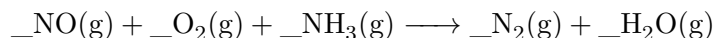


Solve each problem on separate sheets of paper, and clearly indicate the problem number and your name on each. Carefully and neatly document your answers. You may use a mathematical solver like Jupyter/iPython. Use plotting software for all plots.

1 All in balance

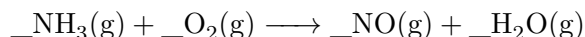
- 1.1 One way under consideration for removing harmful “NO_x” (NO + NO₂) from flue gas is the thermal deNO_x process, in which NH₃ is used to reduce the NO to NO₂:



The research lab has several gas tanks available to study this reaction, including one containing 2.0% NO in an N₂ diluent, one containing 10% O₂ in an N₂ diluent, and a bottle of 4% anhydrous ammonia in N₂. You can assume all gases behave ideally.

1. Balance the thermal deNO_x reaction, assuming each NH₃ titrates one NO.
2. What mass flow rates are necessary to create a stoichiometric mixture at 1 bar total pressure, 400 °C, and 10 l/s total volumetric flow rate?
3. Plot the molar flow rates of all five gases as a function of reaction advancement.
4. Plot the total volumetric flow rate as a function of reaction advancement.

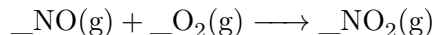
- 1.2 NH₃ oxidation is an undesirable side-reaction of thermal deNO_x:



1. Balance the NH₃ oxidation reaction.
2. Under the stoichiometric conditions described above, the reactor generates 0.036 g/s NO and 0.017 g/s NH₃. How effectively is the NH₃ being used for thermal deNO_x? (*Hint*: What are the advancements of the two reactions?)

2 NO_x, NO_x, who's there?

- 2.1 A simpler and confounding reaction of NO is its oxidation to NO₂:



You can assume all gases behave ideally under the conditions considered in this problem.

1. Determine $\Delta H^\circ(298 \text{ K})$, $\Delta S^\circ(298 \text{ K})$, $\Delta G^\circ(298 \text{ K})$, and $K_p(298 \text{ K})$ for the NO oxidation reaction. Be sure to specify your source and the standard state.
2. Calculate the equilibrium partial pressure ratio of NO₂ to NO in the atmosphere near the surface of the earth. Assume the mixing ratio of O₂ to be 0.2 and a temperature of 25 °C.
3. From standard compilations and at 1 atm standard state, $\Delta H^\circ(250) = -116.532 \text{ kJ mol}^{-1}$ and $\Delta S^\circ(250) = -152.179 \text{ J/mol/K}$. Use the van't Hoff relationship to plot $\Delta G^\circ(T)$ vs T from room temperature to 600 °C. Add a point on your plot for the $\Delta G^\circ(298 \text{ K})$ you found from a tabulation.

-
4. NO oxidation is catalyzed over diesel oxidation catalysts (DOCs) on diesel vehicles. Plot the equilibrium conversion of NO to NO₂ vs T from room temperature to 600 C for an isobaric 1 atm reactor presented with 0.1% NO and 5% O₂, and balance N₂.