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The role of E90 and ST80_25 in understanding the tropopause and their implementation in E3SM

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Outline

The intangible yet important tropopause

Earlier implementations of the E90 and ST80_25 tracers

Implementation within E3SM

Validation of implementation

Next steps and application

The intangible yet important tropopause

The tropopause is the border between the troposphere (temperature decreases with height, thus strong vertical mixing) and stratosphere (temperature increases with height, thus weak vertical mixing). Air parcels from the troposphere and stratosphere are significantly different in composition (e.g. water vapor is very scarce in the stratosphere) and many models handle tropospheric and stratospheric air parcels in different ways. It is therefore important to have a clear idea of exactly which type any given air parcel may be.

Diagram from Seinfeld and Pandis textbook.

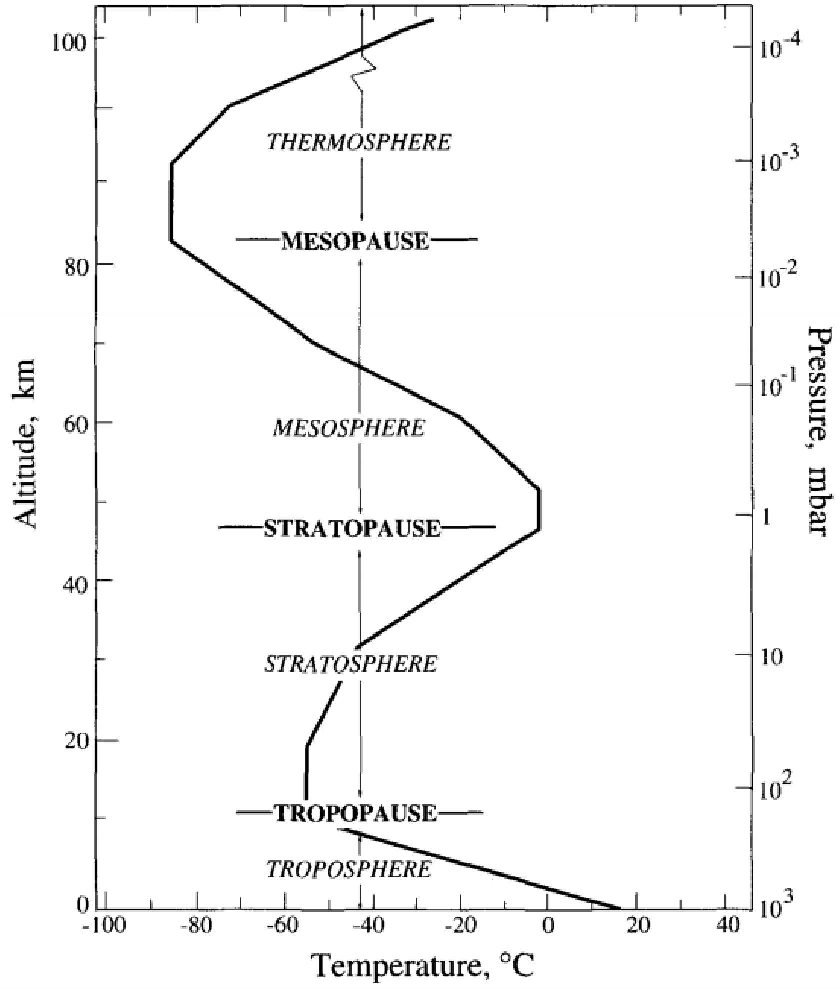


FIGURE 1.1 Layers of the atmosphere.

about 217 K (−56°C). The troposphere can be divided into the *planetary boundary laye*

What is a passive tracer?

To address this issue, we employ passive tracers. A passive tracer is handled just like any other species within the model, but does not react with any other species. It may have no reactions at all, or only have a decay reaction (react with itself to produce nothing). Effectively, they serve as flags or markers, allowing us to track air parcels within the model simply by looking at the concentration of the tracers.

The first passive tracer we employ is E90. It is emitted evenly at the Earth's surface (regardless of land or ocean) and has an e-folding time of 90 days. This serves as a useful tool for looking at tropospheric air parcels, even if they enter the stratosphere.

The second passive tracer is ST80_25. It has a specified, fixed concentration above 80 hPa altitude and an e-folding time of 25 days. As 80hPa is generally above the tropopause, this tracer is used for following stratospheric air parcels.

Both tracers have a molecular weight of 28 (like CO).

Previous implementations

E90 is first mentioned in Prather et al. (2011), which primarily dealt with finding the tropopause to improve the UC Irvine model. Citing Prather et al. (2001), where they found that the tropopause contained 80% of the atmosphere's mass as a rule of thumb, they found that the portion of the atmosphere where E90 concentration was greater than 90 ppb coincided well with the above assumption. Therefore the layer of air where E90 concentration was 90 ppb was assumed to be the tropopause within the UC Irvine model. The concentration of ozone at the tropopause was then compared with observations from 23 ozone sonde sites at the corresponding altitude – generally agreed well with a few exceptions

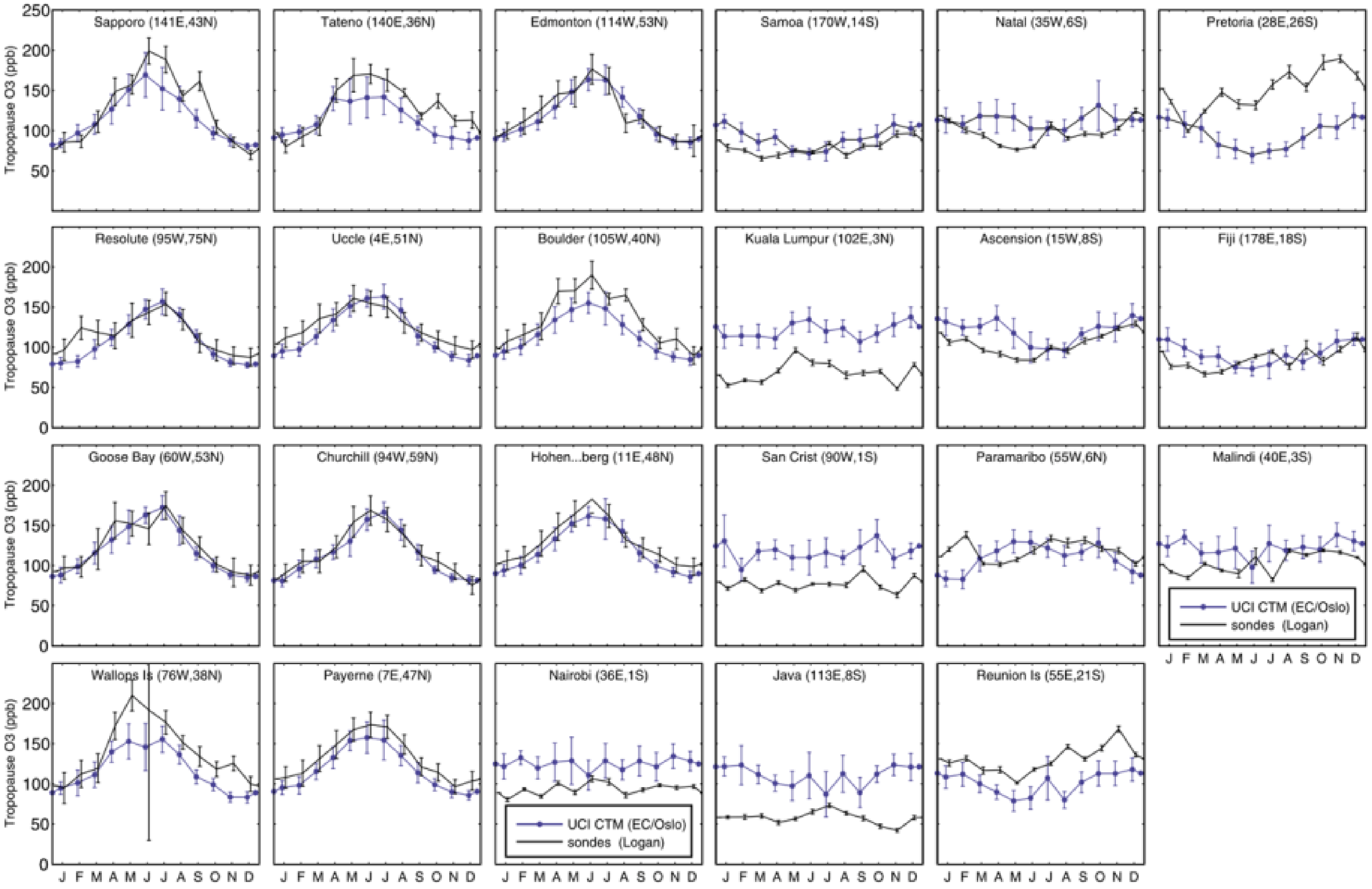


Figure 2. Monthly mean O_3 abundance (ppb) at the tropopause for the 23 sonde sites. See Figure 1. Both observations (black) and model (blue) shown with standard deviations as whiskers.

Previous implementations

E90 and ST80_25 are used by Abalos et al. (2017) and Abalos et al. (2020) to track the height of the tropopause and troposphere-stratosphere exchange over long periods of time

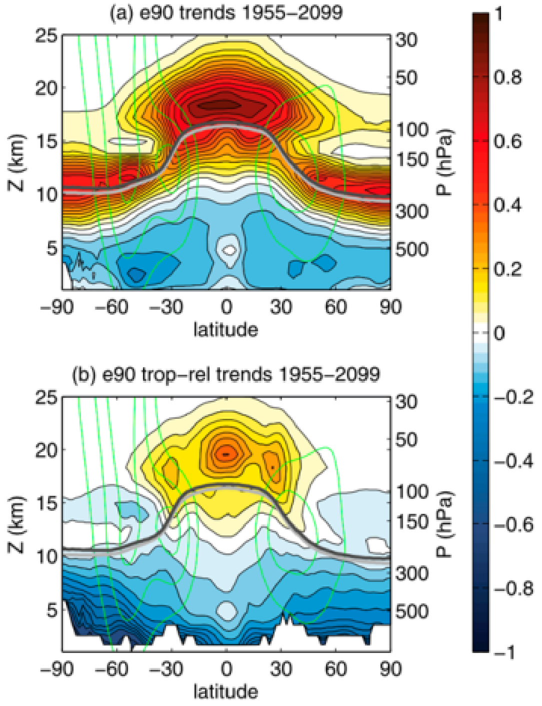


FIG. 8. Annual-mean trends in e90 (ppbv decade^{-1}) using (a) log-pressure altitude and (b) tropopause-relative log-pressure altitude as the vertical coordinate. The gray lines indicate the altitude of the tropopause for the past (light gray) and the future (dark gray), using the first and last 10 years of the simulation, respectively. Note that the tropopause-relative trends have been remapped onto pressure coordinates using the climatological mean tropopause altitude.

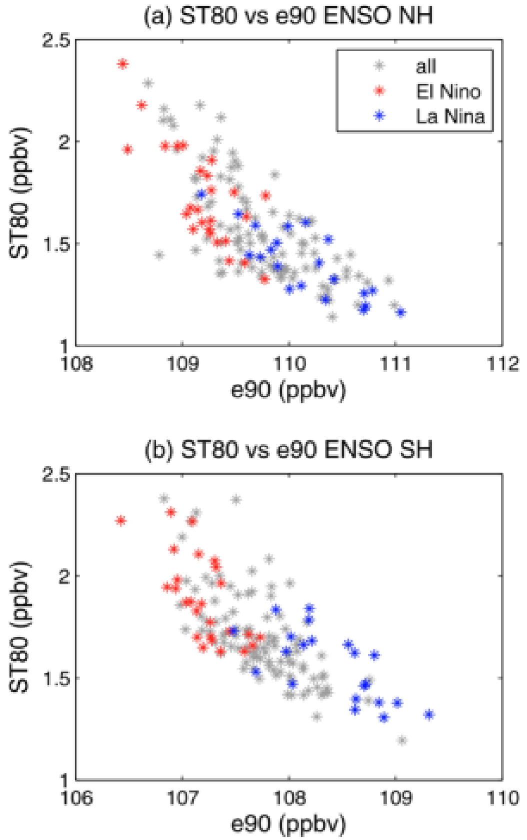


FIG. 7. Tracer–tracer correlation plot (ppbv) of annual-average ST80 vs e90 over 1955–2099, with warm and cold ENSO events indicated. The points correspond to the concentrations averaged over 500–200 hPa and 20°–30° latitude in the (a) NH and (b) SH.

Implementation within E3SM

Fortunately, these tracers are already implemented in CESM, which E3SM split off from less than a decade ago. The two models are fairly similar, and I could use the grep command to find all mention of the tracers in CESM

E3SM utilizes a chemistry preprocessor. It is essentially a list of all the chemical species that participate in calculations, what sort of approximation is made in solving their differential equations, and the chemical reactions they participate in.

Any changes made to the chemistry preprocessor are automatically converted to source code changes if the user uses a special command to swap in the new file.

There are minor additional steps to add an option to input E90 emissions files, and specify a fixed concentration for ST80_25 above 80hPa – again, just copy from CESM.

Input file

```
BEGSIM

  Preprocessor Specs

  Comments
  End Comments

  SPECIES
  End SPECIES

  Solution Classes
  End Solution Classes

  CHEMISTRY
  END CHEMISTRY

  SIMULATION PARAMETERS
  END SIMULATION PARAMETERS

ENDSIM
```

```
*AH -- added E90 and ST80
      Solution
 E90 -> CO
 ST80_25 -> CO
 O3
 H2O2, H2SO4, SO2, DMS -> CH3SCH3, SOAG -> C
```

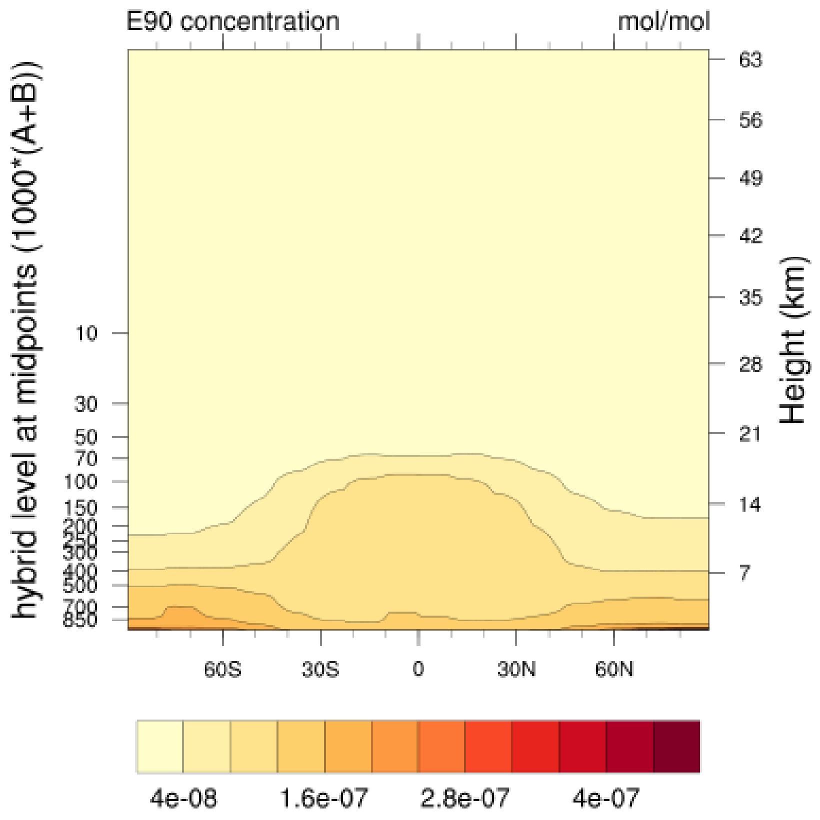
```
*AH -- Added both tracers
   Solution Classes
      Explicit
        O3
        ST80_25
        E90
      End Explicit
```

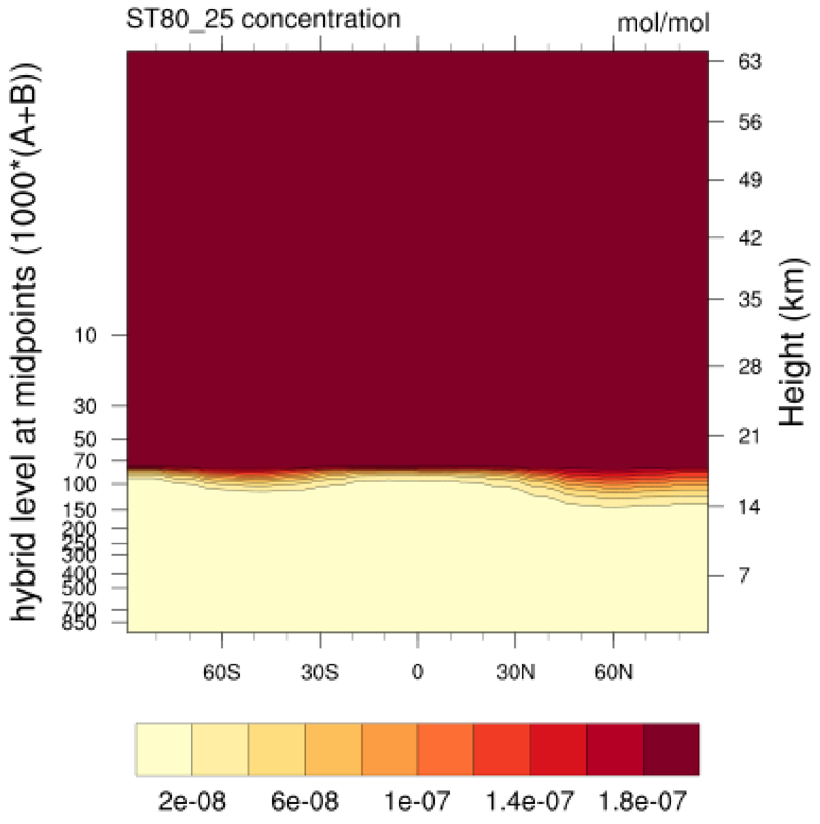
```
[E90_tau]     E90 -> sink                                              ; 1.29e-07
[ST80_25_tau]          ST80_25  ->                                      ; 4.63e-07
```

Validation and next steps

- Check whether or not any other species were influenced. Run the same model under the same settings with and without the tracers, subtract the concentration fields for other species – all zeroes, as intended
- Check whether the decay rate is working correctly – run the model with the tracers turned on for a certain period of time, then shut off E90 emissions and remove all ST80_25 above 80hPa and continue the run. Integrate all tracer concentrations within the atmosphere and check whether the curve is correct
- Run the model until it reaches a stable state – tracer spatial distribution should be roughly similar (i.e. within an order of magnitude at least) to CESM run under the same conditions
- If the above works correctly, run the model with tracers implemented in the context of the Pinatubo eruption – maybe compare it against a control run with the eruption removed

E90 and ST80_25 contour plots





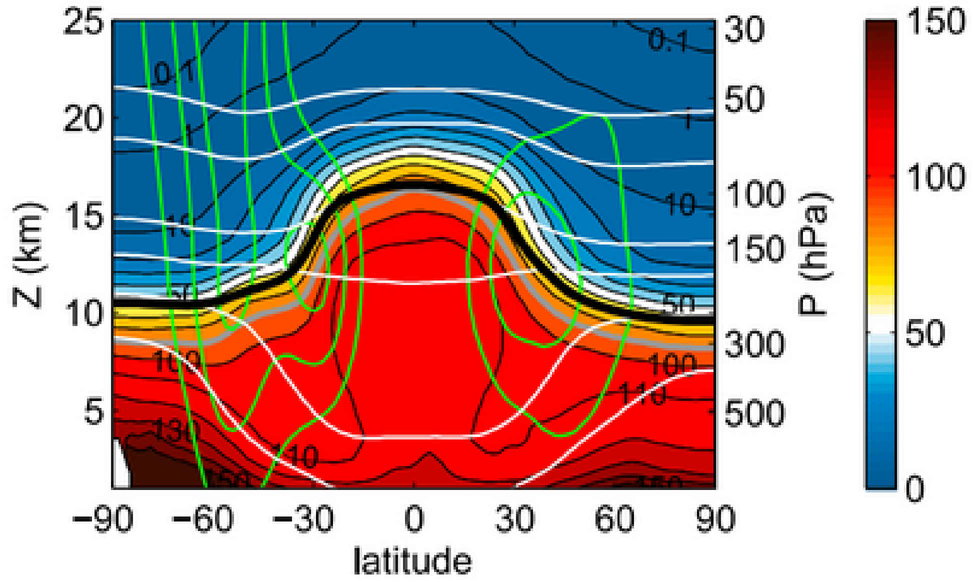


FIG. 1. Climatology of e90 concentrations (shading; ppbv) for the annual mean in the REF-C2 WACCM run as a function of latitude and log-pressure altitude $Z = -H \ln(p/p_0)$ with $H = 7$ km and $p_0 = 1000$ hPa. The 90-ppbv contour is shown in gray. The thick black contour shows the lapse-rate tropopause. The green contours show the zonal-mean wind ($10\,\mathrm{m\,s^{-1}}$ spacing; zero omitted), and the white contours show selected isentropes (300, 320, 350, 380, 450, and 500 K).

References

Seinfeld, J., & Pandis, S. (2008). Atmospheric chemistry and physics. 1997. *New York*.

Prather, M. J., Zhu, X., Tang, Q., Hsu, J., & Neu, J. L. (2011). An atmospheric chemist in search of the tropopause. *Journal of Geophysical Research: Atmospheres*, *116*(D4).

Abalos, M., Randel, W. J., Kinnison, D. E., & Garcia, R. R. (2017). Using the artificial tracer e90 to examine present and future UTLS tracer transport in WACCM. *Journal of the Atmospheric Sciences*, *74*(10), 3383-3403.

Abalos, M., Orbe, C., Kinnison, D. E., Plummer, D., Oman, L. D., Jöckel, P., ... & Dameris, M. (2020). Future trends in stratosphere-to-troposphere transport in CCMI models. *Atmospheric Chemistry and Physics*, *20*(11), 6883-6901.

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Thanks for listening!

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