Simulating Particle Transport and Diffusion

Sakura Takahashi, Hongwei Sun[1]

[1] Dr. Hongwei Sun is a Tenure-Track Assistant Professor in Atmospheric Sciences at the University of Hawaii at Manoa

Introduction

Stratospheric transport and turbulence play a critical role in regulating the distribution of trace gases and aerosols, influencing ozone chemistry, Earth's radiative balance, and stratosphere-troposphere coupling. These processes also affect weather and climate predictability, yet they remain a major source of uncertainty in atmospheric models. Recent observations further suggest strong links between stratospheric dynamics, extreme weather events, and climate change. Accurately representing small-scale mixing in the stratosphere is particularly challenging for traditional Eulerian computational fluid dynamics (CFD) approaches due to resolution limits and simplifying assumptions.

Methods

Meteorological Data & Model

ERA5 reanalysis data (ECMWF) at 6-hourly temporal resolution and ∼31 km horizontal resolution were used to drive the LAGRANTO Lagrangian trajectory model (Sprenger & Wernli, 2015). ERA5 provides the large-scale resolved wind field used to advect air parcels. Simulations were performed on the Bridges2 HPC cluster.

Observational Data

Vertical ozone (O_3) profiles were obtained from B2SAP balloon soundings at Hilo, Hawai'i (19.72°N, 155.05°W) on Nov. 4, 2019. These profiles serve as the observational benchmark for model validation.

Trajectory Setup

A total of 74 parcels were initialized along the observed vertical profile at each measured pressure level and advected forward for 10 days using ERA5 winds. To represent unresolved small-scale vertical mixing, a stochastic vertical displacement was applied at each timestep:

$$\delta X = \mathbf{V}(X,t)\delta t + \delta\eta(t)\mathbf{k}$$

where $\mathbf{V}(X,t)$ is the resolved wind, $\mathbf{k}$ is the vertical unit vector, and $\delta\eta(t) \sim \mathcal{N}(0, 2D_v\delta t)$ (Legras et al., 2003). This formulation models vertical diffusion as a random walk process superimposed on resolved advection.

- Diffusivity values tested: $D_v = 0.01,\ 0.02,\ 0.03,\ 0.05,\ 0.07,\ 0.09,\ 0.1,\ 0.15,\ 0.2,\ 0.3,\ 0.5,\ 1.0\ \mathrm{m^2/s}$

Ozone Reconstruction & Comparison

O_3 was treated as a tracer over the 10-day simulation period. At trajectory endpoints, ozone mixing ratios were sampled from GEOS-CF 3D chemistry model output using spatial interpolation. Ensemble-mean vertical profiles were reconstructed by averaging parcel concentrations within pressure bins.

Parcels that descended below 200 hPa were excluded from analysis, as ozone conservation does not hold across the tropopause. Of the 74 initialized parcels, 66-69 remained in the stratosphere across ensemble members and were used for comparison.

Model performance was evaluated using root mean square error (RMSE) between simulated and observed ozone profiles. RMSE was computed for each ensemble member and averaged across members, with standard error reported.

The optimal diffusivity D_v is identified as the value that minimizes RMSE and maximizes agreement with observations.

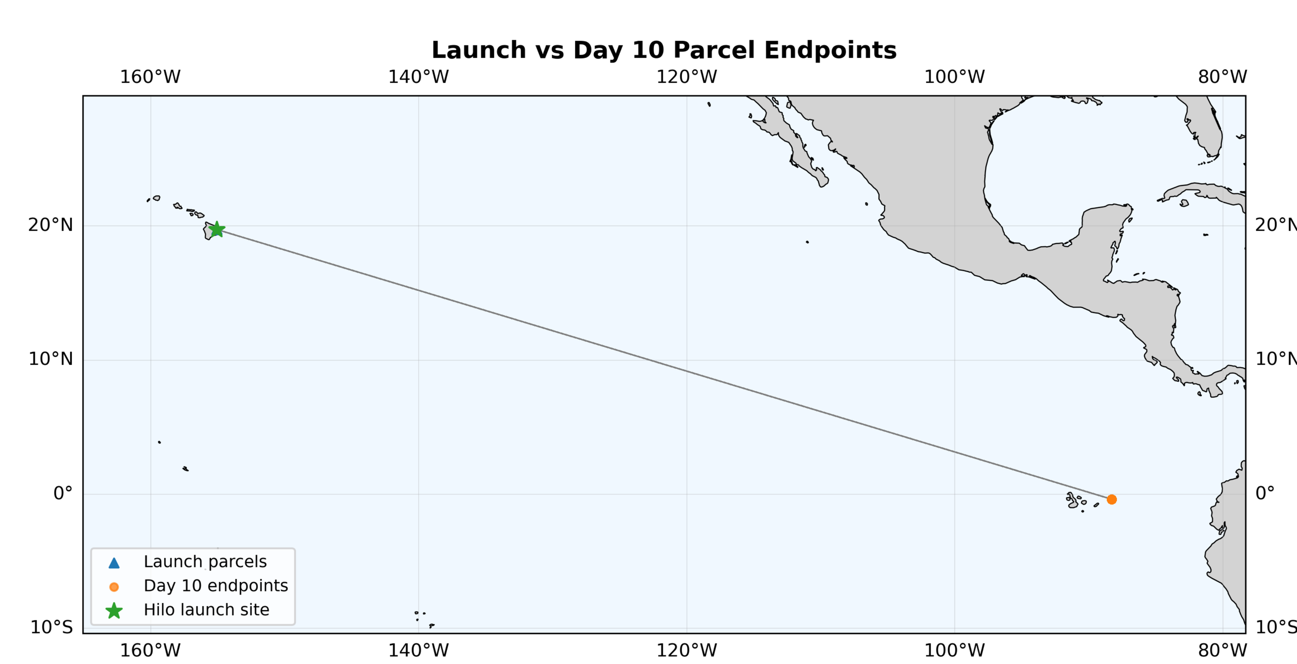
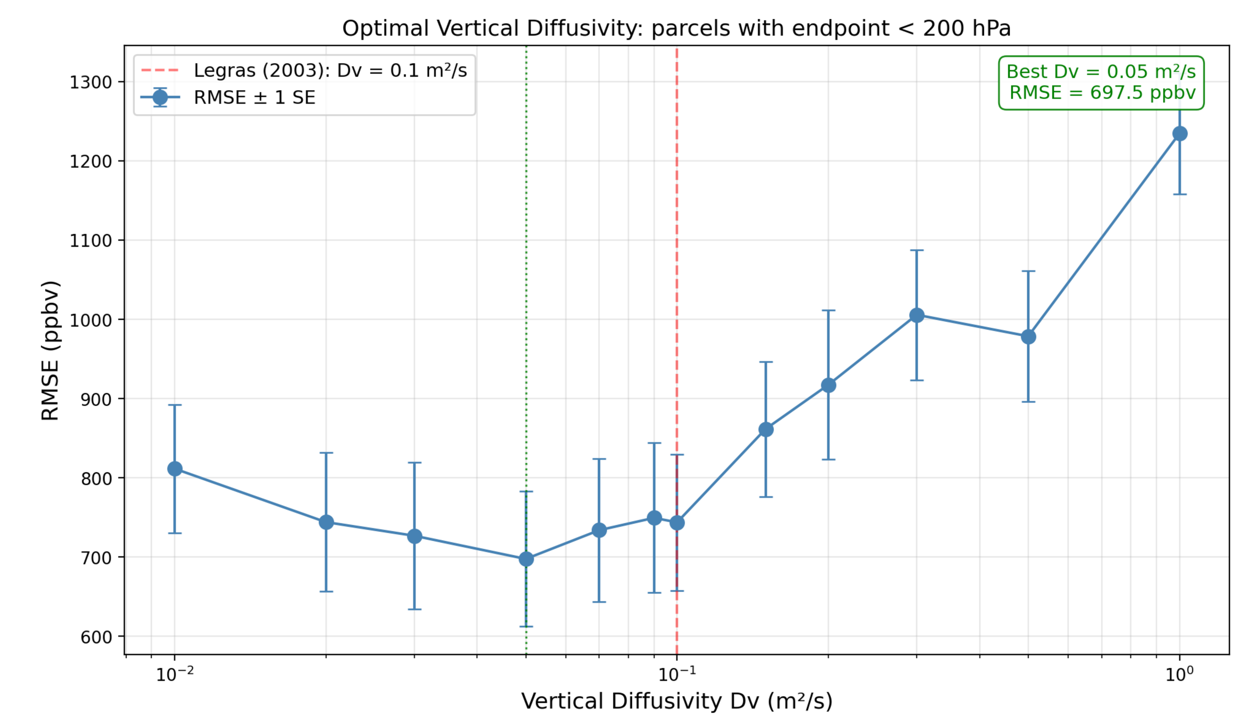


Figure 1. Simulated parcel distribution for $D_v = 1.0\ \mathrm{m^2/s}$ (Nov. 4, 2019).

Results

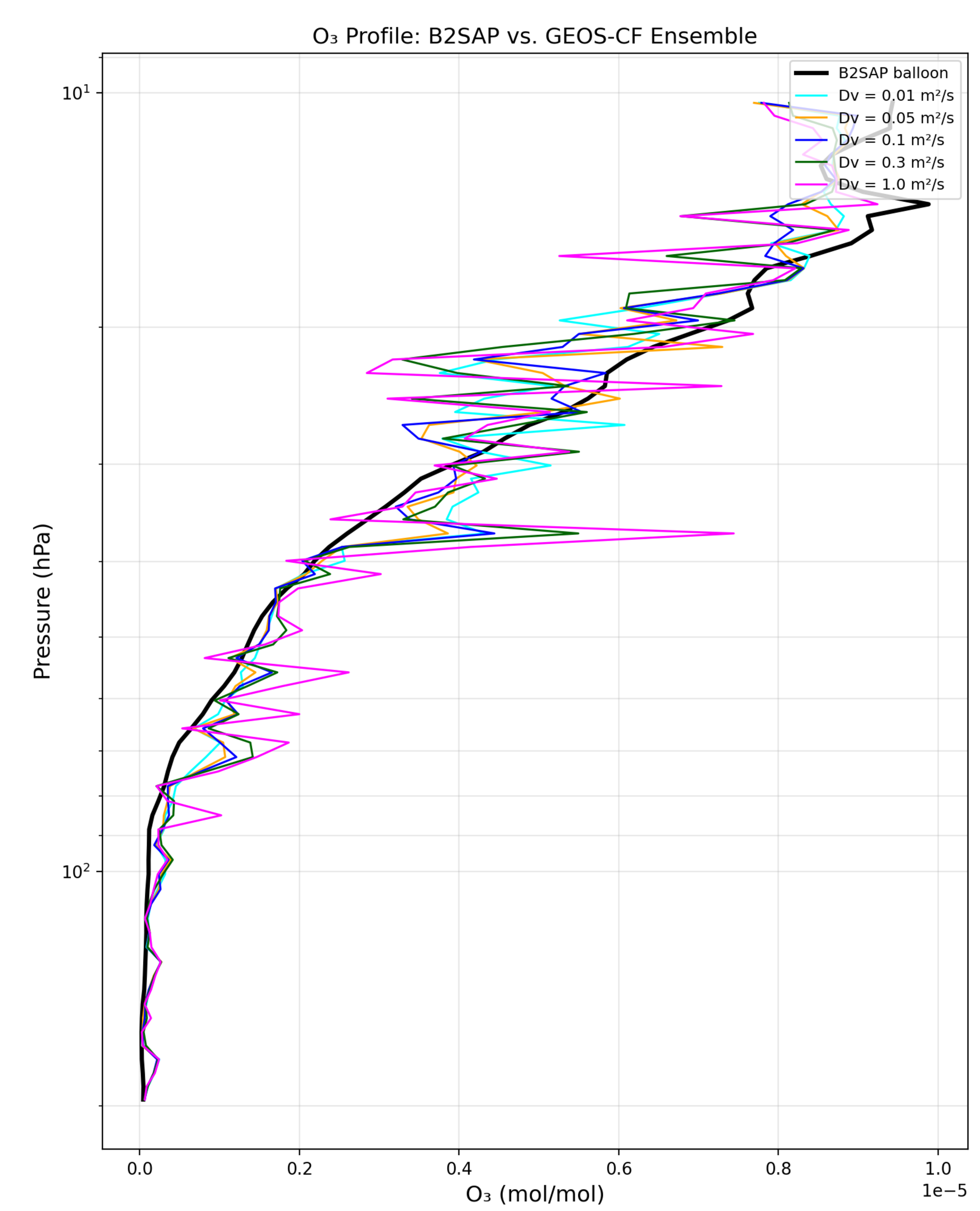
Optimal Vertical Diffusivity



RMSE vs. vertical diffusivity. Minimum at $D_v = 0.05\ \mathrm{m^2/s}$.

- Parcels below 200 hPa were excluded, leaving 66–69 of 74 parcels
- Best-fit diffusivity: $\mathbf{D_v = 0.05\ m^2/s}$ (RMSE ≈ 700 ppbv)
- Similar range: 0.03–$0.1\ \mathrm{m^2/s}$
- RMSE increases sharply for $D_v > 0.1$

Ozone Profile Comparison



Ensemble mean O_3 profiles vs. B2SAP balloon observations.

- Low D_v $(0.01$–$0.1)$ reproduces observed vertical structure across ∼10–200 hPa
- High diffusivity ($D_v = 1.0$) smooths gradients, especially at 50–150 hPa

Results Continued

Model Validation (Best D_v)

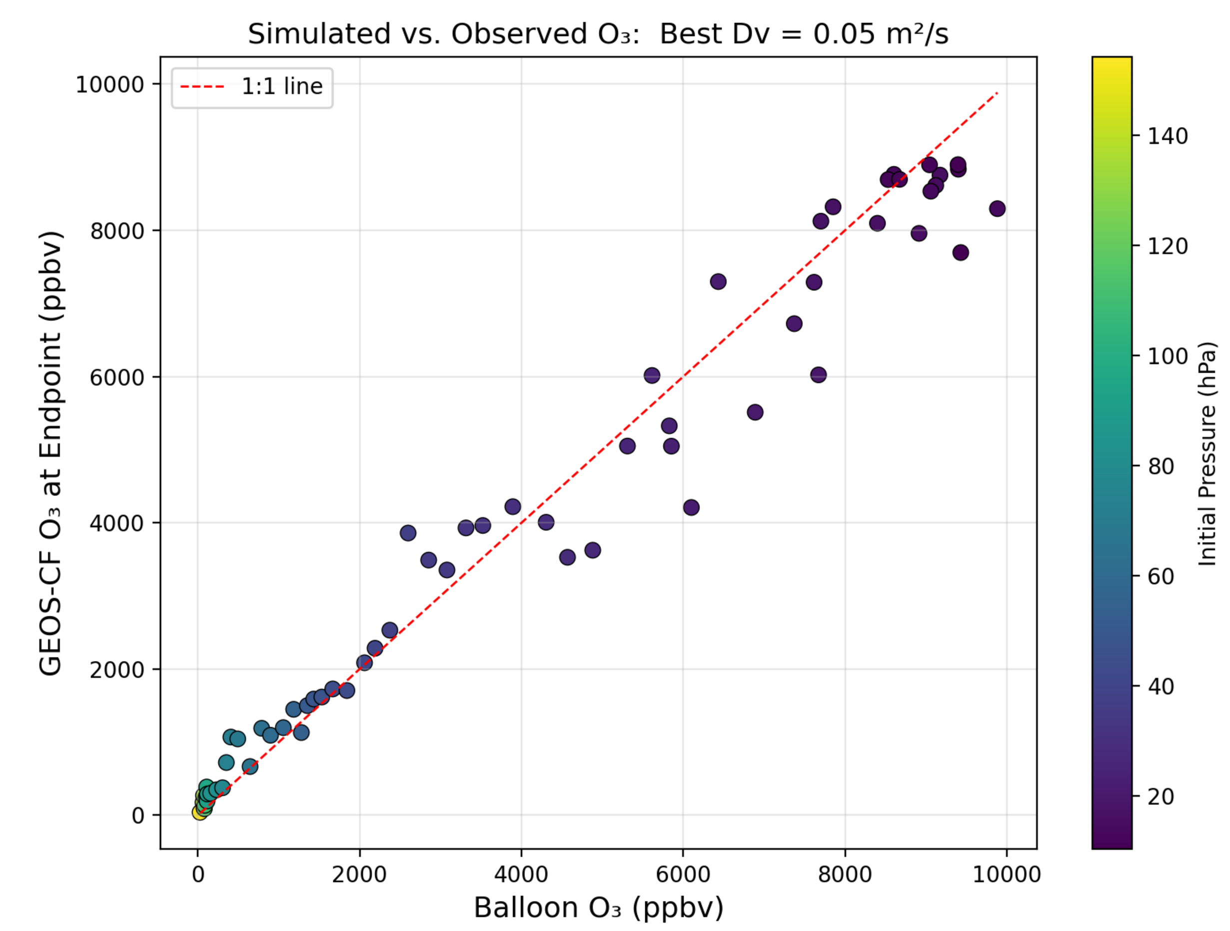


Figure 4. Simulated vs. observed ozone at $D_v = 0.05\ \mathrm{m^2/s}$.

- Strong agreement along the 1 to 1 line
- Largest scatter at high ozone values

Discussion & Future Work

- The optimal diffusivity $\mathbf{D_v = 0.05}\ \mathrm{m^2/s}$ is consistent with the $\sim 0.1\ \mathrm{m^2/s}$ value reported by Legras et al. (2003), representing agreement between two methods?
- Future work will extend this analysis to the Aug. 21, 2019 B2SAP for more comparisons
- A maximum likelihood framework could refine the diffusivity estimate by replacing RMSE with a probabilistic metric that accounts for ensemble spread.

References

[1] Bernard Legras, B. Joseph, and François Lefèvre.
Vertical diffusivity in the lower stratosphere from lagrangian back-trajectory reconstructions of ozone profiles.
Journal of Geophysical Research: Atmospheres, 108(D18):ACL 1–ACL 13, 2003.

[2] Michael Sprenger and Heini Wernli.
The lagranto lagrangian analysis tool – version 2.0.
Geoscientific Model Development, 8(8):2569–2586, 2015.

[3] Hongwei Sun, Sylvain Bourguet, Sebastian Eastham, and David Keith.
Optimizing injection locations relaxes altitude-lifetime trade-off for stratospheric aerosol injection.
Geophysical Research Letters, 50(16):e2023GL105371, 2023.

[4] Hongwei Sun, Sylvain Bourguet, Luan Luan, and David Keith.
Stratospheric transport and tropospheric sink of solar geoengineering aerosol: A lagrangian analysis.
npj Climate and Atmospheric Science, 7:115, 2024.

[5] Hongwei Sun, Sebastian Eastham, and David Keith.
Developing a plume-in-grid model for plume evolution in the stratosphere.
Journal of Advances in Modeling Earth Systems, 14(4):e2021MS002816, 2022.