

The goal of this project is to have you compute and then explain how photolysis rate constants depend on solar zenith angle (SZA) and altitude, and how the ratio of long wavelength to short wavelength photolysis rate constants varies with SZA and altitude.

You **may not** work with other students **at all** on this project.

Preliminary Steps

- A) From the course web page, download the spreadsheet “Calculating Photolysis Rates” (for 0 km) and “F0_40.xls” for calculations at 0 and 40 km. Combine these into one spreadsheet (you can split the calculations for 0 and 40 km between two tabs).
- Delete all the tabs from the spreadsheet at 0 km except the one labeled “NO₂” which has the calculation.
 - Modify the spreadsheet to delete data at SZA other than 30 or 70 degrees.
 - Within the same Excel file, make a copy of the tab for the calculations.
 - Name one copy “HOOH” and the other “O₃”
- B) Take quantum yields for the two photolysis pathways of O₃ from *Burkholder*. For the spectral region in which the cross-section changes rapidly, use the data labeled “Matsumi(2002)_298K_220-340nm” in http://satellite.mpic.de/spectral_atlas.

Take absorption cross sections from http://satellite.mpic.de/spectral_atlas:

For O₃, use the two sets of data labeled “IUPAC(2004)”

For HOOH, use the data for 298 K, not 355 K.

NOTE: Set up your spreadsheet so that I can see how you computed the answers to questions 2, 3, and 4. I should be able to diagnose any errors in the hardcopy of your answers by looking at your spreadsheet.

Part A. (~65%) Photolysis Calculations: Due date To be Determined.

Turn in **hardcopy** with your answer to question (1) and tables of your answers to questions 2-4.

Also, e-mail me your spreadsheet calculations as a **single Excel file**.

1) EXPLAIN how you determined the values of absorption cross-sections to enter in the spreadsheet. Show examples to clarify any types of cases that are less than obvious. Many students lose points because they do not show examples.

2) Calculate the total photolysis rate constants for HOOH and O₃ at both 40 km and 0 km at both SZA= 30 and SZA= 70 degrees. Use the following format to report results:

	J(HOOH)		J(O ₃)	
	SZA=30	SZA=70	SZA=30	SZA=70
h=40 km				
h=0 km				

- 3) Calculate the photolysis rate constants for $\text{O}_3 \rightarrow \text{O}(^1\text{D})$ and $\text{O}_3 \rightarrow \text{O}(^3\text{P})$ for all four conditions in question 2. **Quantum yields are on page 4-100 of Burkholder.** Use the following format to report your results:

	SZA=30		SZA=70	
	$\text{O}_3 \rightarrow \text{O}(^1\text{D})$	$\text{O}_3 \rightarrow \text{O}(^3\text{P})$	$\text{O}_3 \rightarrow \text{O}(^1\text{D})$	$\text{O}_3 \rightarrow \text{O}(^3\text{P})$
h=40 km				
h=0 km				

- 4) What fraction of the total O_3 photolysis occurs at $\lambda \geq 300 \text{ nm}$? Calculate the answer for all four conditions in question 2. Use the following format:

	SZA=30	SZA=70
h=40 km		
h=0 km		

NOTE: Set up your spreadsheet so that I can see how you computed the answers to questions 2, 3, and 4. I should be able to diagnose any errors in the hardcopy of your answers by looking at your spreadsheet.

Part B. (~35%) Qualitative Analysis of Trends: Due date To be Determined.

For this part you will use **MY** answers to Part A, which will be posted to Blackboard after the due date for Part A.

Explain the direction and size of the following trends based on the physical phenomena that control photolysis rate constants:

- 1) Trend in J versus altitude **and** SZA for HOOH and CH₂O. Include causes of the differences in the magnitude of the trends for HOOH versus CH₂O.
- 2) Trend in the answers to questions (3) versus altitude **and** SZA. Include an analysis of the differences between the two pathways for CH₂O photolysis.
- 3) Trend in the answers to question (4) versus altitude **and** SZA.

In explaining the answers to question (4), you will be re-using some of the logic from your answer to previous questions. You do not need to repeat **all** the logic in the same level of detail, but you should repeat certain basic concepts.