

# CHEMISTRY IN CESM2

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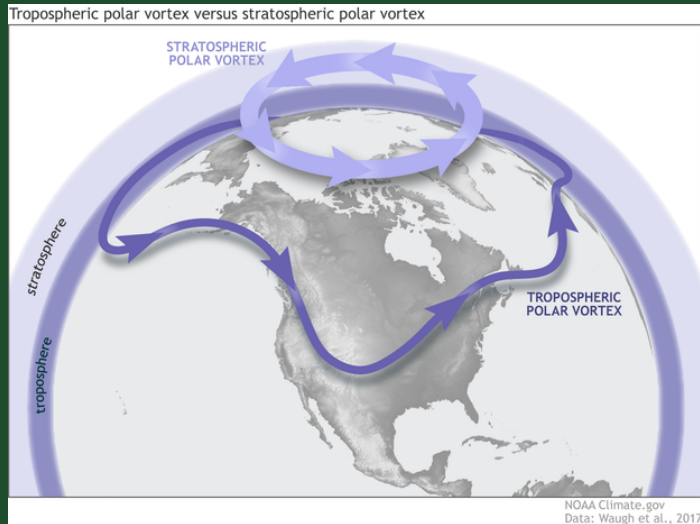


Colorado State University

## MOTIVATION

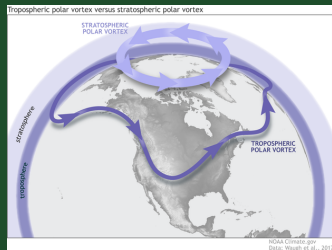
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# STRATOSPHERIC SUDDEN WARMINGS



- SSWs, or stratospheric sudden warmings, are when the stratosphere is warmed by many kelvins. This is preceded by a wind reversal of the stratospheric polar vortex. I.e., the westerlies go eastward.

# STRATOSPHERIC SUDDEN WARMINGS

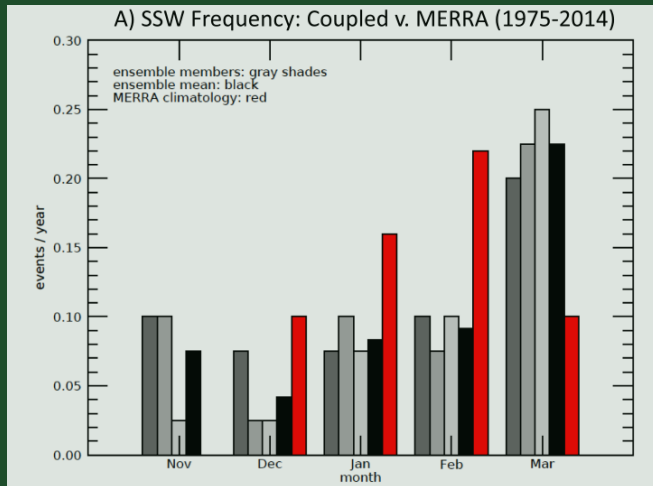


climate.gov

- Defined as a wind reversal (eastward) at 10 hPa ( $\sim 25$  km),  $60^\circ\text{N}$
- Big improvement from including updated parametrizations of turbulent mountain stress (TMS), surface stress due to unresolved topography
- A lack of stratospheric internal variability without a high-top atmosphere

- The change in direction is what is used to define their occurrence and frequency.
- With the inclusion of turbulent mountain stress from unresolved topography, the SSW's saw a big improvement.
- Even though this is also part of the low-top version (CAM), the frequencies are too small, and WACCM get much closer to observation.

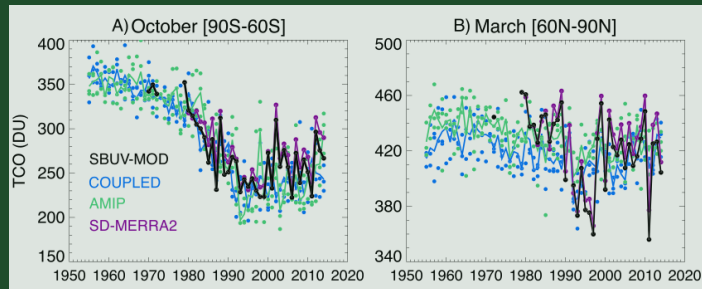
# STRATOSPHERIC SUDDEN WARMINGS



- Here we see frequency of SSW's between 1975 and 2014, in events per year. Three ensemble members in grayscale, the ensemble mean in black and observations in red.

# EVOLUTION OF THE OZONE LAYER

- WACCM6 is able to reproduce the evolution of the ozone layer (also SH polar ozone hole)
- Ozone variability in the tropical stratosphere improves on the inclusion of an internally generated quasi-biennial oscillation (QBO)



- The figure is showing total column ozone in Dobson units from a WACCM6 coupled simulation (blue) together with a specified SST (AMIP, green), specified dynamics (purple) and observations (black).
- If one look at ozone the biggest improvement is in the polar regions. WACCM6 is able to reproduce the evolution of the ozone layer, and also the SH polar ozone hole.
- One important improvement is the inclusion of an internally generated QBO. So again, stratospheric winds (but now in the tropical stratosphere) are needed to more precisely simulate a different physical process, ozone variability.
- Not shown are the tropics, where there are larger biases.
- *(This is due to tropical upwelling; since the lower stratospheric ozone field is dynamically controlled, vertical velocity impact the total column ozone. And, larger vertical velocities in the lower stratosphere are expected to be associated with reduced ozone due to vertical advection of ozone poor air from the troposphere.)*

# ATMOSPHERIC BLOCKING

Frequency of the meridional gradient of 500-hPa geopotential height below a threshold of  $\text{GHGS} > 0$ ,  $\text{GHGN} < -5 \text{ m/degree}$

$$\text{GHGS} = \frac{Z(\phi_0) - Z(\phi_S)}{\phi_0 - \phi_S}$$

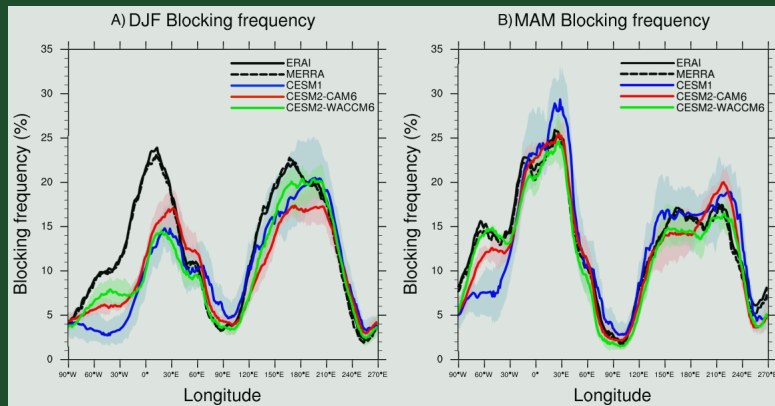
$$\text{GHGN} = \frac{Z(\phi_N) - Z(\phi_0)}{\phi_N - \phi_0}$$

where  $\phi_N = 78.75^\circ\text{N} + \Delta$ ,  $\phi_0 = 60^\circ\text{N} + \Delta$ ,  $\phi_S = 41.25^\circ\text{N} + \Delta$  and  $\Delta = -3.75^\circ, 0^\circ, 3.75^\circ$  [1].

- Blocking frequency is another way tropospheric variability improve.
- A definition from D'Andrea et al. (1998) defines it as the frequency of the meridional gradient at 500-hPa geopotential height to be below a threshold of  $-5 \text{ m/}^\circ$ .
- A given longitude is locally defined as blocked on a specific day if these conditions are satisfied for at least one of the three deltas.

[1] D'Andrea et al. "Northern Hemisphere atmospheric blocking as simulated by 15 atmospheric general circulation models in the period 1979–1988". 1998

# BLOCKING FREQUENCY



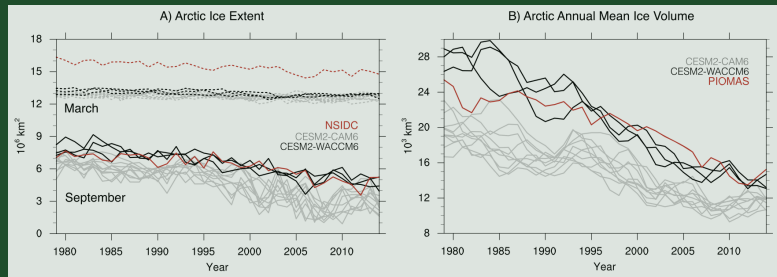
- All simulations coupled to an active ocean. CESM1 has 35 simulations, CESM2-CAM6 5 simulations and CESM-WACCM6 3 simulations.
- CESM2 better than CESM1 in the Greenland blocking bump in March–May (30 °W)
- CESM2 still has a DJF bias in the Atlantic sector.
- CESM2-WACCM6 significantly better than CESM2-CAM6 in the Pacific sector during DJF.
- With blocking frequency closer to observations, this indicates that stratospherical dynamical processes are important for high-latitude tropospheric climate variability.



# SEA ICE

- The September NH sea ice extent is better in WACCM6 than in CAM6
- Less downward surface SW and LW in WACCM6 due to higher LWP<sup>1</sup> which in turn is due to higher aerosol number.

⇒ Tropospheric aerosol chemistry impacts Arctic sea ice.



<sup>1</sup> liquid water path

[3] Gettelman et al. "The Whole Atmosphere Community Climate Model Version 6 (WACCM6)". 2019

- With sea ice, you have an example of a process on the very bottom of the model that is noticeably affected by improving the resolution of the top of the atmosphere component.
- Annual mean sea ice extent is similar in CAM6 and WACCM6, both coupled, but WACCM6 has less melt in summer, resulting in thicker ice.
- The September NH sea ice extent is higher and in better accordance with observations in WACCM6 than in CAM6.
- The sea ice volume is dropping faster in WACCM6, faster than observations, while in CAM6 the rate is better while the volume is smaller.
- Have found that WACCM6 has less downward surface SW and LW because of slightly higher liquid water path. In winter this is around the ice edge, in summer over the ice. This again is a result of higher aerosol number.
- We therefore find that tropospheric aerosol chemistry can make an impact on Arctic sea ice.

## IMPLEMENTATION

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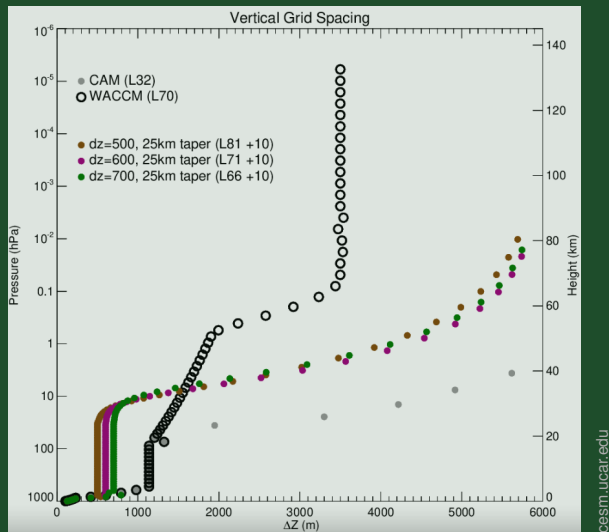
# COMPUTATIONAL COST

**Table 1:** Approximate costs of running different atmosphere models  
(From lecture by Mills)

Configuration	Resolution	Chemistry	Core-hours/simulation years
CAM6	1°, 32 L	CAM	3700
WACCM6	2°, 70 L	MA	5400
WACCM6	1°, 70 L	TSMLT	22 000
WACCM6-SC	1°, 70 L	SC	6000
WACCM6-SD	1°, 88 L	TSMLT	23 000

- We have now seen some of the improvements one might expect when using WACCM6 in favour of CAM6. But this comes at a cost. Let us see what that might be, before we look more closely at how and what extra is implemented in WACCM6.
- CAM is cheapest by quite a lot.
- Even the older MA version, which can only run at nominal two degrees is close.
- SC: specified chemistry. Radiatively active chemical species (e.g., ozone) are prescribed.
- SD: specified dynamics. Winds and temperatures are relaxed to a specific set of data (e.g., reanalysis from NASA GEOS).

## SPATIAL



cesm.ucar.edu

- The most obvious change is in vertical resolution.
- Brown, Purple and Green are just suggested new coordinates.
- Circles are WACCM6 and grey are CAM6, equivalent up to about 100 hPa.

See more at: <https://www.cesm.ucar.edu/events/wg-meetings/2018/presentations/amwgjoint/richter.pdf>

# CHEMISTRY VERSIONS

- Neutral chemistry model versions of WACCM6

- There are four chemistry packages to choose from when running WACCM6.
- TSMLT is the default in WACCM6, with troposphere, stratosphere, mesosphere and lower thermosphere included.
- TS is the troposphere and stratosphere mechanism.
- MA is the middle atmosphere version, included as a two degree option. It is very similar to the older default package used in WACCM4, and thus also has a reduced set of tropospheric reactions.
- But there is more! Mad! Middle atmosphere with D region ion chemistry included, that is.
- The D region is often used when talking about the ionosphere, as it is the lowest region in the ionosphere. It sits at around 60-80 km during the day and disappears during night.
- This version adds 15 positive and 21 negative ions, making it so that below 75 km, electrons are no longer the main negative charge carrier.
- Might also mention the eXtended versions while we're at it.

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  - MA (Middle atmosphere)
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    - Reduced set of tropospheric reactions
  - MAD (Middle atmosphere with D region ion chemistry)

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  - MAD (Middle atmosphere with D region ion chemistry)
    - Adds 15 positive and 21 negative ions
    - Thus, below 75 km electrons are no longer the main negative charge carrier
- Additional thermosphere eXtension (WACCM-X)

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# CHEMISTRY IN TSMLT

MAM4 (*Modal Aerosol Model*), also used in CAM6, but WACCM6 adds chemistry.

- Includes the chemical families  $O_x$ ,  $NO_x$ ,  $HO_x$ ,  $ClO_x$  and  $BrO_x$ , as well as  $CH_4$
- Allows growth of sulfate aerosols, so the prognostic stratospheric aerosols can increase in width
- Maximum altitude of 20 km for eruptions outputting more than 3.5 Tg  $SO_2$

MOZART (*Model for OZone And Related chemical Tracers*)

- The chemical mechanism in CESM2, available from WACCM6, but also CAM-chem
- See table 2<sup>2</sup> for a complete list of chemical reactions included in CESM2 when run with the TSMLT (troposphere, stratosphere, mesosphere, lower thermosphere) configuration.

<sup>2</sup>[https://agupubs.onlinelibrary.wiley.com/action/downloadSupplement?doi=10.1029%2F2019MS001882&file=jame21103-sup-0003-2019MS001882+Table\\_SI-S02.pdf](https://agupubs.onlinelibrary.wiley.com/action/downloadSupplement?doi=10.1029%2F2019MS001882&file=jame21103-sup-0003-2019MS001882+Table_SI-S02.pdf)

- In charge of chemistry we find MAM and MOZART, not to be confused with MOSART (MOdel for Scale Adaptive River Transport).
- MAM includes the chemical families  $O_x$ ,  $NO_x$ ,  $HO_x$ ,  $ClO_x$  and  $BrO_x$ , as well as  $CH_4$ .
- Also included are prognostic stratospheric aerosols. MAM4 was updated to allow for growth of sulfate aerosols into the coarse, or larger size, mode. This is important to represent aerosol sources (including volcanic emissions).
- The  $SO_2$  emissions from volcanic eruptions are derived from Volcanic Emissions for Earth System Models, which is based on observations. These observations then has to be accounted for, which is done by placing a maximum altitude on eruptions outputting more than 3.5 Tg  $SO_2$ . (The maximum altitude is to account for aerosol self-lofting due to in situ absorption of longwave radiation in estimating the initial altitude of large volcanic  $SO_2$  clouds.)
- MOZART takes care of the chemical mechanism, and can also be run in CAM-chem. A complete list of chemical reactions can be seen via link.

# LUMPING

- TSMLT has 231 solution species
- Species are lumped together to reduce the computational cost
- Example:  $C_{10}H_{16}$  in MOZART-4 turned into five new lumped species, with APIN, BPIN, LIMON, MYRC and BCARY giving the primary degradation rates.

- With that many reactions, 231 solution species, you have to draw the line at some point, but where?
- Lumping of chemical species is common.
- As an example, take  $C_{10}H_{16}$  which was one lumped species in MOZART-4. This was turned into four monoterpenes and one sesquiterpene, with corresponding expansion of the oxidation scheme. The primary degradation rates were now based on alpha-pinene (APIN), beta-pinene (BPIN), limonene (LIMON), myrcene (MYRC) and beta-caryophyllene (BCARY).



# SOLAR AND GEOMAGNETICS

- Photoionization and heating rates uses parametrization of Solomon and Qian (2005), with input from the  $F_{10.7}$  index
- Ion-pair production rates are prescribed
- Low energy electrons included by the parametrized auroral oval model by Roble and Ridley (1994)
- Input to the model is HP, hemispheric power, related to the  $K_p$  index:

$$HP = \begin{cases} 16.82 \exp(0.32K_p) - 4.86, & K_p \leq 7 \\ 153.13 + 73.4(K_p - 7.0), & K_p > 7 \end{cases}$$

- Since WACCM3, E region ionosphere is represented with a chemistry consisting of  $O^+$ ,  $O_2^+$ ,  $N^+$ ,  $N_2^+$ ,  $NO^+$

- Photoionization and heating rates at wavelengths shorter than Lyman- $\alpha$ , WACCM6 uses the parametrization of Solomon and Qian. This uses the  $F_{10.7}$  index as input.
- Ion-pair production rates by galactic cosmic rays, solar protons, and medium-energy electrons are prescribed
- For lower-energy electrons that precipitate in the auroral regions, WACCM6 use the parametrized auroral oval model by Roble and Ridley (1994) (implementation described in Marsh et al. (2007)). This model takes as input the power input to the atmosphere from energetic particle bombardment integrated over either the Northern or Southern Hemisphere, known as the Hemispheric Power in gigawatts.
- $HP$  is assumed to be related to the  $K_p$  index only, show here, formulation by Zhang and Paxton. If one wish to simulate for example solar storms, higher frequency forcing files can also be used.



F. D'Andrea et al. "Northern Hemisphere atmospheric blocking as simulated by 15 atmospheric general circulation models in the period 1979–1988". In: *Climate Dynamics* 14.6 (May 1998), pp. 385–407. ISSN: 1432-0894. DOI: [10.1007/s003820050230](https://doi.org/10.1007/s003820050230). URL: <https://doi.org/10.1007/s003820050230>.



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Daniel R. Marsh et al. "Modeling the whole atmosphere response to solar cycle changes in radiative and geomagnetic forcing". In: *Journal of Geophysical Research: Atmospheres* 112.D23 (2007). DOI: <https://doi.org/10.1029/2006JD008306>. eprint: <https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1029/2006JD008306>. URL: <https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2006JD008306>.



Michael J. Mills et al. "Global volcanic aerosol properties derived from emissions, 1990–2014, using CESM1(WACCM)". In: *Journal of Geophysical Research: Atmospheres* 121.5 (2016), pp. 2332–2348. DOI: <https://doi.org/10.1002/2015JD024290>. eprint: <https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1002/2015JD024290>. URL: <https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1002/2015JD024290>.



Michael J. Mills et al. “Radiative and Chemical Response to Interactive Stratospheric Sulfate Aerosols in Fully Coupled CESM1(WACCM)”. In: *Journal of Geophysical Research: Atmospheres* 122.23 (2017), pp. 13, 061–13, 078. DOI: <https://doi.org/10.1002/2017JD027006>. eprint: <https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1002/2017JD027006>. URL: <https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1002/2017JD027006>.



R. G. Roble and E. C. Ridley. “A thermosphere-ionosphere-mesosphere-electrodynamics general circulation model (time-GCM): Equinox solar cycle minimum simulations (30–500 km)”. In: *Geophysical Research Letters* 21.6 (1994), pp. 417–420. DOI: <https://doi.org/10.1029/93GL03391>. eprint: <https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1029/93GL03391>. URL: <https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/93GL03391>.



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