Exercises

A. Given data in the text (Tables B4-6 in Appendix B) and \([\text{OH}]_{\text{day}} = 1.6 \times 10^6 \text{ molecules cm}^{-3}, [\text{NO}_3]_{\text{night}} = 5 \times 10^8 \text{ molecules cm}^{-3}, [\text{O}_3]_{\text{day}} = 100 \text{ ppbv and } [\text{O}_3]_{\text{night}} = 30 \text{ ppbv.}\)

QUESTION: is cyclohexene removed more rapidly at night or during the day?

B. Re-calculate \([\text{C}_2\text{H}_5\text{O}_2]_{\text{ss}}\) and \([\text{C}_2\text{H}_5\text{O}•]_{\text{ss}}\) from Exercise D on Homework #5, given:

the following reaction added to the mechanism:

\[ \text{C}_2\text{H}_5\text{O}_2 + \text{HOO} \rightarrow \text{C}_2\text{H}_5\text{OOH} + \text{O}_2 \quad k_5 = 8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}.\]

Assume \([\text{HOO}] = 0.03 \text{ ppbv}\) and change \([\text{NO}]\) to 0.05 ppbv

C. Sketch out the fates of the organic species formed in the degradation of 2-pentene in polluted air during the day (initiated by OH) with rural NOx concentrations.

Follow all significant branches until all organic species are converted to non-radicals. You can omit the formation of RONO2.

D. Compute \([\text{NO}_2]_{\text{ss}}\) at \(t=190.6\) on the graphs from Homework #5 Given:

\[ \text{ROO}• + \text{NO} \rightarrow \text{RO}• + \text{NO}_2 \quad k \approx 8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}.\]

\[ \text{HOO}• + \text{NO} \rightarrow \text{OH} + \text{NO}_2 \quad k \approx 8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}.\]

E. If an OH radical reacts with a VOC molecule in a remote area, is it likely that subsequent radical chemistry is going to lead to an NO-to-NO2 conversion?

F. Given the mechanism and rate constants (in the “model” worksheet) and the concentration data in the file CO_oxidation_model_results.xls (available on the Homework page of the course website). The conditions are 1 atm air at 298 K.

a) Verify that at \(t=0\) and \(t=3600\) seconds there is a mass balance in carbon, hydrogen and reactive nitrogen (N-containing compounds other than N2).

b) Considering the mechanism, would you expect the concentration of \([\text{HO}_x]\) to be constant over the course of the simulation?

c) Use numerical differentiation to determine the rate of the OH + CO reaction at \(t = 2400\) sec.

Problems

I. Compare \([\text{C}_2\text{H}_5\text{O}_2]_{\text{ss}}\) and \([\text{C}_2\text{H}_5\text{O}•]_{\text{ss}}\) in Exercise B, above, to the values in Exercise D on Homework #5. Explain with quantitative arguments why \([\text{C}_2\text{H}_5\text{O}_2]_{\text{ss}}\) and \([\text{C}_2\text{H}_5\text{O}•]_{\text{ss}}\):

- rise or fall
- why they rise or fall as much or as little as they do (in approximate terms)
II.A. Show that the answer to Exercise D in this Homework barely changes if you omit the reaction: \( \text{OH} + \text{NO}_2 \rightarrow \text{HONO}_2 \).

II.B. If this reaction barely changes the answer to Exercise D, how can we also claim (correctly) that it is an important reaction for \([\text{NO}_2]\) under the conditions of the graph?  

Type of answer: Quantitative arguments.

III. Use calculations to verify that \([\text{O}]\) is near steady state at \(t=2400\) sec in the file \(\text{CO_oxidation_model_results.xls}\) from Exercise F.

IV. Do any of the competing reaction pathways of alkoxy radicals in Exercise C lead to more NO-to-NO\(_2\) conversions than others?

V. Write one question at each of levels 1, 2, and 3 of Boom’s Taxonomy of Knowledge (defined below). That is a total of three (3) questions, only! The questions should be based on the material in section 16.A.1 of the book by Finlayson-Pitts and Pitts (on reserve at Moon Library).

Questions should be designed so that they can be answered without using resources other than
- the specified section of the Finlayson-Pitts and Pitts
- general concepts taught in the course
- minimal use of a calculator (for example, no Arrhenius expressions)

Finally, specify whether the answer should be quantitative, qualitative, a calculation, or some combination.

**Bloom’s Taxonomy of Knowledge (revised)**
(a famous way to think about levels of knowledge)

<table>
<thead>
<tr>
<th>Level Of Learning</th>
<th>Examples</th>
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| 1. Remembering    | What is the average \([\text{CH}_4]\) in atmosphere?  
  *The answer is a data point which is in the textbook and easily found online.* |
| 2. Understanding  | Why is \([\text{CH}_4]\) greater than \([\text{CO}]\) in the atmosphere despite the fact that CO emissions are much larger than \([\text{CH}_4]\) emissions?  
  *This was a level 3 question on Homework #3, but now it should be Level 2.*  
  Part A of Exam 1 |
| 3. Applying       | Part A of the Project  
  Part B of Exam 1. The calculation questions should be level 2 by mid-December. |
| 4. Analyzing      | Part B of the Project  
  In Figure 16.7 of FP+P, what are some compounds likely formed in abundance comparable to the species shown, but whose concentrations are not shown? |
| 5. Evaluating     |          |
| 6. Creating       |          |

See https://www.cloud.edu/Assets/PDFs/assessment/revised-blooms-chart.pdf