SPARC CCMVal PhotoComp-2008 *(version 1 July 2008)*

GOALS. Evaluate how models calculate photolysis (and indirectly heating) rates in the stratosphere and troposphere with the incentive of locating errors or biases and identifying improved and practical methods. There are three basic parts to PhotoComp2008:

(1) Basic test of ***all*** J- values for high sun (SZA=15º), w/ & w/o additional scattering layers (stratiform clouds & stratospheric volcanic aerosols).

(2) Test of twilight, sphericity, and 24-hour averages (SZA = 84º - 96º).

(3) Test of wavelength integration w/o scattering (SZA = 15º).

There will be one standard atmosphere, whose primary definition will include air mass, ozone mass, and temperature in each layer. This atmosphere is typical of the tropics, ozone column = 260 DU. For efficiency, we will use this same atmosphere in all sections, even the low-sun, polar cases.

PARTICIPATION. This study is designed to aid development and testing of the photolysis and short-wave heating codes used in chemistry-transport models and coupled chemistry-climate models. This project is open: any research group can participate by running the experiments and reporting the results as specified below. We also encourage participation from groups (without CTMs or CCMs) who have participated in other model-measurement studies (e.g., IPMMI, POLARIS). Many CTM/CCMs will be using "the same" photolysis scheme (e.g., fast-TUV, fast-J) and think their participation redundant – this is false. The implementation of a standard scheme into any CTM/CCM will likely alter (intended or inadvertent) how the J-values are calculated: thus it is very important when you perform these tests that the photolysis module that is as close a possible to that embedded within the CTM/CCM and not the original, standalone version that you used to derive your inline model.

EXPERIMENTS.

Part 1 is a basic test of all J-values for high sun (SZA = 15º) over the ocean (albedo = 0.10, Lambertian). **Part 1a**: **Clear sky** (only Rayleigh scattering) and no aerosols. **Part 1b: Pinatubo aerosol** in the stratosphere (layer 10). **Part 1c: Stratus cloud** (layer 2). The primary atmosphere (Table 1a) is specified in terms of pressure layers, mean temperature, and column O_3 in each layer. Please do not include absorption by NO_2 or other species in calculating optical depths. For 1b and 1c we recommend that you use the specified optical properties in Table 1c, interpolating across the 5 specified wavelengths.

Part 2 tests the simulation of a spherical atmosphere and twilight conditions that are critical to the polar regions. Use the same atmosphere as Part 1 without clouds or aerosols. Assume equinox (solar declination = 0º) and a latitude of 84ºN. The surface SZA (not including refraction) varies from 84º (noon) to 96º (midnight). Report all J-values at noon, midnight, and the 24-hour average (integrating as you would in your CTM/CCM). With a spherical atmosphere, the local solar zenith angle changes with altitude and if refraction is included it will change the surface angle. Please note how you treat the solar ray path in your model description.

Part 3 tests the accuracy of wavelength binning in the critical region 290-400 nm that dominates tropospheric photolysis. Shut off all Rayleigh scattering and surface reflection (albedo = 0) giving effectively a simple Beer's Law calculation. Repeat the calculation in Part 1, but report only J-values for J-O3 (i.e., total), J-O3(1d) [$O_3 \Rightarrow O_2 + O(^1D)$], and J-NO2 [$NO_2 \Rightarrow NO + O$]. These are the two critical J-values for the troposphere, and they both have unusual structures in absorption cross section and quantum yields. The organizers will make these calculations using very high resolution (0.05 nm) cross sections and solar fluxes and for different options (e.g., JPL-06 vs. IUPAC cross sections) to provide a benchmark. NOTE that we will only use results below 20 km (L=1:11) for this comparison.

DIAGNOSTICS.

Model Documentation should include a brief outline of the methods and any references (limit: one page). Please include brief notes on: how you treat sphericity and refraction, the Schumann-Runge bands (J-O_2 and J-NO), Rayleigh scattering, multiple scattering, clouds and aerosols, seasonal changes in sun-earth distance, solar variability, and any specific parameterizations. Default cross sections are JPL-2006, please note if you are using alternate.

Report all J-values and all standard model layers since this is a check on all modeled J-values, not just the radiative transfer solution. See Appendix for data formatting. We are not specifying the day-of-the-year, so use solar fluxes for sun-earth distance = 1.0 au and average over the 11-yr solar cycle if possible. UCI's high-resolution solar spectrum used in these experiments is the average of two high and low SUSIM spectra (29 Mar 1992 and 11 Nov 1994), this is not meant to be the 11-yr average. It will be provided at 0.05 nm resolution, but we encourage you to use your own solar fluxes for the primary tests since changing solar fluxes will mostly likely require a complete re-averaging of all cross-sections (see Fast-J paper, Wild, Zhu, Prather, 2000). Please report in model documentation what you are using for the solar spectrum and how the solar cycle is represented in your submissions, and if possible submit it as a separate file so that it may be used to address differences later. (With different wavelength binning, this will not be trivial.) Reported photolysis rates should be calculated for the mass mid-point of each layer, this brings PhotoComp closer to current CTM usage rather than the original grid-point formulation used in M&M. Results in the form of clearly labeled ascii text files should be uploaded to BADC CCMVal archive or emailed to the organisers (see web posting for specific details).

DISCUSSION.

Implementation into a particular model's code will up to the participant. For example, at UCI we have two models that we will use in PhotoComp: a fast-JX model within the CTM that uses layers of uniform composition defined by mass (kg/m^2); and a stand-alone photochemical box model that defines altitude (in cm) as the vertical grid and uses number densities for air and ozone. For the latter, we have re-mapped the primary atmosphere (Table 1a) onto a grid-point structure (Table 1b) that has the same mid-layer properties as the layer mean value and the same columns of O_2 and O_3.

One question will be: What is the correct answer? In some cases we may be able to define a "best" answer based on obvious physics or convergence of some of the more resolved models, but in others we may not. Thus in all of our proposed experiments we will begin with a "standard model" result (not necessarily the best answer) from one of the models and then determine a best answer, if possible, after analysis of the results.

One approach to defining the correct answer would be to merge observed radiation fields or photolysis rates (e.g., IPMMI, POLARIS, see references below), but we feel this may be too difficult to match the exact observing conditions. One way to include the knowledge gained by these field studies is to ensure participation from some of the models (e.g., NCAR-TUV, APL).

We do not recommend reporting detailed actinic fluxes as a function of wavelength since everyone selects different ways of integrating over wavelength (e.g., bins) and trying to reconcile the different wavelength scales is not worthwhile. If major problems show up, then a subgroup of models can consider how to resolve the differences.

Another major issue with photolysis and heating rates is the treatment of clouds and cloud fraction. This is very important, but probably beyond the current PhotoComp. It would require a special workshop. We do include an option for a plane-parallel volcanic aerosol layer (aka Pinatubo) and a stratiform cloud.

APPENDIX

Standard Atmosphere & Other Specifications

Table 1a. PhotoComp 2008 standard atmosphere

L	edge p(hPa)	T	O3(mass/mass)	DU(**redundant)
1	1000.0	299.9	3.844E-08	2.4532
2^^	866.0	289.5	4.704E-08	4.8514
3	649.4	278.8	4.720E-08	3.6498
4	487.0	267.2	4.972E-08	2.8831
5	365.2	253.9	5.551E-08	2.4140
6	273.8	239.7	5.977E-08	1.9491
7	205.4	224.6	6.390E-08	1.5627
8	154.0	209.4	9.012E-08	1.6527
9	115.5	198.2	1.486E-07	2.0441
10**	86.60	195.8	3.885E-07	4.0065
11	64.94	203.1	1.533E-06	11.8582
12	48.70	209.9	3.790E-06	21.9783
13	36.52	215.5	6.849E-06	29.7855
14	27.38	220.1	1.034E-05	33.7361
15	20.54	224.5	1.326E-05	32.4219
16	15.40	228.9	1.577E-05	28.9124
17	11.55	233.3	1.653E-05	22.7293
18	8.660	237.8	1.670E-05	17.2239
19	6.494	242.6	1.578E-05	12.2053
20	4.870	248.3	1.363E-05	7.9054
21	3.652	254.1	1.236E-05	5.3734
22	2.738	259.5	9.733E-06	3.1740
23	2.054	262.9	8.158E-06	1.9951
24	1.540	265.1	6.721E-06	1.2325
25	1.155	266.9	5.511E-06	0.7578
26	0.8660	264.7	4.810E-06	0.4960
27	0.6494	261.8	4.009E-06	0.3100
28	0.4870	259.7	3.325E-06	0.1928

29	0.3652	254.3	2.820E-06	0.1226
30	0.2738	247.0	2.323E-06	0.0758
31	0.2054	239.4	1.909E-06	0.0467
32	0.1540	234.4	1.585E-06	0.0291
33	0.1155	232.7	1.335E-06	0.0184
34	0.08660	226.4	1.102E-06	0.0114
35	0.06494	216.4	8.927E-07	0.0069
36	0.04870	210.8	7.372E-07	0.0043
37	0.03652	208.0	6.168E-07	0.0027
38	0.02738	205.2	5.162E-07	0.0017
39	0.02054	202.4	4.317E-07	0.0011
40	0.01540	199.4	3.607E-07	0.00066
41	0.01155	197.6	3.032E-07	0.00042
42	0.00866			

above model top layer=41 @ 0.0866 hPa, assume uniform T & O3

42	0.00866	197.6	3.032E-07	0.00125
43	0.00000			

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^^ layer for stratiform cloud: OD (600 nm) = 20.0

** layer for Pinatubo sulfate aerosol: OD(600 nm) = 1.00
see Table 1c.

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Table 1b. Standard atmosphere shown mapped into grid points

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L	alt(km)	air(#/cm^3)	O3(#/cm^3)	T(K)
1	0.0	2.416E+19	5.611E+11	299.9
2	2.5	1.877E+19	5.335E+11	289.5
3	4.9	1.462E+19	4.169E+11	278.8
4	7.2	1.144E+19	3.436E+11	267.2
5	9.4	9.025E+18	3.027E+11	253.9
6	11.4	7.169E+18	2.589E+11	239.7
7	13.4	5.737E+18	2.215E+11	224.6
8	15.2	4.615E+18	2.513E+11	209.4
9	16.9	3.656E+18	3.283E+11	198.2
10	18.6	2.775E+18	6.514E+11	195.8
11	20.3	2.006E+18	1.858E+12	203.1
12	22.0	1.456E+18	3.334E+12	209.9
13	23.8	1.063E+18	4.399E+12	215.5
14	25.7	7.807E+17	4.879E+12	220.1
15	27.5	5.740E+17	4.598E+12	224.5
16	29.4	4.222E+17	4.022E+12	228.9
17	31.4	3.106E+17	3.102E+12	233.3
18	33.4	2.285E+17	2.306E+12	237.8
19	35.4	1.680E+17	1.602E+12	242.6
20	37.5	1.231E+17	1.014E+12	248.3
21	39.6	9.018E+16	6.732E+11	254.1
22	41.7	6.622E+16	3.894E+11	259.5
23	43.9	4.902E+16	2.416E+11	262.9
24	46.2	3.645E+16	1.480E+11	265.1
25	48.4	2.715E+16	9.039E+10	266.9
26	50.6	2.053E+16	5.966E+10	264.7
27	52.8	1.557E+16	3.771E+10	261.8
28	55.0	1.177E+16	2.364E+10	259.7
29	57.2	9.011E+15	1.535E+10	254.3
30	59.3	6.957E+15	9.766E+09	247.0
31	61.4	5.383E+15	6.210E+09	239.4
32	63.4	4.123E+15	3.949E+09	234.4
33	65.3	3.114E+15	2.512E+09	232.7
34	67.3	2.400E+15	1.597E+09	226.4
35	69.1	1.883E+15	1.016E+09	216.4
36	70.9	1.450E+15	6.458E+08	210.8
37	72.7	1.102E+15	4.107E+08	208.0
38	74.4	8.374E+14	2.612E+08	205.2
39	76.1	6.367E+14	1.661E+08	202.4
40	77.8	4.846E+14	1.056E+08	199.4
41	79.5	3.667E+14	6.717E+07	197.6

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above-top extend with 6.3-km scale-height for air & O3

	air(#/cm^2)	O3(#/cm^2)
columns:	2.129E+25	6.985E+18

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Table 1c. Scattering properties of Pinatubo and stratus layers

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Definitions:

W = wavelength (nm)

Q = scattering efficiency (average of cross-section / (pi * r**2))
typically Q ~ 2 for large clouds and large aerosols

fn of aerosol size distrib N(r), index of refraction, wavelength.

K = extinction (m2/g), the cross-sectional area per gram of material
K(m2/g) = Q / [4/3 * Reff(micron) * Rho(g/cm3)]

Reff = effective radius (microns)
= Average[N(r) * r**3] / Average[N(r) * r**2]

Rho = density of particles (g/cm3)

n = index of refraction

OD = optical depth (column) = column mass (g/m2) * K (m2/g)

SSA = single scattering abledo

LG(1:8) = coefficients of Legendre expansion of scattering phase fn.
both polariztions are added. By definition SLEG(1) = 1.
Fast-JX uses these first 8 terms to define the scattering.

g = asymmetry factor = LG(2) / 3.

Pinatubo: OD = 1.0 in layer 10 (86.6 to 64.9 hPa)
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Stratospheric aerosol composed of 75%-wt H2SO4.
Rho = 1.630
n = 1.514 + 0.000i (200 nm)
1.473 + 0.000i (300 nm)
1.459 + 0.000i (400 nm)
1.448 + 0.000i (600 nm)
1.435 + 0.000i (999 nm)
Log-normal distribution with R0 = 0.08 micron & sigma = 0.800
**check that you are using the right log-normal by deriving Reff
Reff = 0.386 micron

K (600nm) = 2.610
OD (@600nm) = 1.00 ==> aerosol = 1.00/K = 0.3832 g/m2

W	Q	SSA	LG(2)	LG(3)	LG(4)	LG(5)	LG(6)	LG(7)	LG(8)
200	2.5935	1.0000	2.092	2.914	2.880	3.295	3.185	3.430	3.379
300	2.6669	1.0000	2.121	2.861	2.792	2.936	2.733	2.703	2.568
400	2.5588	1.0000	2.144	2.813	2.711	2.695	2.425	2.257	2.069
600	2.1893	1.0000	2.149	2.713	2.547	2.362	2.018	1.740	1.499
999	1.4540	1.0000	2.118	2.537	2.277	1.951	1.555	1.229	0.972

(fast-JX v61 scatter #15)

Stratus: OD = 20.0 in layer 2 (866 to 649 hPa)
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Pure water cloud
Rho = 1.000
n = 1.335 + 0.000i (assumed 200-999 nm)
Deirmendjian Cumulus C1 (Gamma, n(r) = a r**alpha exp[-b r**gamma])
mode radius Rc = 4 microns, alpha=6, b=3/2, gamma = 1
Reff = 6.00 micron

K (600nm) = 0.2668
OD (@600nm) = 20.0 ==> aerosol = 20.0/K = 75.0 g/m2

W	Q	SSA	LG(2)	LG(3)	LG(4)	LG(5)	LG(6)	LG(7)	LG(8)
200	2.0650	1.0000	2.610	3.998	4.771	5.450	6.196	6.829	7.721
300	2.0835	1.0000	2.596	3.973	4.725	5.406	6.129	6.751	7.607
400	2.1064	1.0000	2.571	3.936	4.660	5.345	6.056	6.670	7.492
600	2.1345	1.0000	2.557	3.902	4.596	5.263	5.923	6.507	7.267
999	2.1922	1.0000	2.499	3.799	4.418	5.081	5.667	6.213	6.851

(fast-JX v61 scatter #08)

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Table 2. Standard diagnostics and file names

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Ascii tables will be fine given small data sets.
Report J-values at the mid-point of Layers 1 through 40.
File names: PC08_{model name + version if need be}_{PhotoPart#}
Write format: J-title, J-value(1:41) '(a8,1x,41e9.2)'

File Examples:
PC08_UCIref_doc.txt (or .pdf or .doc if need formatting)
UCI old reference code, documentation
PC08_UCI-JX_doc.txt
UCI version of fast-JX, documentation
PC08_UCIref_P1a.txt

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PC08_UCIref_P1b.txt
PC08_UCIref_P1c.txt
        UCI-ref results for Part 1 clear, Pinatubo & stratus (see sample below)
PC08_UCIref_P2n.txt
PC08_UCIref_P2m.txt
PC08_UCIref_P2a.txt
        UCI-ref results for Part 2 noon, midnight and average
PC08_UCIref_P3.txt
        UCI-ref results for Part 3 (J-O3(1d) and J-NO2 only).

PC08_UCIref_P1.txt
----------file: PC08_UCIref_P1a.txt  ----------------
PhotoComp2008:  UCI pratmo P1a '(a8,1x,41e9.2)' ** note that UCIref does not calculate
L=1(933) but at surface(1000)
pressure    933.**     750.     562.   .....    .0237    .0178    .0133    .0100
J-NO      7.02E-31 6.85E-28 7.42E-25  ......  4.71E-06 4.91E-06 5.10E-06 5.26E-06
J-O2      1.16E-23 6.49E-22 4.67E-20  ......  4.80E-09 5.57E-09 6.45E-09 7.51E-09
J-O3      4.55E-04 5.09E-04 5.37E-04
J-O3(1D)  4.84E-05 7.00E-05 8.02E-05
J-H2COa   3.08E-05 4.43E-05 5.22E-05
.......
J-Acet-b  4.26E-07 3.94E-07 2.79E-07   .....
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Table 3. Standard J-value names.

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Please use these abbreviations (if possible in the following order) so that J’s can be sorted.   For new J's please add with unique name. (available as PC08_J-labels.txt) Note that for some J's, the branching ratios do not have different cross-sections associated with them and the branching ratios are fixed, hence we report only one J. For many organics, the quantum yields are complex and have been incorporated into these J's. If you do not calculate one of these, please keep that row in your table with zero or blank values.

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```
    1  J-NO      NO      =N+O
    2  J-O2      O2      =O+O
    3  J-O3      O3      =O+O2 (total = both O(3P) and O(1D))*
    4  J-O3(1d)  O3      =O(1D)+O2
    5  J-H2COa   H2COa   =H+HCO
    6  J-H2COb   H2COb   =H2+CO
    7  J-H2O2    H2O2    =OH+OH
    8  J-CH3OOH  CH3OOH  =CH3O+OH
    9  J-NO2     NO2     =NO+O
   10  J-NO3     NO3     =NO+O2(11.4%) & NO2+O(88.6%)*
   11  J-N2O5    N2O5    =NO2+NO3
   12  J-HNO2    HONO    =OH+NO
   13  J-HNO3    HNO3    =OH+NO2
   14  J-HNO4    HO2NO2  =OH+NO3
   15  J-ClNO3a  ClNO3a  =Cl+NO3
   16  J-ClNO3b  ClNO3b  =ClO+NO2
   17  J-Cl2     Cl2     =Cl+Cl
   18  J-HOCl    HOCl    =OH+Cl
   19  J-OClO    OClO    =O+ClO
   20  J-Cl2O2   Cl2O2   =Cl+Cl+O2
   21  J-ClO     ClO     =Cl+O
   22  J-BrO     BrO     =Br+O
   23  J-BrNO3   BrNO3   =Br+NO3(29%) & BrO+NO2(71%)*
   24  J-HOBr    HOBr    =OH+Br
   25  J-BrCl    BrCl    =Br+Cl
   26  J-N2O     N2O     =N2+O
   27  J-CFCl3   CFCl3   =...
   28  J-CF2Cl2  CF2Cl2  =...
   29  J-F113    CF2ClCFCl2=...
   30  J-F114    CF2ClCF2Cl=...
   31  J-F115    CF3CF2Cl=...
   32  J-CCl4    CCl4    =...
   33  J-CH3Cl   CH3Cl   =CH3+Cl
   34  J-MeCCL3  CH3CCl3=...
   35  J-CH2Cl2  CH2Cl2  =...
   36  J-CHF2Cl  CHF2Cl  =...
   37  J-F123    CF3CHCl2=...
   38  J-F141b   CH3CFCl2=...
   39  J-F142b   CH3CF2Cl=...
   40  J-CH3Br   CH3Br   =CH3+Br
   41  J-H1211   CF2ClBr=...
   42  J-H1301   CF3Br   =...
   43  J-H2402   C2F4Br2=...
   44  J-CH2Br2  CH2Br2  =...
   45  J-CHBr3   CHBr3   =...
   46  J-CH3I    CH3I    =CH3+I
   47  J-CF3I    CF3I    =CF3+I
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   48  J-OCS     OCS    =CO+S
   49  J-PAN     CH3C(O)O2NO2 =CH3C(O)O2+NO2(60%) & CH3C(O)O+NO3(40%)*
   50  J-CH3NO3  CH3ONO2=CH3O+NO2
   51  J-ActAld  CH3CHO =CH3+HCO
   52  J-MeVK    CH3C(O)CH=CH2 =C3H6+CO(60%) & CH2=CHCO+CH3(40%)*
   53  J-MeAcr   CH2C(CH3)CHO =CH2=C(CH3)+HCO
   54  J-GlyAld  HOCH2CHO  =HOCH2+HCO
   55  J-MEKeto  CH3COC2H5 =CH3+C2H5CO(15%) & C2H5+CH3CO(85%)*
   56  J-EAld    C2H5CHO =C2H5+HCO
   57  J-MGlyxl  CH3COCHO =CH3CO+HCO
   58  J-Glyxla  (CHO)2 =HCO+HCO
   59  J-Glyxlb  (CHO)2 =H2+CO+CO
   61  J-Acet-a  C3H6O  =CH3CO+CH3
   62  J-Acet-b  C3H6O  =CH3+CH3+CO
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* In preliminary comparisons, we have found it best to compare
the total O3 photolysis rate and the rate leading to O(1D),
skipping the O(3P) path.  When branching paths with % are
indicated in the table, they indicate the values derived for
fast-JX, please just report the total J-value.
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