Illustration of calculus used in ChE804:

This summary is an overview of calculus used in ChE804. The summary is meant to be representative, not comprehensive. The examples provide an overview of the types of problems that are solved. Some of the examples here integrate concepts that are introduced within the course. Use these examples as a guide to the use of calculus, recognizing that the other concepts are discussed in course lessons.

Topic 3 - 5: Integration of single variables.

Example 1. Work for an isothermal (constant $T$) compression of fluid is calculated by

$$W = -\int_{V_i}^{V_f} PdV.$$  

Calculate the work done to compress an ideal gas from 7L to 3L at 320K.

Solution:
The ideal gas law is $PV = RT$ where $R = 8.314 \text{ J/(molK)}$ is a constant. Need to write $P$ in terms of $V$: $P = RT/V$. Inserting into the formula for work, recognizing that $T$ is constant so that it can come out of the integral, and applying limits of integration:

$$W = -\int_{V_i}^{V_f} PdV = -RT\int_{V_i}^{V_f} \frac{dV}{V} = -RT \ln(V_f/V_i) = -(8.314)(320) \ln(3/7) = 2.25 \text{ kJ}$$
Example 2. For the compression of an ideal gas in a piston/cylinder, the energy balance simplifies to:

\[ C_V dT = -\frac{RT}{V} dV. \]

Where \( C_V \) and \( R \) are constants. Find the relationship between temperature and volume for the ideal gas.

**Solution:**

To perform the integration, we must separate variables.

\[
\frac{C_V}{R} \frac{dT}{T} = -\frac{dV}{V} \Rightarrow \frac{C_V}{R} \ln\left(\frac{T_2}{T_1}\right) = -\ln\left(\frac{V_2}{V_1}\right) = \ln\left(\frac{V_1}{V_2}\right)
\]
Example 3. The entropy, $S$, is a property of a fluid that is used in the course. Entropy depends on temperature and volume by the following relation:

$$dS = C_v \frac{dT}{T} + \left( \frac{\partial P}{\partial T} \right)_{V} dV,$$

and an ideal gas follows $P=RT/V$, where $C_v$ and $R$ are constants. Provide the integrated formula that relates entropy to $T$ and $V$.

Solution:

$P$ depends on both $T$ and $V$. Evaluating the partial derivative, $\left( \frac{\partial P}{\partial T} \right)_{V} = \frac{R}{V}$, and inserting into the given relation: $dS = C_v \frac{dT}{T} + \frac{R}{V} dV$. Since $C_v$ and $R$ are constants and all variables are separated, the terms may all be integrated independently, $S_2 - S_1 = C_v \ln(T_2 / T_1) + R \ln(V_2 / V_1)$. 

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Example 4. The enthalpy, $H$, is a property of a fluid that is used in the course. The enthalpy departure is introduced in the course, which quantifies the difference between the actual fluid enthalpy and the enthalpy of an ideal gas $H_{ig}^{\text{ig}}$. To illustrate the mathematics, this example uses the enthalpy departure. The enthalpy departure is calculated by

$$\frac{H - H_{ig}^{\text{ig}}}{RT} = \int_0^\rho -T\left(\frac{\partial Z}{\partial T}\right)_{\rho} \frac{\partial \rho}{\rho} + Z - 1$$

$Z = PV/RT$ which depends on $P$ and $T$ for a real fluid.

For a fluid that follows the van der Waals equation of state, $P = \frac{RT}{V - b} - \frac{a}{V^2}$, find the enthalpy departure. Note: $a$ and $b$ are constants, and $V = 1/\rho$.

Solution:

rearranging the equation of state:

$$\frac{PV}{RT} = Z = \frac{V}{V - b} - \frac{a}{VRT}$$

$$Z = \frac{1}{1 - b\rho} - \frac{a\rho}{RT}$$

$$Z - 1 = \frac{1}{1 - b\rho} - \frac{a\rho}{RT} - \frac{1 - b\rho}{1 - b\rho} = \frac{b\rho}{1 - b\rho} - \frac{a\rho}{RT} \left(\frac{\partial Z}{\partial T}\right)_{\rho} = \frac{a\rho}{RT^2} \rightarrow$$

$$\frac{H - H_{ig}^{\text{ig}}}{RT} = \int_0^\rho -\frac{a\rho}{RT} \frac{\partial \rho}{\rho} + Z - 1 = -\frac{a\rho}{RT} + Z - 1 = \frac{b\rho}{1 - b\rho} - \frac{2a\rho}{RT}$$
Example 5: This section of the course focuses on design of chemical reactors using the kinetic rate laws. The rate laws are typically given in problem statements in terms of the concentration. Then the concentrations are expressed in terms of the conversion of the limiting reactant, $X_A$. These steps are algebraic, so they are not summarized here. Depending on the type of reactor, problem solutions may require integration. Sometime the integrals are straightforward and can be done quickly or by using integral tables. Sometimes the integrals are more complicated. For a particular reactor engineering example, the volume of the reactor that provides 80% conversion of the limiting reactant is given by:

$$V \text{(in Liters)} = 75 \int_{0}^{0.8} \left( \frac{1 - X_A}{1 + X_A} \right)^{1/2} dX_A$$

Solution: The above integral could be solved by substitution, but frequently the integrals that are ‘messy’ are solved by numerical integration. We provide a spreadsheet tool for numerical integration in the course to use on homework problems such as this.