Inclusion of Inline photolysis module (TUV-x) in CESM2 MUSICAv0

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Presentation Outline

- Briefly describe the "new" TUV-x
- Show how TUV-x fits into the master plan for photolysis needs at NCAR
- Why do we need to move on from the LUT approach for global modeling?
- First results using inline TUV-x in CESM2 (MUSICAv0), i.e., CAM-Chem
- Special needs for WACCM

Tropospheric Ultraviolet Visible extension TUV-x (Madronich et al., Original TUV Code)

- Portable... presents a single interface that is usable in multiple contexts
- Builds as a software library. Build once and link to from any application
- Configurable (data-driven)
- Maintainable (ready for new science)
- Can include a representation aerosols and clouds in radiative transfer

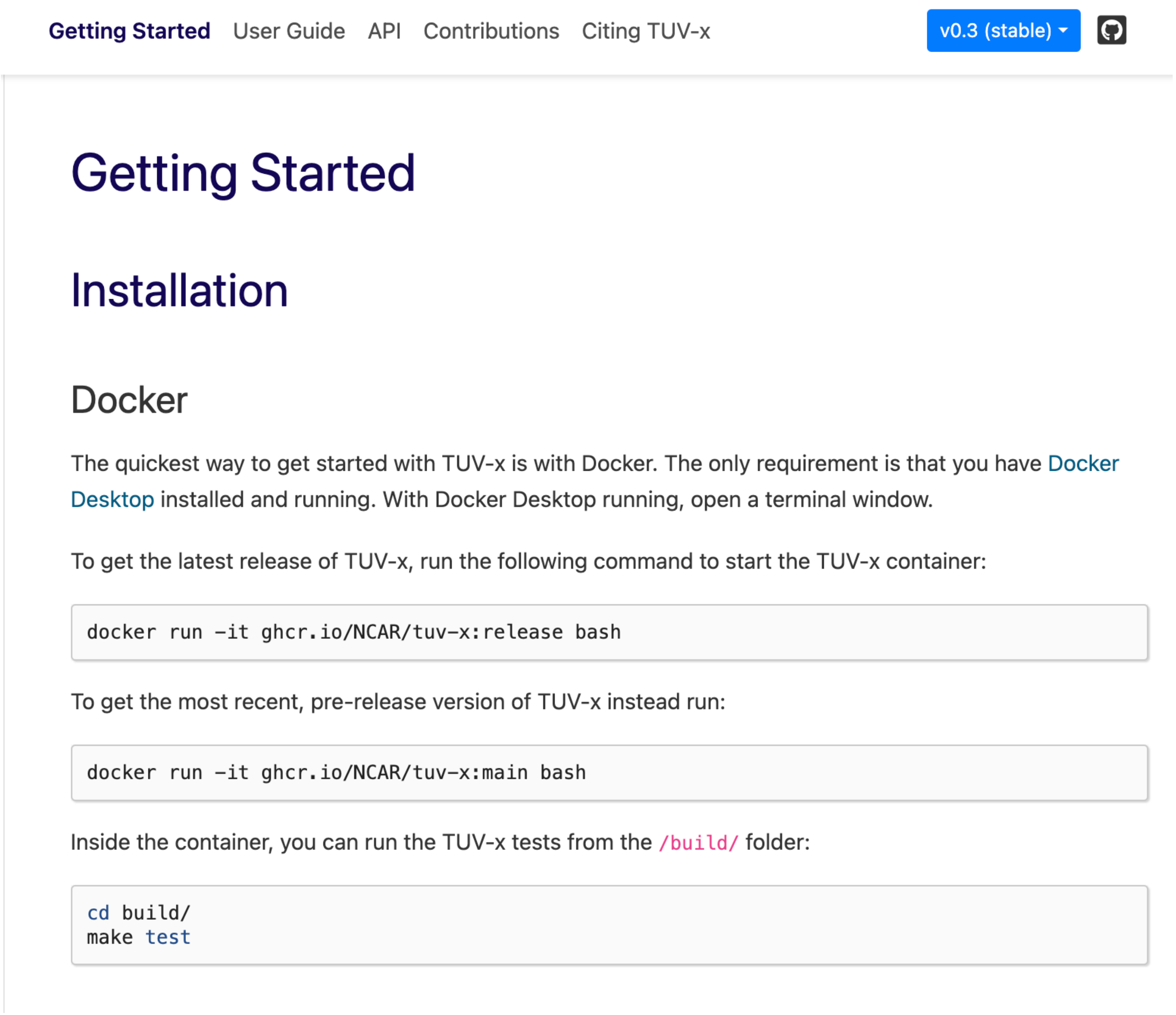
TUV-x Configurability

- Moved hard-coded configuration details to JSON data files
- Reusable datatypes allow run-time addition/modification of:
  - Cross sections
  - Quantum yields
  - Absorbing species
  - *and more!*

```
},
{
  "name": "BrONO2+hv->BrO+NO2",
  "cross section": {
    "netcdf files": [
      { "file path": "data/cross_sections/BrONO2_1.nc" }
    ],
    "type": "base"
  },
  "quantum yield": {
    "type": "base",
    "constant value": 0.15
  }
},
{
  "name": "BrONO2+hv->Br+NO3",
  "cross section": {
    "netcdf files": [
      { "file path": "data/cross_sections/BrONO2_1.nc" }
    ],
    "type": "base"
  },
  "quantum yield": {
    "type": "base",
    "constant value": 0.85
  }
},
{
  "name": "BrCl+hv->Br+Cl",
  "cross section": {
    "netcdf files": [
      { "file path": "data/cross_sections/BrCl_1.nc" }
    ],
    "type": "base"
  },
  "quantum yield": {
    "type": "base",
    "constant value": 1.0
  }
},
```

Tropospheric Ultraviolet Visible extension TUV-x Access

- Try out stand-alone TUV-x (https://github.com/NCAR/tuv-x)
    - Quick-start instructions on the GitHub repo for running stand-alone TUV-x in a Docker containers
- Send feedback to Matthew Dawson: mattdawson@ucar.edu


Getting Started User Guide API Contributions Citing TUV-x v0.3 (stable)

Getting Started

Installation

Docker

The quickest way to get started with TUV-x is with Docker. The only requirement is that you have Docker Desktop installed and running. With Docker Desktop running, open a terminal window.

To get the latest release of TUV-x, run the following command to start the TUV-x container:

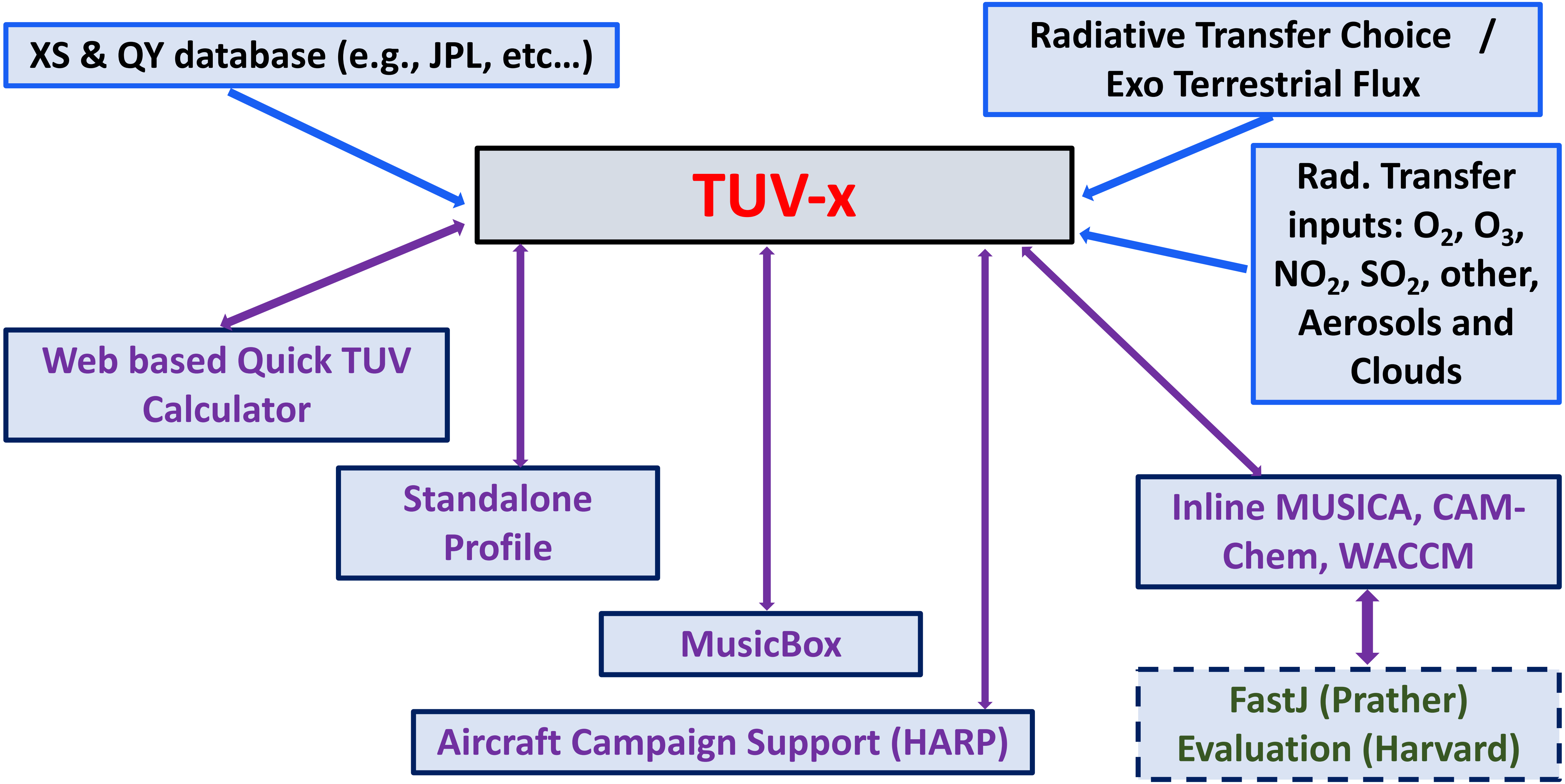
```
docker run -it ghcr.io/NCAR/tuv-x:release bash
```

To get the most recent, pre-release version of TUV-x instead run:

```
docker run -it ghcr.io/NCAR/tuv-x:main bash
```

Inside the container, you can run the TUV-x tests from the `/build/` folder:

```
cd build/
make test
```


XS & QY database (e.g., JPL, etc…)
Radiative Transfer Choice / Exo Terrestrial Flux
TUV-x
Rad. Transfer inputs: O_2, O_3, NO_2, SO_2, other, Aerosols and Clouds
Web based Quick TUV Calculator
Standalone Profile
MusicBox
Aircraft Campaign Support (HARP)
Inline MUSICA, CAM-Chem, WACCM
FastJ (Prather) Evaluation (Harvard)

TUV-Webpage

231,663 calculations since 2016-02-09 (113 photolysis rates).

https://www.acom.ucar.edu/Models/TUV/Interactive_TUV/

QUICK TUV CALCULATOR

This web page runs the *5.3* version of the TUV model. You can run the model for a specified latitude, longitude and time (input option 1), or for a given solar zenith angle (input option 2). In either case, you must also specify the additional parameters in the second column. Also, you may select to print out the photolysis rates and/or the solar actinic flux spectrum at a given altitude above the surface (output option 1), or the erythemal UV and/or solar irradiance at that altitude (output option 2). For any problem, or to send comments, email TUV administrators.

Wavelength

Start:	End:	Increments:
280	700	420

◉ **INPUT OPTION 1**

LATITUDE (deg): 0

LONGITUDE (deg): 0

DATE (YYYYMMDD): 20150630

TIME (hh:mm:ss, GMT): 12:00:00

○ **INPUT OPTION 2**

SOLAR ZENITH ANGLE (deg): 0

OTHER INPUT PARAMETERS

OVERHEAD OZONE COLUMN (du): 300

SURFACE ALBEDO (0-1): 0.1

GROUND ELEVATION (km asl): 0

MEASUREM. ALTITUDE (km asl): 0

Clouds

Opt. Depth:	Base:	Top:
0.00	4.00	5.00

Aerosols

Opt. Depth:	S-S Alb:	Alpha:
0.235	0.990	1.000

Sunlight

Direct beam:	Diffuse down:	Diffuse up:
1.0	1.0	1.0

◉ **OUTPUT OPTION 1**
(for Atmospheric Science)

☑ MOLECULAR PHOTOLYSIS FREQUENCIES (s-1)

☐ ACTINIC FLUX, SPECTRAL (quanta s-1 cm-2 nm-1)

○ **OUTPUT OPTION 2**
(for Biology)

☑ IRRADIANCE, WEIGHTED (W m-2)

☐ IRRADIANCE, SPECTRAL (W m-2 nm-1)

RADIATION TRANSFER MODEL

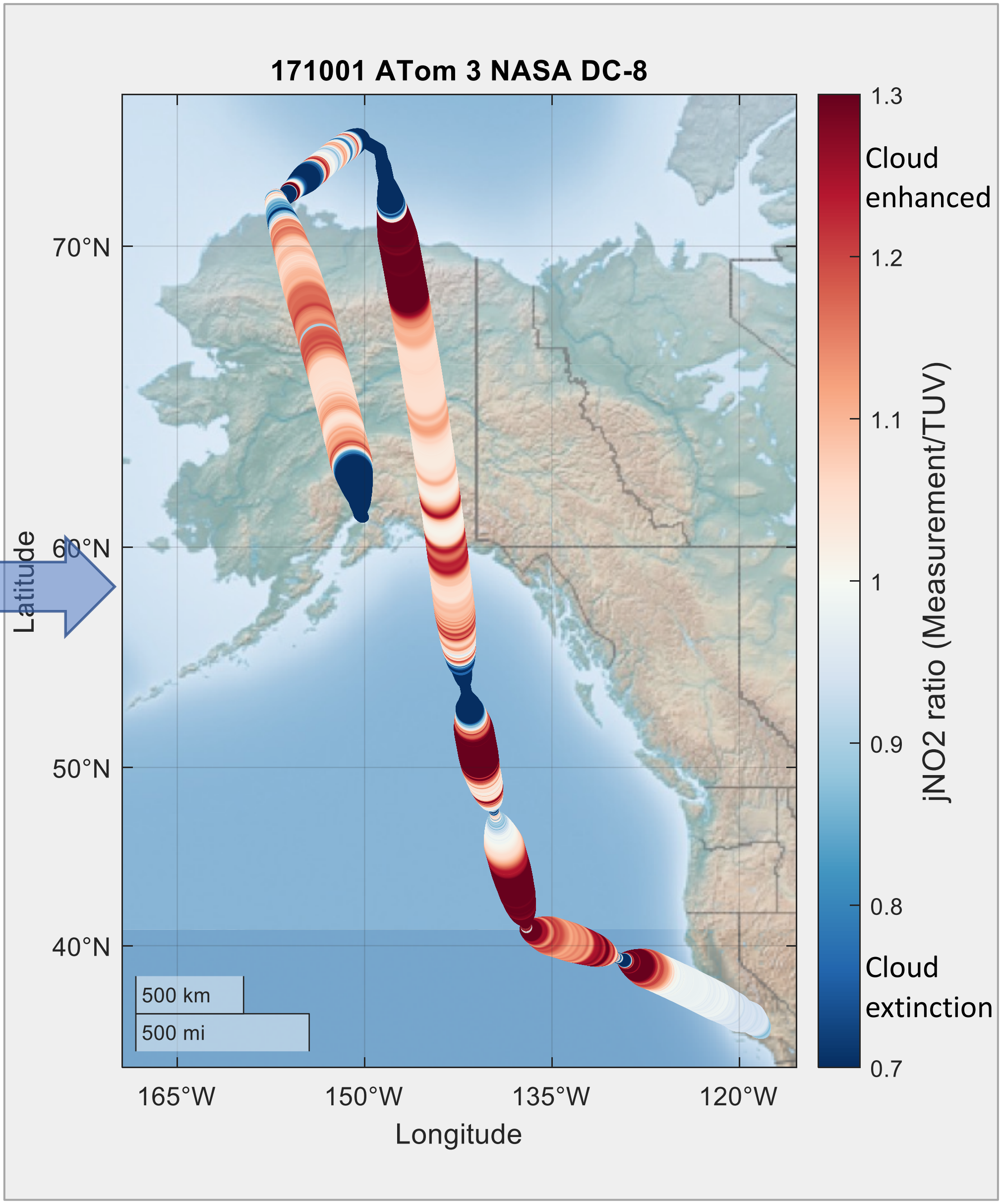
◉ Pseudo-spherical 2 streams (faster, less accurate)

○ Pseudo-spherical discrete ordinate 4 streams (slower, more accurate)

GO! Reset

TUV connections to HARP/CAFS airborne actinic flux measurements

TUV provides	Benefits/examples
Photolysis frequency calculations for measured and modeled actinic flux	Measurement/model consistency • Identical absorption cross-sections • Identical quantum yields
Clear-sky calculations of up/down actinic flux and photolysis frequencies along flight track	• Project continuity (since 1996) • ACCLIP calibration issue identification and analysis
Measurement/TUV ratio removes SZA and altitude impacts	• **Identification of cloud, aerosol, albedo and ozone column impacts** • **Statistical comparisons to global models (Hall et al., 2018)**
Cloud/aerosol, ozone column, albedo parameters	• ACCDAM satellite trace gas retrievals • DC3 optical depths • KORUS-AQ aerosol impacts • CONTRAST jet stream ozone
Spectral absorption analysis	Remote sensing smoke detection (up/down)



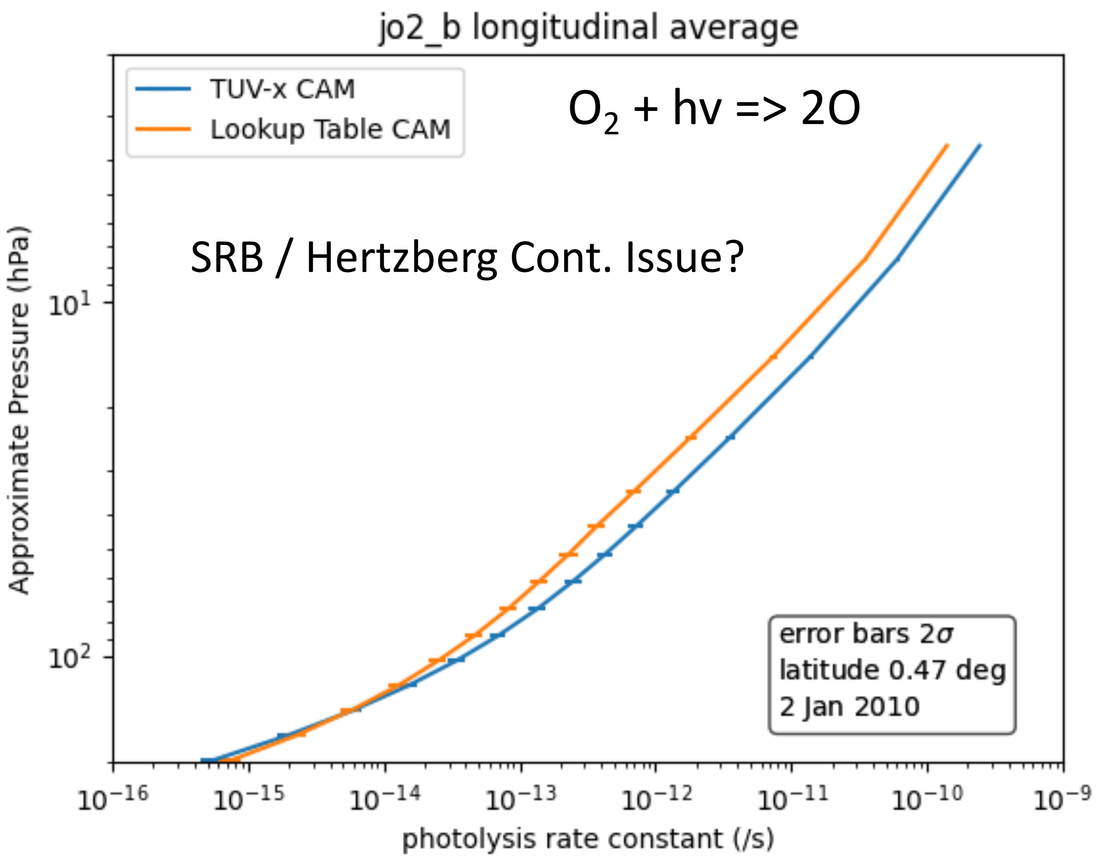
Contact: Sam Hall (halls@ucar.edu) and Kirk Ullmann (ullmannk@ucar.edu)

Global modeling needs for influence of species and aerosols that impact the radiative transfer / photolysis rates

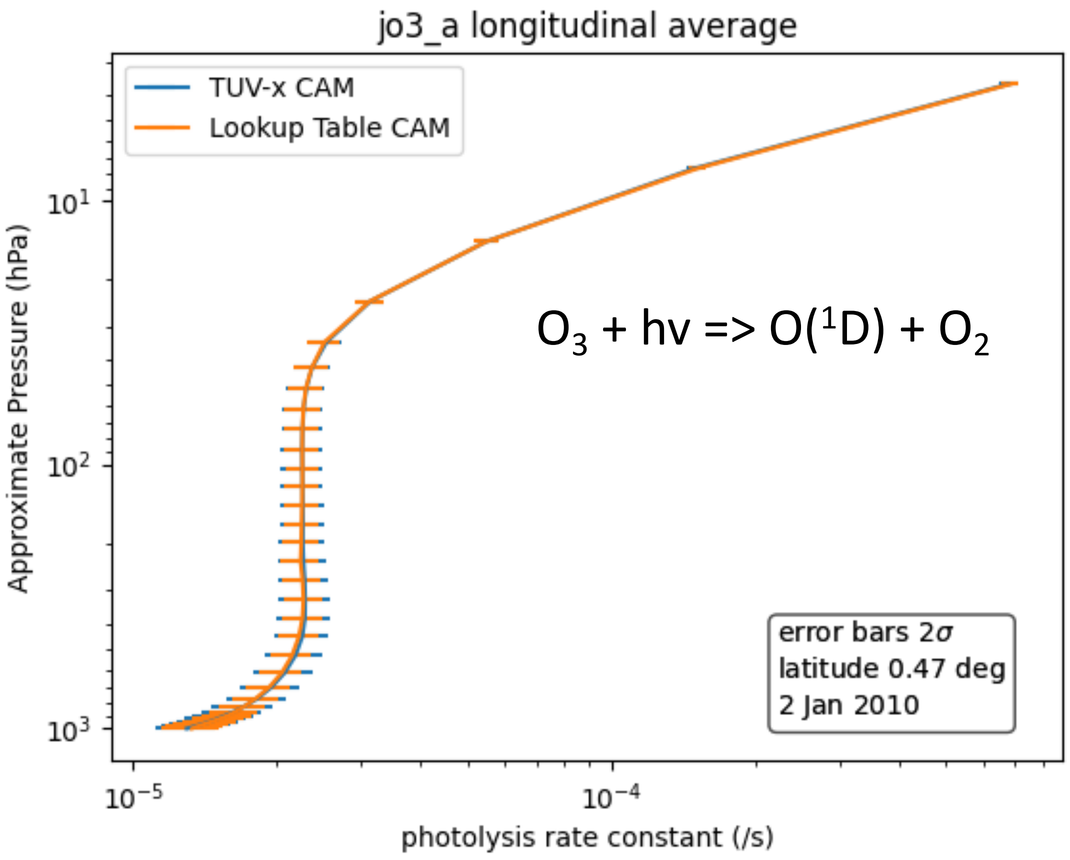
Representation of a wide range of Science Projects, e.g.

- Present day atmosphere under various volcanic sulfate/soot loadings and possible Geoengineering studies (Tilmes).
- Large wildfire (pyroCb) towers where injections of soot, organic aerosols are included (Solomon).
- Early earth atmospheres where O_2 and O_3 are not major absorbers (Marsh).
- Asteroid impact scenarios where there is a large perturbation of soot, H_2O, NOx, and halogens (Bardeen, Garcia).
- Nuclear war scenarios where soot, organic aerosols, NOx are elevated (Bardeen, Kinnison).

CESM2 Inline vs LUT

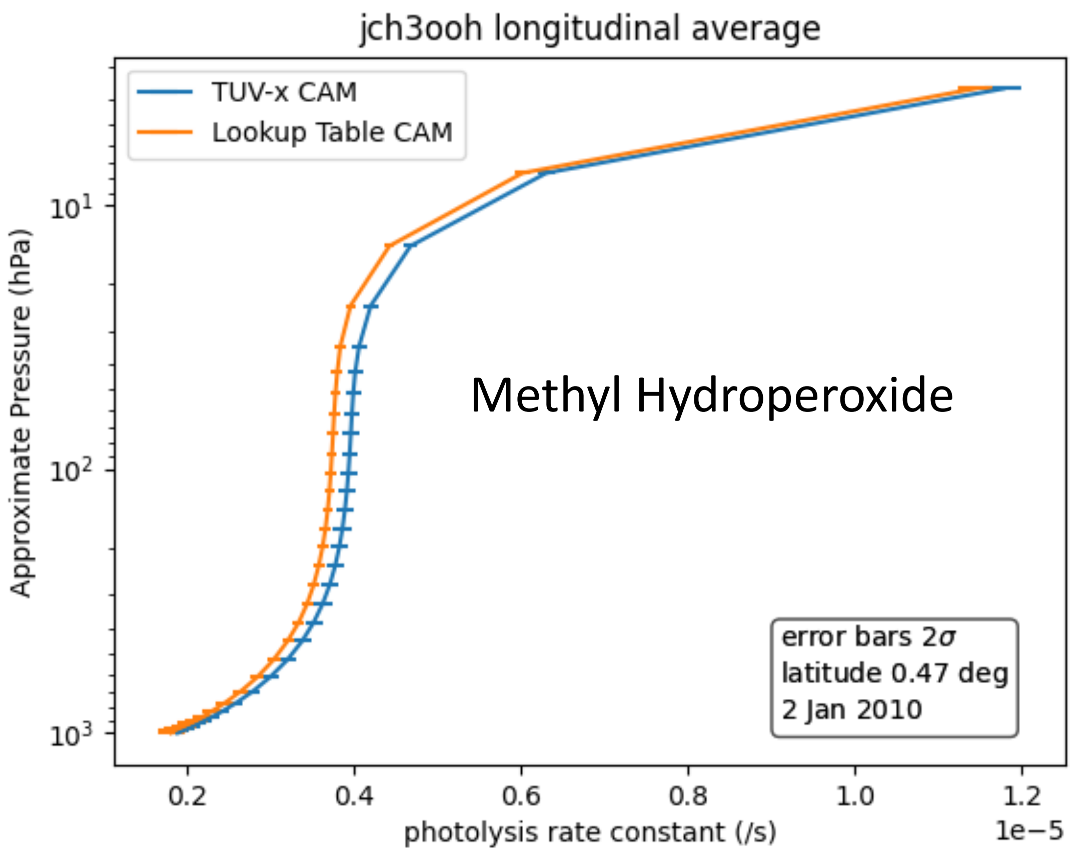


Wavelength range: 175-205nm

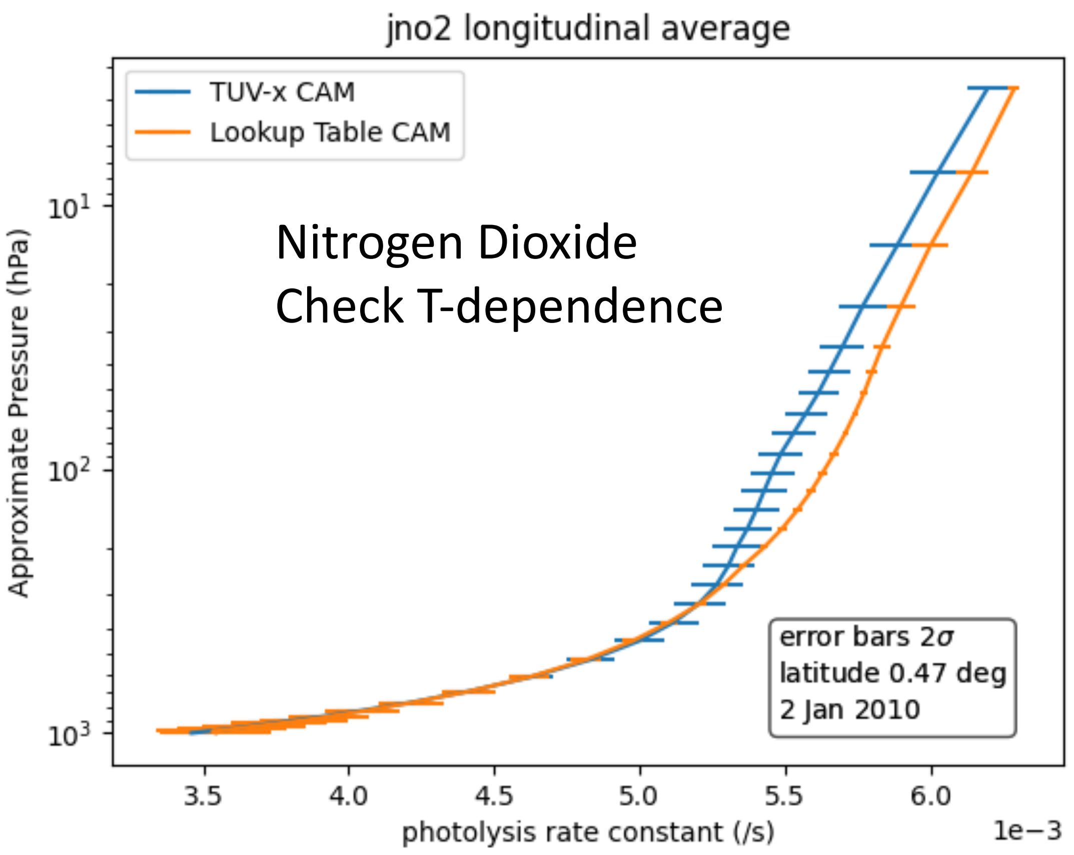


Wavelength range: ~310-411nm

CESM2 Inline vs LUT



Wavelength range: 210-365nm

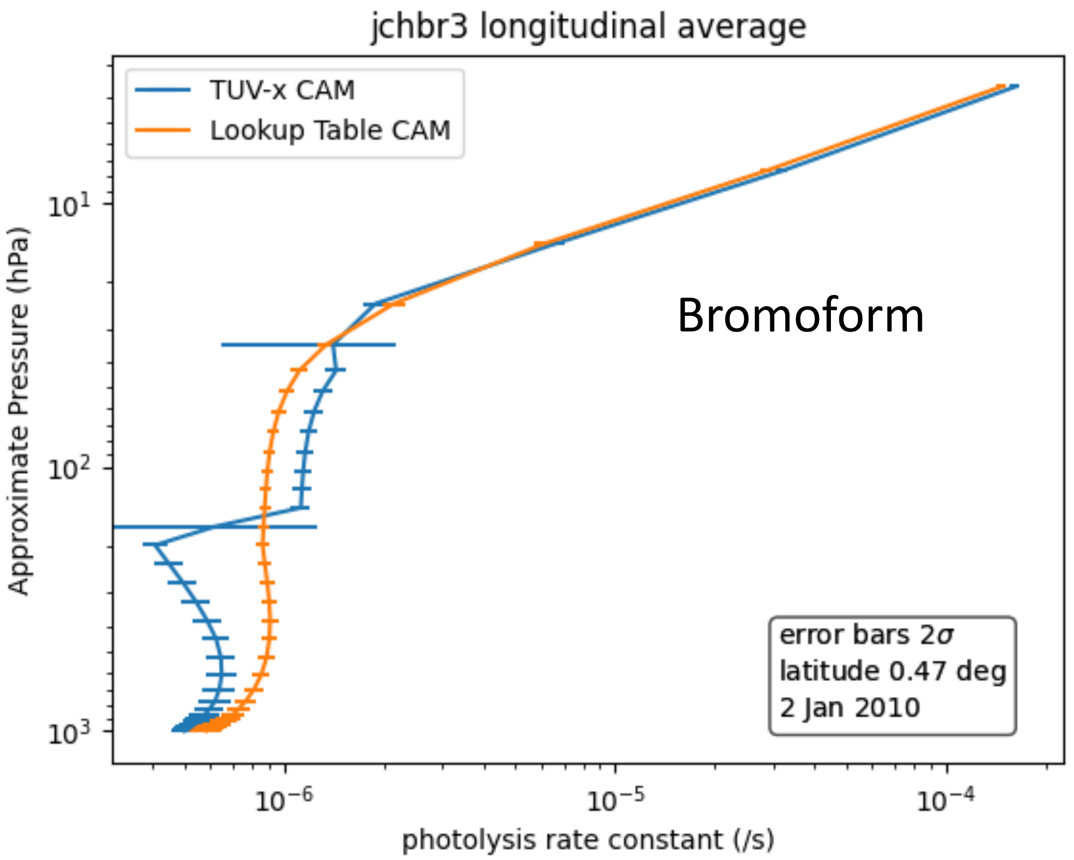


Wavelength range: 240-650nm

CESM2 Inline vs LUT

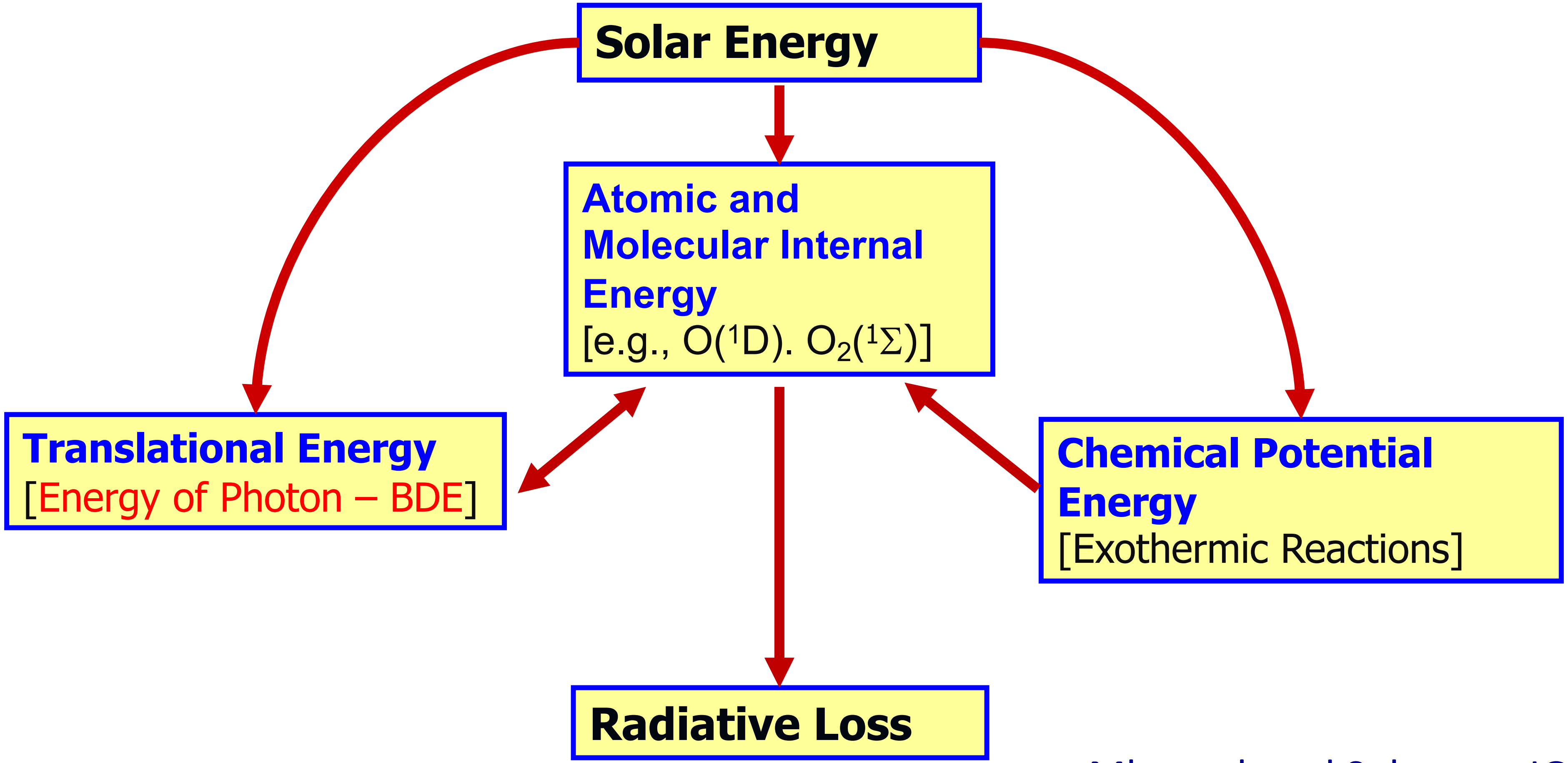
Summary: Need to check all cross section and quantum yield values and implementation in TUV-x.

Will compare to TUV (v5.3) and the LUT databases.



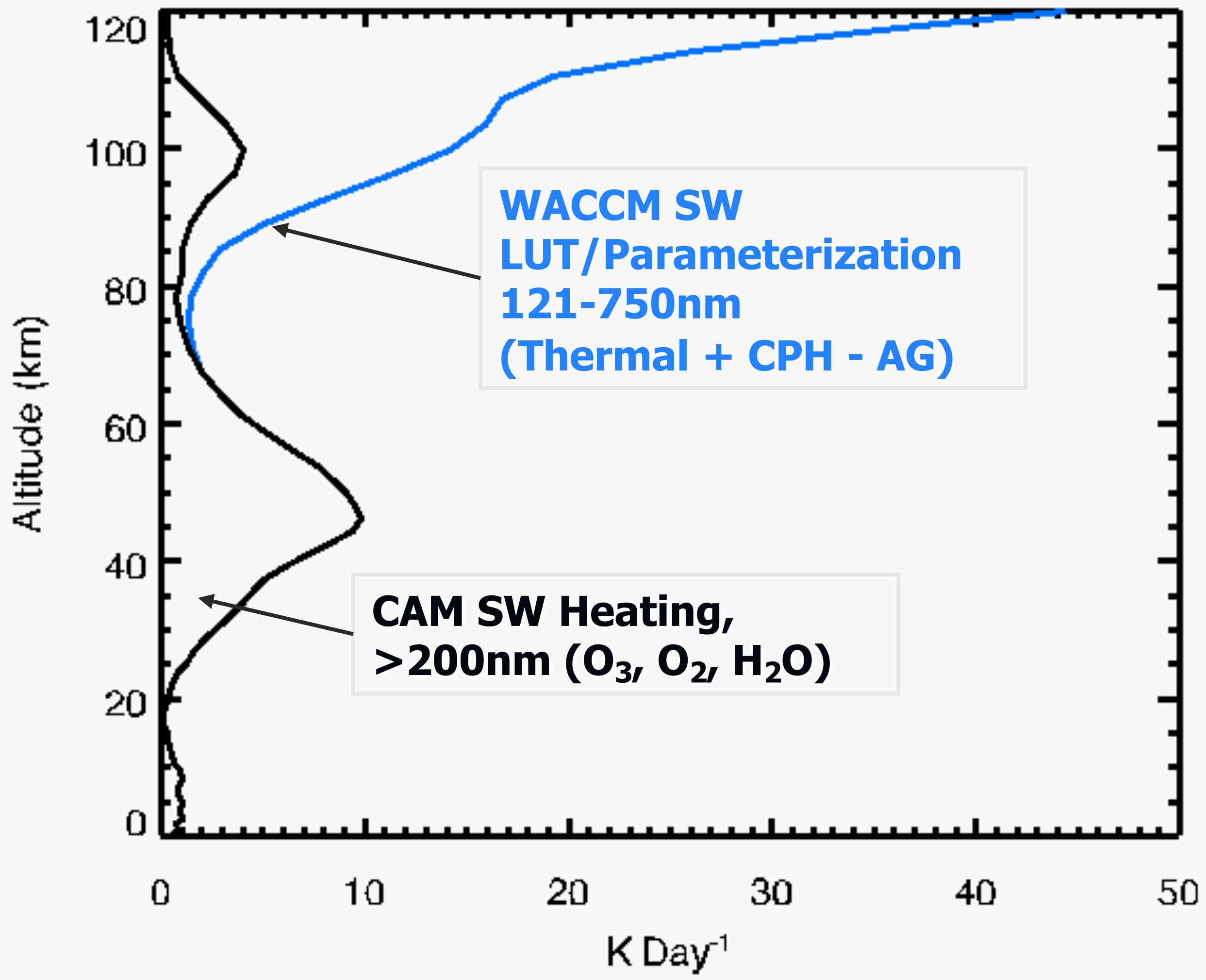
Wavelength range: 170-362nm

Solar Heating Rate Approach in WACCM



Mlynczak and Solomon, JGR, 1993.

Merge Solar Heating Approaches for WACCM



Next Step

- Finish integration of TUV-x into MUSICAv0
- Test with aerosol input (e.g., Sulfate, Soot)
- Aim for 4-stream discrete ordnance radiative transfer (RT)
  - May need to optimize wavelength grid for computational efficiency?
  - Could also use 2-stream RT
- Derive heating rates for high top (WACCM) to address chemical potential heating.
- Add cloud fraction approach to RT

Evaluate model chemical composition with LUT approach and Observations

Evaluate with CloudJ (Prather) when available

Extra Slide

CESM2-MUSICAv0

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)

CAM4 SW Heating rates

Heating and Photolysis rates

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