MAE 164 Final Project

Problem Description

Imagine that you are a member of a group of research scientists working for an air quality regulatory agency, such as the South Coast Air Quality Management District or the California Air Resources Board. Within this agency, you are part of a group that specializes in modeling the effects of emissions concentrations on local ambient air quality. Your group has recently been assigned the task of investigating the interaction between ethene (C_2H_4) emissions and other species typically found in the urban airshed. Of particular interest is the interaction between ethene emitted into the atmosphere and the concentrations of NO_X and ozone (O_3) that will result.

In order to develop this understanding, you have been tasked with creating a model that dynamically simulates the evolution of various species' concentrations within the airshed with a wide range of initial ethene concentrations. The goal of these investigations will be to help identify a proper ethene mitigation strategy that provides the greatest benefit to the ambient air quality. In addition, it has been proposed that a NO_x mitigation strategy may play a similar role, and you are asked to investigate this strategy as well.

Thus, it is your job to develop a model that solves the set of ordinary differential equations (ODEs) describing the rates of reactions of all the relevant species. The chemical mechanism you are asked to investigate is provided in the table below, with most rates given in ppm^{-1} $min^{-1.}$

#	Reaction	Rate
1	$NO_2 + h\nu \rightarrow NO + O$	$k_1(t)$
2	$O + O_2 + M \rightarrow O_3 + M$	2.183E-05
3	$O_3 + NO \rightarrow NO_2 + O_2$	26.6
4	$HO_2 + NO \rightarrow OH + NO_2$	1.2E+04
5	$OH + NO_2 \rightarrow HNO_3$	1.6E+04
6	$C_2H_4 + OH \rightarrow HOCH_2CH_2O_2$	1.3E+04
7	$HOCH_2CH_2O_2 + NO \rightarrow NO_2 + 0.72\ HCHO + 0.72\ CH_2OH + 0.28\ HOCH_2CHO + 0.28\ HO_2$	1.1E+04
8	$CH_2OH + O_2 \rightarrow HCHO + OH$	2.1E+03
9	$C_2H_4 + O_3 \rightarrow HCHO + 0.4\ H_2COO + 0.18\ CO_2 + 0.42\ CO + 0.12\ H_2 + 0.42\ H_2O + 0.12\ HO_2$	2.6E-02
10	$H_2COO + H_2O \rightarrow HCOOH + H_2O$	0.034

Reaction #1 is a photocatalyzed reaction, and its rate of reaction therefore depends on the variation of solar irradiation with time. The time-dependent rate of reaction accounting for this variation is given in the equation below.

$$k_1(t) = 0.2053t - 0.02053t^2, \qquad 0 \le t \le 10 \text{ hours}$$

$$k_1(t) = 0, \qquad t \ge 10 \text{ hours}$$

Specific Questions

In order to provide a complete analysis and understanding of the chemical reaction system, you are asked to complete the following steps:

1) Prepare a table that lists all the participating species and indicate which species can be treated as constant, which are active, and which can be treated using the pseudo steady-state assumption (PSSA).

2) List the expressions for the reaction rates for all ten reactions. Using these, derive the differential equations that govern the concentrations of all active and steady state species.

3) Use the PSSA to derive and list expressions for the concentrations of the steady state species as a function of the concentrations of the active and constant species.

4) Solve the system for a period of 12 hours using the following initial conditions as a base case:

   $$[NO_x]_0 = 0.5 \text{ ppm}, \ [NO_2]_0/[NO_x]_0 = 0.25, \ [C_2H_4]_0 = 3.0 \text{ ppm}$$

   Plot and discuss the resulting concentrations of ozone (O_3), nitric oxide (NO), nitrogen dioxide (NO_2), ethane (C_2H_4), hydroxyl (OH), and nitric acid (HNO_3).

5) Discuss the effect of the hydrocarbon on the maximum ozone values by repeating the above simulation for initial ethane values of 1, 2, and 4 ppm.

6) Assume that in an effort to reduce ozone levels, the initial concentration of NO and NO_2 are both reduced by 20%. Repeat the simulation of Step 4) with only this change and compare the two ozone curves. Explain the results you observe.