Project #4 : Chemical Equilibrium

A classic nonlinear optimization problem is determining the equilibrium concentration of chemical species in a homogeneous mixture. As a specific example, consider the following scenario. A mixture of one part N_2H_4 and one part O_2 is brought to equilibrium at a temperature of $T = 3500°K$ and a pressure of $P = 750\ psi$. The constituent molecules dissociate and form some combination of the $n = 10$ components shown in the table below.

(j)	component	c_j
1	H	-6.089
2	H_2	-17.164
3	H_2O	-34.054
4	N	-5.914
5	N_2	-24.721
6	NH	-14.986
7	NO	-24.100
8	O	-10.708
9	O_2	-26.662
10	OH	-22.179

The goal is to determine the number of moles, x_j, of the constituent components. This is determined by the minimization of the Gibbs free energy:

$$f(x) = \sum_{j=1}^{n} x_j \left(c_j + \ln \frac{x_j}{s} \right),$$

where $s := \sum_{j=1}^{n} x_j$. The c_j are temperature and pressure dependent free-energy quantities that are determined by other methods. The logarithmic term takes into account the free energy of mixing. Notice that the free energy is defined only for positive values of the mole quantities, $x > 0$. That is, the equilibrium mixture will contain a nonzero quantity of all ten components. The only additional problem constraints are that the total mole count of each element must conform to the totals given by each component:

$$\begin{aligned} x_1 + 2x_2 + 2x_3 + x_6 + x_{10} &= 4 \quad (H) \\ x_4 + 2x_5 + x_6 + x_7 &= 2 \quad (N) \\ x_3 + x_7 + x_8 + 2x_9 + x_{10} &= 2 \quad (O) \end{aligned}$$

Here we have enforced an initial mixture of one mole N_2H_4 and one mole O_2.

Task 1. Create your own Sequential Quadratic Programming (SQP) code or Augmented Lagrangian code (AL) to solve a general constrained nonlinear optimization problem. Your code should appropriately call either your Quadratic Programming code or your unconstrained optimization code as the subproblem.

Task 2. Create an objective function and constraint functions for the chemical equilibrium problem. Your objective function should employ a reasonable method of enforcing a real-valued objective.

Task 3. Solve the chemical equilibrium problem using your SQP or AL code. Explore the sensitivity of your results to different initial guesses and to any hyperparameters you have employed.

Task 4. Provide a short report on code and results.