Inclusion of Inline photolysis module (TUV-x) in CESM WACCM / MUSICA

Douglas Kinnison
Matt Dawson, Francis Vitt
Stacy Walters, Kyle Shore

Atmospheric Chemistry Observations and Modeling Laboratory
NSF NCAR

WACCM Working Group Meeting
Boulder CO
February 13, 2024

NCAR
WACCM
Whole Atmosphere Community Climate Model

Outline

Discuss Stratospheric Photochemical Processes (brief)	LUT Table Approach (TUV4.2, Kinnison, 2007)
	TUV-x (TUV5.5, Madronich)
Comparisons between LUT and TUV-x	Compare important photolytic species. Use 4-Stream radiative transfer from only TUV-x
	Compare photolytic species with radiative transfer from LUT and TUV-x
Heating Processes in WACCM	Photolysis Heating
	Chemical Potential Heating
Run 1-year Specified Dynamics	Initial attempt using TUV-x inline in a SD-WACCM6 (MERRA2) simulation.
Conclusions / Next Step	Optimization
	Test inclusion of aerosols in Radiative Transfer
	Develop Cloud Overlap Approach

CESM WACCM LUT Approach

Photolysis: e.g., $O_2 + hv \rightarrow O(^3P) + O(^1D)$

$$d[O_2]/dt = -J_{O2}[O_2]$$

$$J_{O2}(p) = \sum_{\lambda} F_{exo}(\lambda) \times N_{flux}(p, \lambda) \times \sigma(\lambda) \times \phi(\lambda)$$

<= EUV (LUT)

Inline (33 Bins)	LUT (67Bins)

121 nm **200 nm** **750 nm**

Inline Calculation:

- JO_2 Lyman Alpha
- JO_2 SRB
- JNO SRB
- $\sigma \times \phi$ for all other J's
- $N_{flux}(p, \lambda)$ is funct. of (O_3, O_2)

F_{exo}: Lean (λ) dependent extraterrestrial flux.
Modified by the Earth-Sun distance (esfact).

N_{flux} (normalized flux) is based on TUV (Madronich), 4-stream radiative transfer.

LUT: $N_{flux}(p, \lambda)$ is function of (pressure, col. O_3, SZA, Albedo)

LUT: $\sigma(\lambda) \times \phi(\lambda)$ is function of (T, p)

RRTMG SW Heating rates

Heating and Photolysis rates

Cloud correction factor is applied to total J (Madronich).

CESM WACCM TUV-x Approach

Photolysis: e.g., $O_2 + h\nu \rightarrow O(^3P) + O(^1D)$

$$d[O_2]/dt = -J_{O2}\,[O_2]$$

$$J_{O2}(p) = \sum_{\lambda} F_{exo}(\lambda) \times N_{flux}(p, \lambda) \times \sigma(\lambda) \times \phi(\lambda)$$

<= EUV (LUT)

Inline	Inline

121 nm **200 nm** **750 nm**

RRTMG SW Heating rates

Heating and Photolysis rates

Merger RRTMG and Photolysis HR at 60km

Aerosols and Clouds included in 4-stream radiative transfer.

Examining Photolysis Reactions for the TSMLT Mechanism

First Step was to examine all the photochemical reactions used in the WACCM TSMLT1 chemical mechanism.

- This mechanism has **241** species, **447** chemical (gas & heterogeneous), **150 photochemical**, equaling **597** total reactions.
- We have examined most of the 150 photochemical reaction. This is a very time consuming processes, i.e., examining cross sections and quantum yields, & **Temperature dependence** properties.
- We have compared the profiles (single timestep) for the TUV-x photochemical reactions to the LUT.
- The first step was to use a **common radiative transfer (from TUV-x)** for both TUV-x and LUT photolysis rates (next slide).

Example Temperature dependence for CFC-11

McGillen et al.[11] used the polynomial expansion:

$$\log_{10}\sigma(\lambda, T) = \Sigma A_i (\lambda-200)^i + (T-273) \times \Sigma B_i(\lambda-200)^i$$

to fit their data. The fit is valid for the temperature range 216–296 K and wavelength range 190–230 nm and reproduces their experimental data to within 2%. The reported A_i and B_i parameters are given below. The fit is in good agreement with the Chou et al.[1] data set, to within 5%, in reasonable agreement with the Mérienne et al.[12] data set, differences of 8% or less, but shows systematic differences with the Simon et al. data set, with 15% differences for the data at 230 K. The McGillen et al. parameterization is recommended.

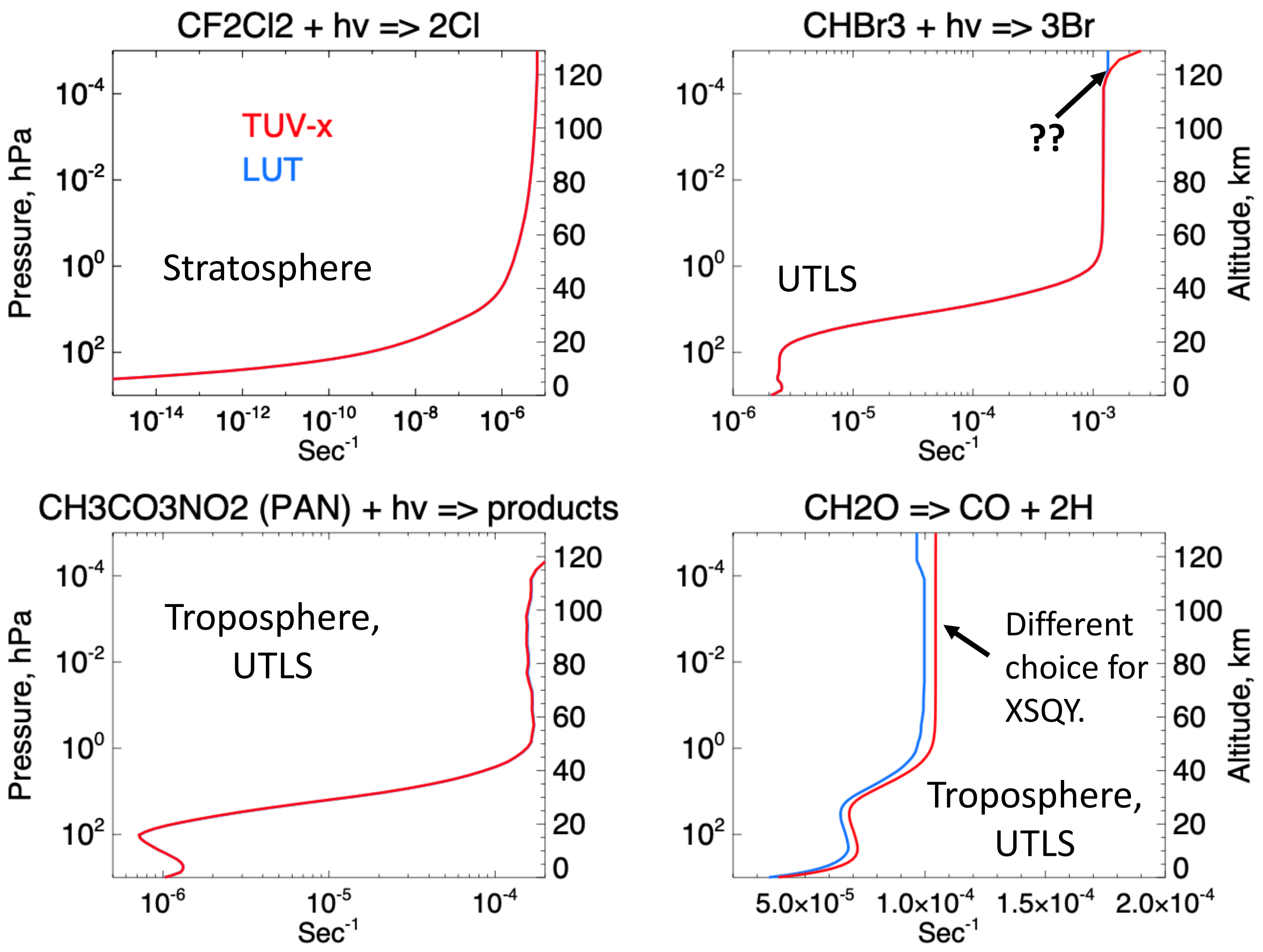
i	A_i	B_i
0	−18.1863	0.0002656
1	−0.0528	4.228×10^{-5}
2	−0.001126	1.4027×10^{-6}
3	-3.0552×10^{-5}	6.44645×10^{-7}
4	2.24126×10^{-6}	-3.8038×10^{-8}
5	-3.2064×10^{-8}	5.99×10^{-10}

Photolysis Quantum Yield and Product Studies: Clark and Husain[2] reported a quantum yield for $Cl^*(^2P_{1/2})$ atom formation in the broadband photolysis of $CFCl_3$ of 0.79 ± 0.27.

Comparison of Select Photolysis Rates between LUT and TUV-x

(Radiative Transfer is from TUV-x for both approaches)

Very Good Agreement of Cross Sections and Quantum Yields between the LUT and TUV-x.



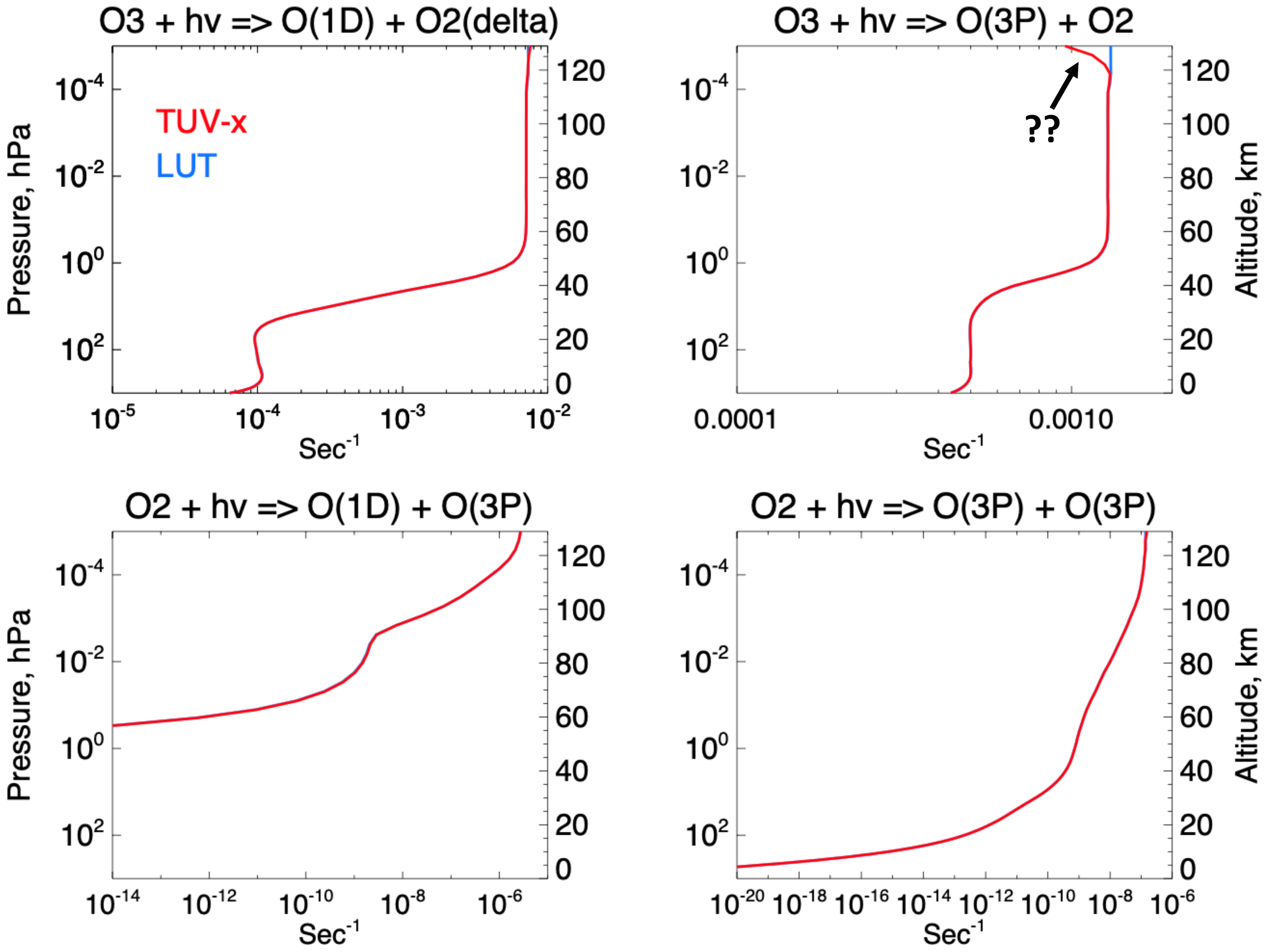
Noon-time output

Comparison of JO_2 and JO_3 between LUT and TUV-x

(Radiative Transfer is from TUV-x for both approaches)

Important photolysis reactions for **both chemistry** and middle atmosphere **heating rates.**

Very Good Agreement of Cross Sections and Quantum Yields between the LUT and TUV-x.



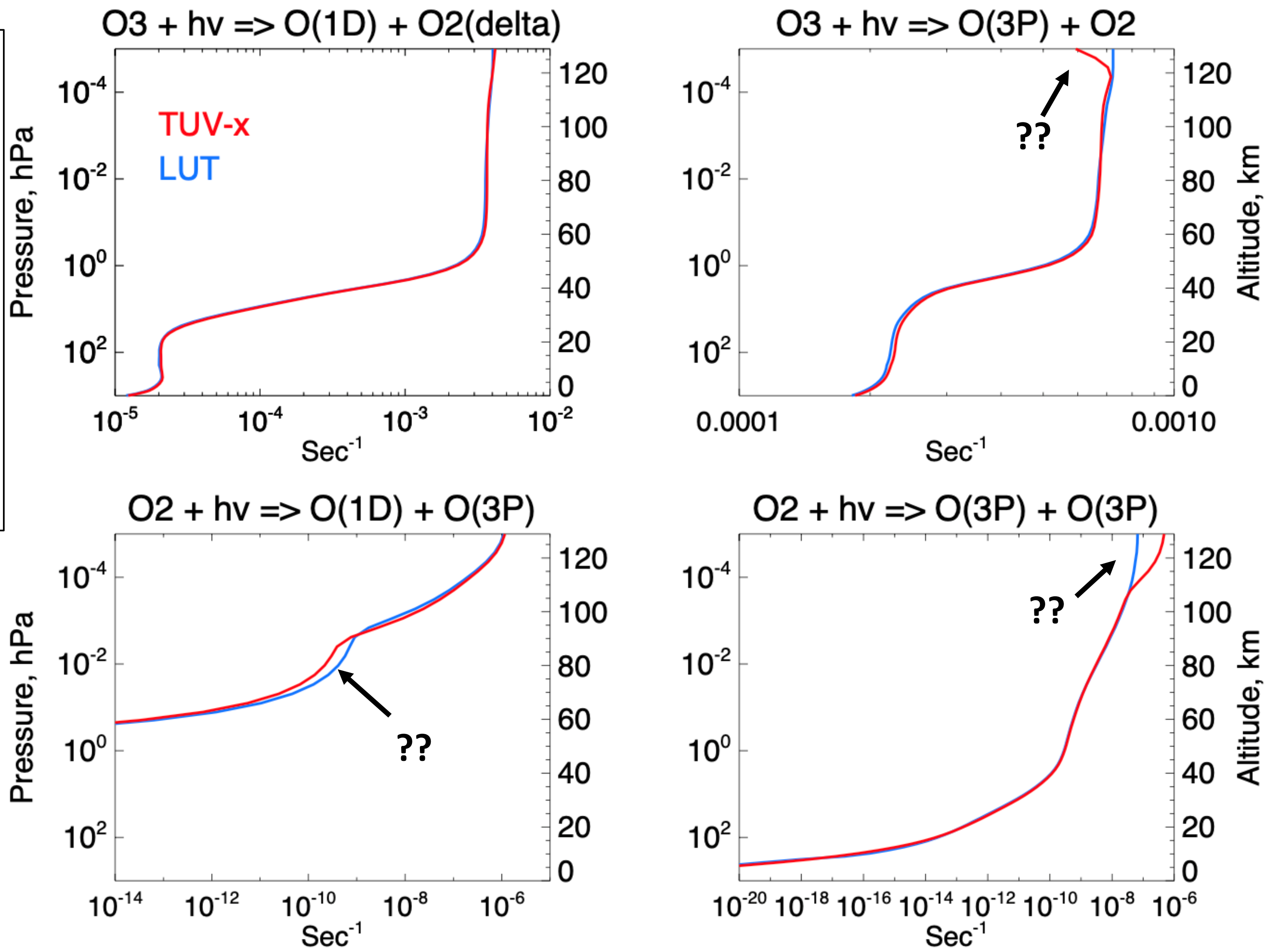
Noon-time output

Comparison of JO_2 and JO_3 between LUT and TUV-x

(Radiative Transfer used from both approaches)

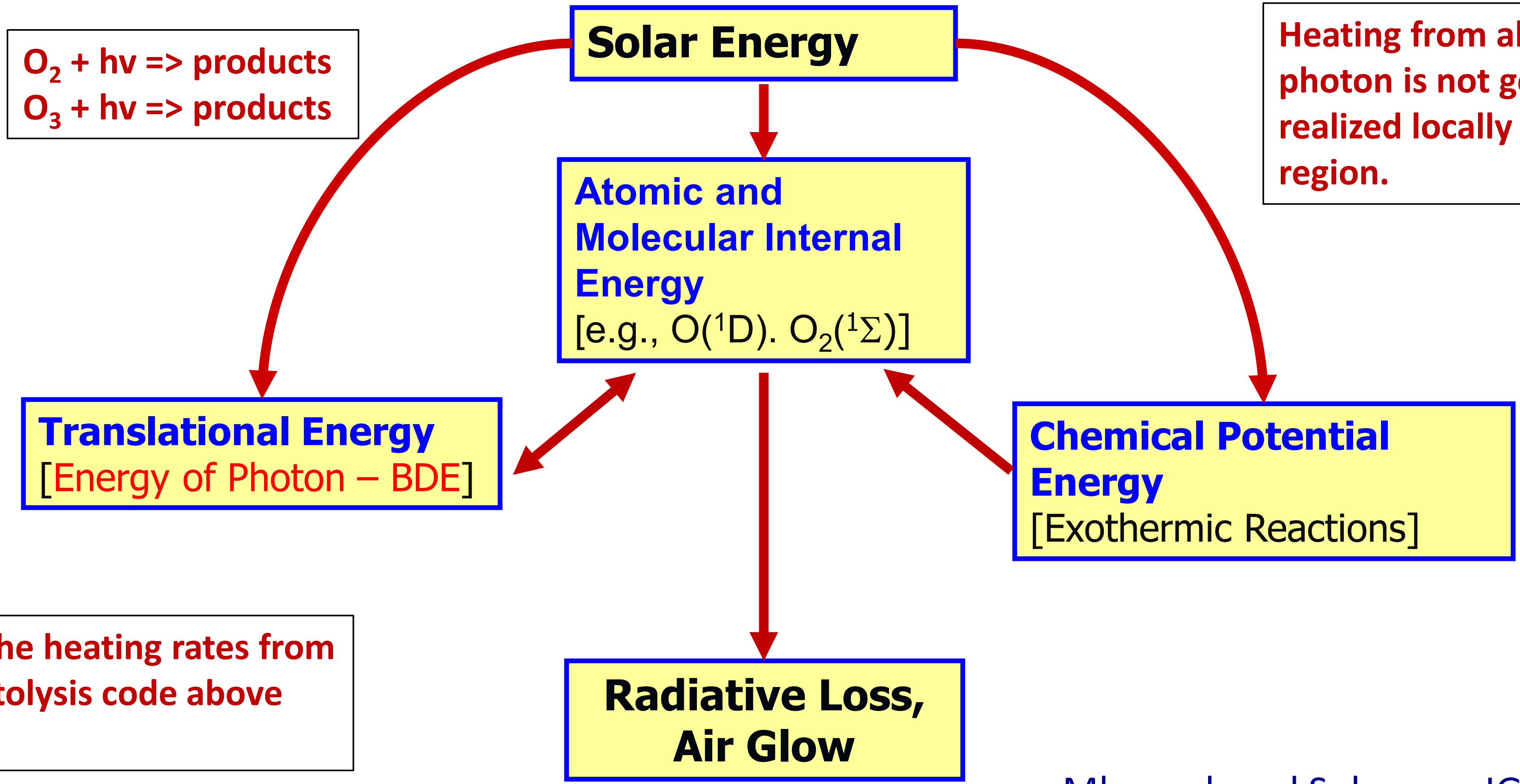
Still Good Agreement of Cross Sections and Quantum Yields between the LUT and TUV-x.

We are continuing to track down any differences between LUT and TUV-x!



24-hr average output

Solar Heating Rate Approach in WACCM MLT



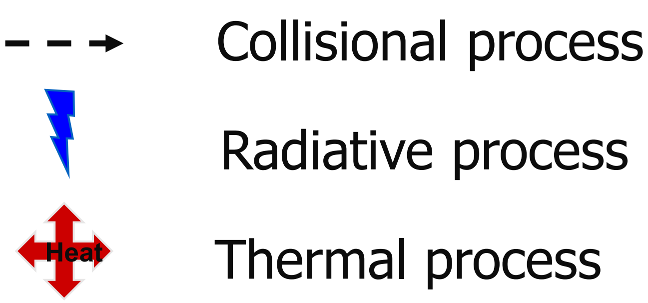
Heating from absorption of a photon is not generally realized locally in the MLT region.

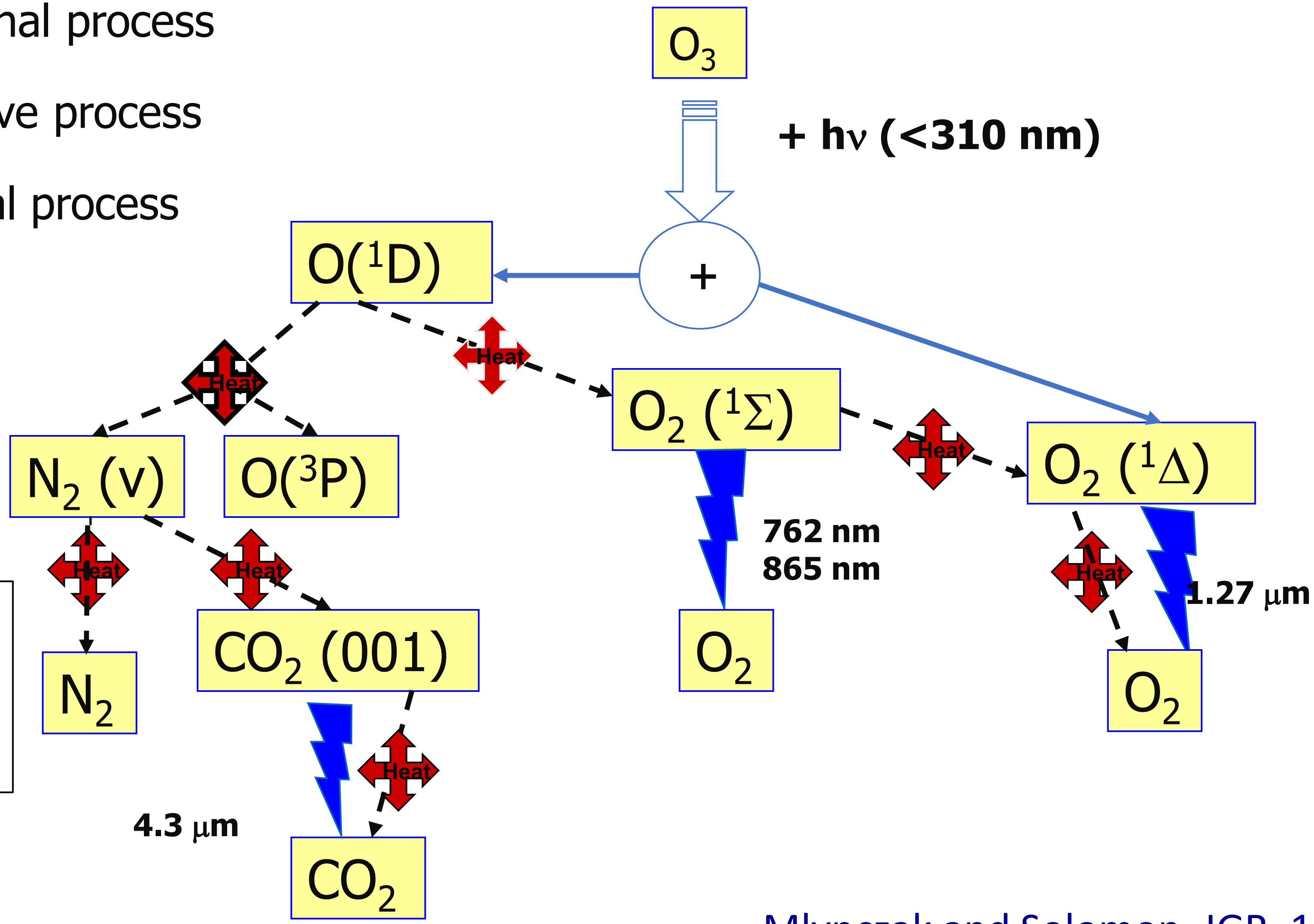
Derive the heating rates from the photolysis code above 60km.

Mlynczak and Solomon, JGR, 1993.

Solar Heating Rate Approach in WACCM Example

$O_3 + h\nu \Rightarrow O(^1D) + O_2(^1\Delta)$



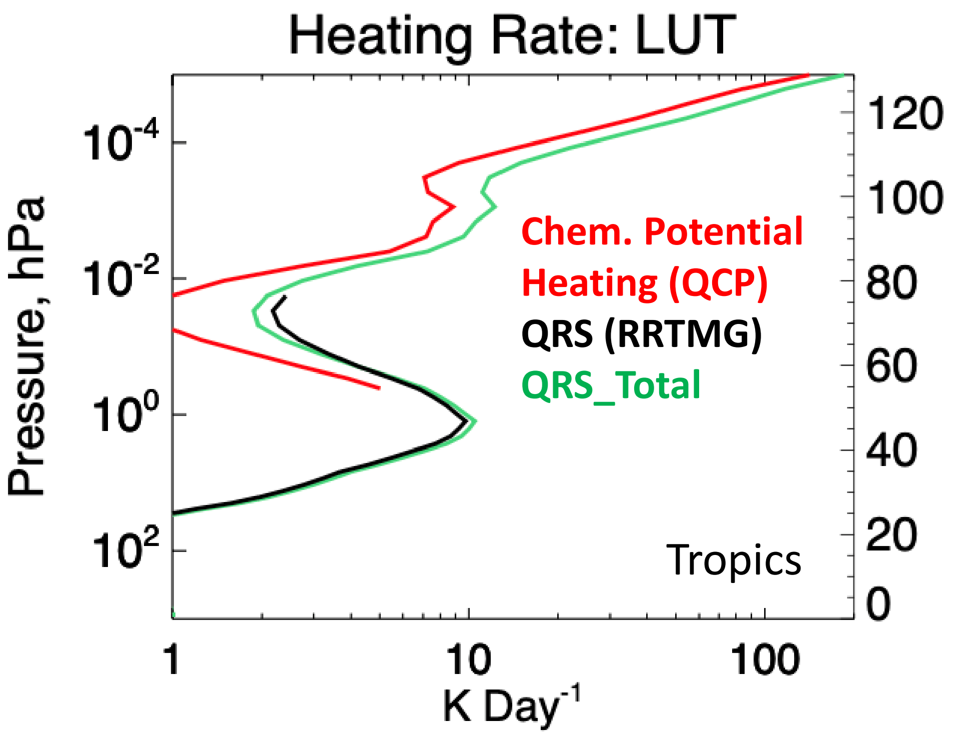


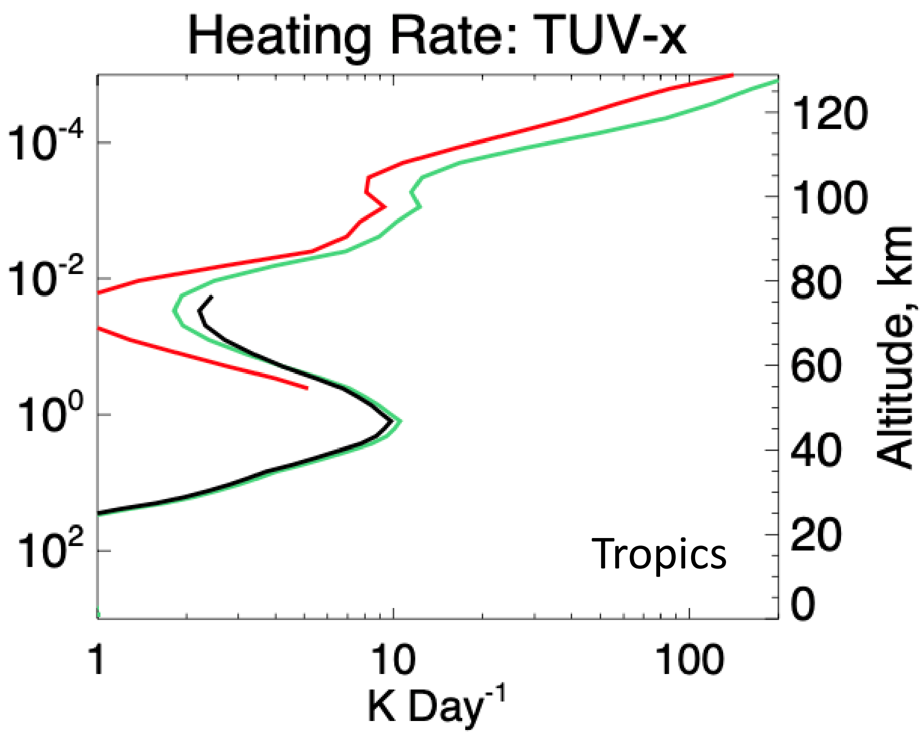
The radiative and thermal processes are dependent on the photolysis package in the MLT region.

Mlynczak and Solomon, JGR, 1993.

WACCM Solar Heating Rates: Merged with CAM6 RRTMG

QRS_Total = QRS +QCP+QTHERMAL+QRS_EUV+QRS_CO2NIR+QRS_AUR

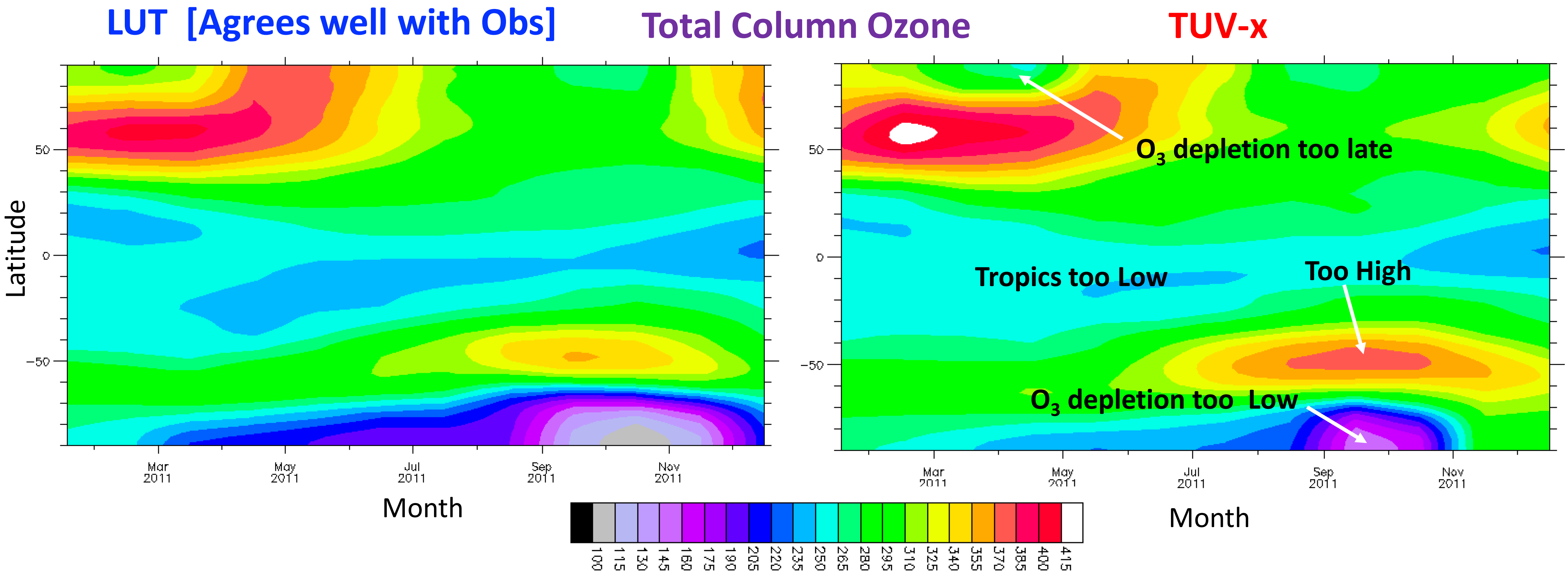




QRS (RRTMG) is merged with other upper atmospheric heating rates starting <u>at 60km</u>.

Initial comparison shows good agreement between LUT and TUV-x

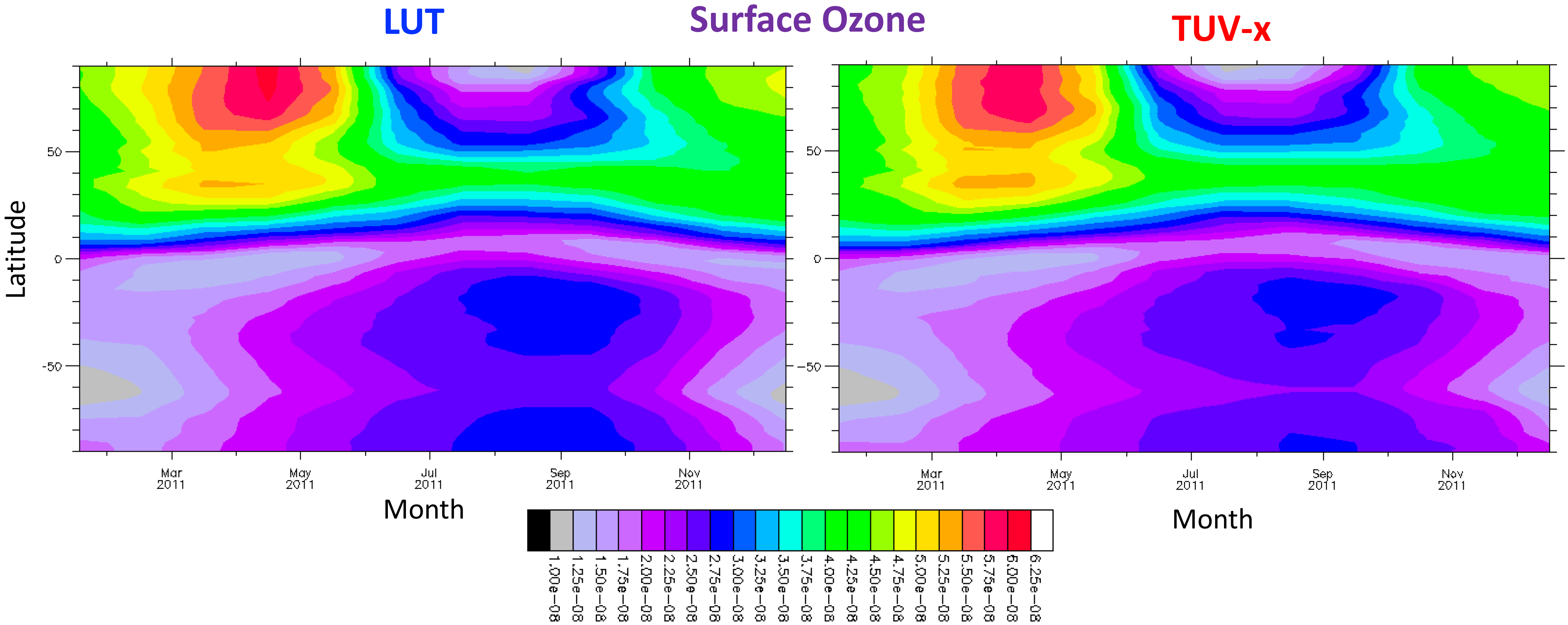
First (preliminary) attempt at 1-year simulation (2011) ** SD-WACCM



Seasonal behavior generally captured in TCO by the TUV-x simulations.

A good first step!

First (preliminary sim) attempt at 1-year simulation (2011) ** SD-WACCM



Excellent Agreement!!!

Summary

- The **TUV-x** **cross sections** and **quantum yield** representation (for the TSMLT chemical mechanism) is currently being evaluated and generally in good agreement with the **LUT** version.
  - More J's are needed to be added to TUV-x for Hg and VSLS Halogen chemistry.

- The **TUV-x** **photolysis heating rates** have been derived and are consistent with the **LUT** approach.

- The **TUV-x photolysis package** has been successfully implemented in **CESM2 WACCM6-SD**. This includes the option of putting aerosols and clouds in the radiative transfer.
  - There are differences in the **TCO** between the **TUV-x** and the **LUT** version that needs to investigated.

- **Next Step (over the next couple months)**
  - Examine the **inclusion** of **aerosols and clouds** in the **TUX-x** radiative transfer for interactive simulations (FCASE, BCASE).
  - **Optimize inline code** to be more computationally efficient with (4-stream radiative transfer).

Extra Slide

Why did we need to "Refactor" the TUV-x Code (Matt Dawson)

- **TUV-x must be configurable:** To have a single codebase that recreates the functionality of the various existing instances of TUV, many hard-coded choices needed to become configuration options. The single TUV-x codebase can now recreate the results of the stand-alone TUV 5.4 as well as the version of TUV used to generate the CAM-Chem lookup table data. Configurability also leads to more code reuse (less need for copy/paste/modify approach to feature addition)

- **TUV-x must be testable and tested:** During the refactoring unit tests were added to ensure the smallest components of the TUV-x code continue to work correctly now and as development continues into the future. Regression testing against older versions of TUV ensures that TUV-x remains able to recreate previous results. Tests are automated and run on every PR into the TUV-x repo and include testing with and without MPI and memory checking with Valgrind. Code coverage by automated testing is at about 80%.

- **Object-oriented design:** The choice to move to an object-oriented design was to improve encapsulation (keeping data and functionality together; separation of concerns) and prepare for eventual porting to a modern language with better compiler support.

- **Computational efficiency:** For the computational cost, we have a SIParCS project in the summer to begin porting the **TUV-x solver to GPUs.** This will involve optimizations (e.g., multi-column solving) applicable to CPU-based solving as well.