Chemical Engineering

Assignment 1 **Due Date: 10 September 2020**

1. Using the appropriate properties of ordinary derivatives, perform the following:

   (a) Find all the first partial derivatives of the following functions $f(x, y)$:

      i. $x^2 y$,

      ii. $x^2 + y^2 + 4$,

      iii. $\sin(x/y)$,

      iv. $\tan^{-1}(y/x)$,

      v. $r(x, y, z) = (x^2 + y^2 + z^2)^{1/2}$.

   (b) For (i), (ii) and (v), find $\partial^2 f/\partial x^2, \partial^2 f/\partial y^2$ and $\partial^2 f/\partial x \partial y$.

   (c) For (iv) verify that $\partial^2 f/\partial x \partial y = \partial^2 f/\partial y \partial x$.

2. Determine which of the following are exact differentials:

   (a) $(3x + 2)y dx + x(x + 1)dy$,

   (b) $y(\tan x)dx + x(\tan y)dy$,

   (c) $y^2(\ln x + 1)dx + 2xy(\ln x)dy$,

   (d) $y^2(\ln x + 1)dy + 2xy(\ln x)dx$,

   (e) $[x/(x^2 + y^2)]\, dy - [y/(x^2 + y^2)]\, dx$.

3. The equation $3y = z^3 + 3xz$ defines z implicitly as a function of x and y. Evaluate all three second partial derivatives of z with respect to x and/or y. Verify that z is a solution of:

$$x\frac{\partial^2 z}{\partial y^2} + \frac{\partial^2 z}{\partial x^2} = 0.$$

4. A possible equation of state for a gas takes the form:

$$PV = RT \exp\left(-\frac{\alpha}{VRT}\right),$$

   in which α and R are constants. Calculate expressions for: $\left(\frac{\partial P}{\partial V}\right)_T$, $\left(\frac{\partial V}{\partial T}\right)_P$, $\left(\frac{\partial T}{\partial P}\right)_V$.

5. In the xy-plane, new coordinates s and t are defined by: $s = \frac{1}{2}(x+y), \quad t = \frac{1}{2}(x-y)$ Transform the equation:
$$\frac{\partial^2 \phi}{\partial x^2} - \frac{\partial^2 \phi}{\partial y^2} = 0\,,$$
into the new coordinates and deduce that its general solution can be written
$$\phi(x,y) = f(x+y) + g(x-y),$$
where $f(u)$ and $g(v)$ are arbitrary functions of u and v, respectively.

6. The function $f(x,y)$ satisfies the differential equation:
$$y\frac{\partial f}{\partial x} + x\frac{\partial f}{\partial y} = 0\,.$$
By changing to new variables $u = x^2 - y^2$ and $v = 2xy$, show that f is, in fact, a function of $x^2 - y^2$ only.

7. Find and evaluate the maxima, minima and saddle points of the function
$$f(x,y) = xy\left(x^2 + y^2 - 1\right)\,.$$

8. Show that
$$f(x,y) = x^3 - 12xy + 48x + by^2, \quad b \neq 0\,,$$
has two, one, or zero stationary points, according to whether $|b|$ is less than, equal to, or greater than 3.

9. By considering the differential
$$dG = d(U + PV - ST),$$
where G is the Gibbs free energy, P the pressure, V the volume, S the entropy and T the temperature of a system, and given further that the internal energy U satisfies:
$$dU = TdS - PdV\,,$$
derive a Maxwell relation connecting $(\frac{\partial V}{\partial T})_p$, and $(\frac{\partial S}{\partial P})_T$.