OH Meinel (3,1) airglow emission model development and comparison with ground-based observations

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Outline

• ERAU WACCM efforts
  – OH(3,1) chemistry
  – OH rotational temperatures measurements comparisons with WACCM results
  – Solar Cycle response of OH temperatures

• Recent studies suitable for WACCM comparisons

• ERAU resources for WACCM development
ERAU-WACCM Efforts

- Develop an OH (3,1) airglow emission model of the earth's middle atmosphere calculating the population at each vibrational level using the Einstein coefficients for spontaneous emission.

- Compare model OH intensities to absolute intensities from a Michelson Interferometer at Resolute Bay (RB), Canada (74.68°N, 94.90°W), which operates continuously (24 hours a day) during the polar night of the winter season (October-March).
Instrumentation

- Michelson Interferometer
  - Resolute Bay, Canada (74.68°N, 94.90°W)
- A low noise InGaAs detector with a narrow field-of-view (~2°)
- Wavelength region, 1.0 μm to 2.0 μm at 4 cm⁻¹ resolution
- 5 minutes time integration
Measurements

• Model Simulations:
  – The species predictions are 10 day averages of instantaneous values at midnight (UT); cover the same 6 year period, 2000-2006, and at the same latitude (74°N) as Resolute Bay time series

• OH Airglow Observations:
  – The peak brightness values of the first six rotational lines of the P branch in OH (3,1) Meinel band were used to derive the rotational temperatures. OH (3,1) band brightness values were also computed from these six rotational. The band brightness time series was sampled and averaged to match the model simulations.
Model Development

- Similar to photochemical developed by *Makhlouf et al.* [1995], including the reactions describing production and loss rates, except we have accounted for multi-quantum quenching of OH by O$_2$ using rate constants calculated by *Adler-Golden* [1997].

\[
\begin{align*}
(1) & \quad k_1(\nu) + k_4(\nu) \\
& \quad H + O_2 \rightarrow OH(\nu) + O_2 \quad \nu=6-9 \\
(2) & \quad k_2(\nu) + k_5(\nu) \\
& \quad O + HO_2 \rightarrow OH(\nu) + O_2 \quad \nu=0-3 \\
(3) & \quad k_3(\nu) \\
& \quad OH(\nu) + O_2 \rightarrow OH(\nu-1) + O_2 \quad \nu=1-9 \\
& \quad \text{where } k_1(\nu), \ldots, k_5(\nu) \text{ are the rate constants and } \nu \text{ is the vibrational level and } A(\nu,\nu-n) \text{ are the Einstein coefficients for spontaneous emission (from personal communication with Sam Yee and U.B. Makhlouf).}
\end{align*}
\]
• OH production determined by Reactions (1) and (2), with the first being the primary source of excited OH.

• Reactions (3) and (4) represent collisional quenching by molecular oxygen and nitrogen and contribute to hydroxyl concentrations at vibrational levels below $\nu=9$.

• Used rate constants for Reaction (3) calculated by Adler-Golden [1997] to include multi-quantum vibrational relaxation of OH by $O_2$.

• The final contribution to OH populations for states below $\nu=9$, comes from Reaction (6), spontaneous emission.

• Reaction (5), which is chemical quenching by atomic oxygen, along with Reactions (3)-(6) comprise the dynamics responsible for loss of vibrationally excited OH.
• Assume steady state and no background wind
• The densities of the species in Reactions (1)-(6) were calculated from their mixing ratios determined from WACCM.

Major species profiles from OH model for midnight (UT), day 281 of year 2000 at 74°N latitude.

Minor atmospheric species altitude profiles produced by WACCM and the OH model for midnight (UT), day 281 of year 2000 at 74°N latitude.
Modeled OH Concentration

- The volume emission rates were vertically integrated over all the altitudes, at 74°N latitude, for a more accurate comparison with ground-based observations at Resolute Bay.

**Graph:**

OH concentrations at 3 vibrational levels generated by the OH model at midnight (UT), day 281 of year 2000 at 74°N latitude.
Results

- OH (3,1) absolute intensities derived from Resolute Bay observations show good agreement with the OH model predictions of band brightness
Future Efforts

- Next the model will be integrated into WACCM, which currently accounts for energy loss due to OH airglow by applying an efficiency factor.
- The fully integrated model would then be used to generate longer time series of predictions to study variations in OH airglow.
WACCM Temperatures at ~87 km Near South Pole

- **Temperature (K)**
  - X-axis: Year
  - Y-axis: Temperature (K)

- **Solar F10.7 flux**
  - X-axis: Year
  - Y-axis: Flux $10^{-22}$ [J/s$^{-1}$ m$^{-2}$ Hz$^{-1}$]
WACCM temperatures at ~ 87 km Near SPS

Solar F10.7 flux

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WACCM Temperature Variation at ~87 km Near South Pole
Solar Cycle Response and Long term trend in WACCM

- WACCM outputs every 5 days covering 1994 to 2003.
- WACCM outputs nearest to South Pole and ~87 km were sampled to replicate fidelity of OH rotational temperature measurements.
- All three realizations of WACCM runs were used.

<table>
<thead>
<tr>
<th>WACCM</th>
<th>Solar Cycle (K/sfu)</th>
<th>Trend term (K/year)</th>
</tr>
</thead>
<tbody>
<tr>
<td>WACCM1</td>
<td>0.03±0.01</td>
<td>-0.5±0.1</td>
</tr>
<tr>
<td>WACCM2</td>
<td>0.01±0.01</td>
<td>0.0±0.11</td>
</tr>
<tr>
<td>WACCM3</td>
<td>0.03±0.01</td>
<td>0.09±0.12</td>
</tr>
</tbody>
</table>
The estimated amplitude of solar cycle variation in observed OH temperatures at South Pole is $\sim 0.04 \pm 0.02$ K/sfu.

The observed 11-year variation in OH temperatures is in phase with the solar flux, with an increase of about 7K between solar min and solar max.

Recent study of OH temperatures at Davis, Antarctica by French et al. [2005] presented solar response amplitude of 5K/100 sfu.
Embry-Riddle Aeronautical University’s High Performance Computer Cluster (Beowulf)

- **Funding Agency:** National Science Foundation
- **Local Partner:** Bethune-Cookman College
- **Objective:** To support all computational research, research training, and education related to that research at ERAU and BCC
ERAU Beowulf

- Vendor: DELL
- 131 dual-processor nodes (3 head, 128 compute)
- 262 processors
- 3.2 GHz Intel Xeon (64-bit)
- Minimum RAM 4 GB per node
- Myrinet Interconnect
- Hard Drives: 2 TB, 73 GB, 36 GB - *all mirrored*
- Redhat Linux OS
- Internet-2 link to BCC and Prescott, AZ
OH and O2 Rotational Temperatures

South Pole OH and O2 rotational temperatures at South Pole during 2002

Adelaide OH and O2 rotational temperatures at South Pole during 2002