Development of the Tangent Linear and Adjoint Models of the Global Online Chemical Transport Model MPAS-CO2

CMS Feng-2020

Tao Zheng [1] Sha Feng [2] Jeffery Stewart [3] Xiaoxu Tian [3] David Baker [4] Martin Baxter [1]

[1]Central Michigan University [2]Pacific Northwest National Laboratory [3]Tomorrow.io [4]Colorado State University

Background

Major gaps and challenges identified in the NASA CMS Phase 2 report include (1) The availability of high-resolution, low-latency global flux and emissions datasets remains an unmet need, and (2) Atmospheric transport remains a sizeable source of uncertainty for inverse estimates at both regional and global scales. The dense spatial and temporal coverage provided by the wide range of atmospheric CO_2 measurements makes it possible to provide flux estimates at higher resolution and multiple scales in order to better support the Global Stocktake.

Objectives

One of the objectives of the project (CMS Feng-2020) is to develop an advanced CO_2 data assimilation system based on an online Eulerian transport model to enable high-resolution flux estimation with improved accuracy and uncertainty quantification. To accomplish this objective, we have successfully developed and evaluated the global online transport model MPAS-CO_2 based on the variable-resolution non-hydrostatic Model for Predictions Across Scales-Atmosphere (MPAS-A). To implement a variational data assimilation system, we have developed the Tangent Linear (TL) and adjoint model of the transport model MPAS-CO_2.

MPAS-CO_2 transport model

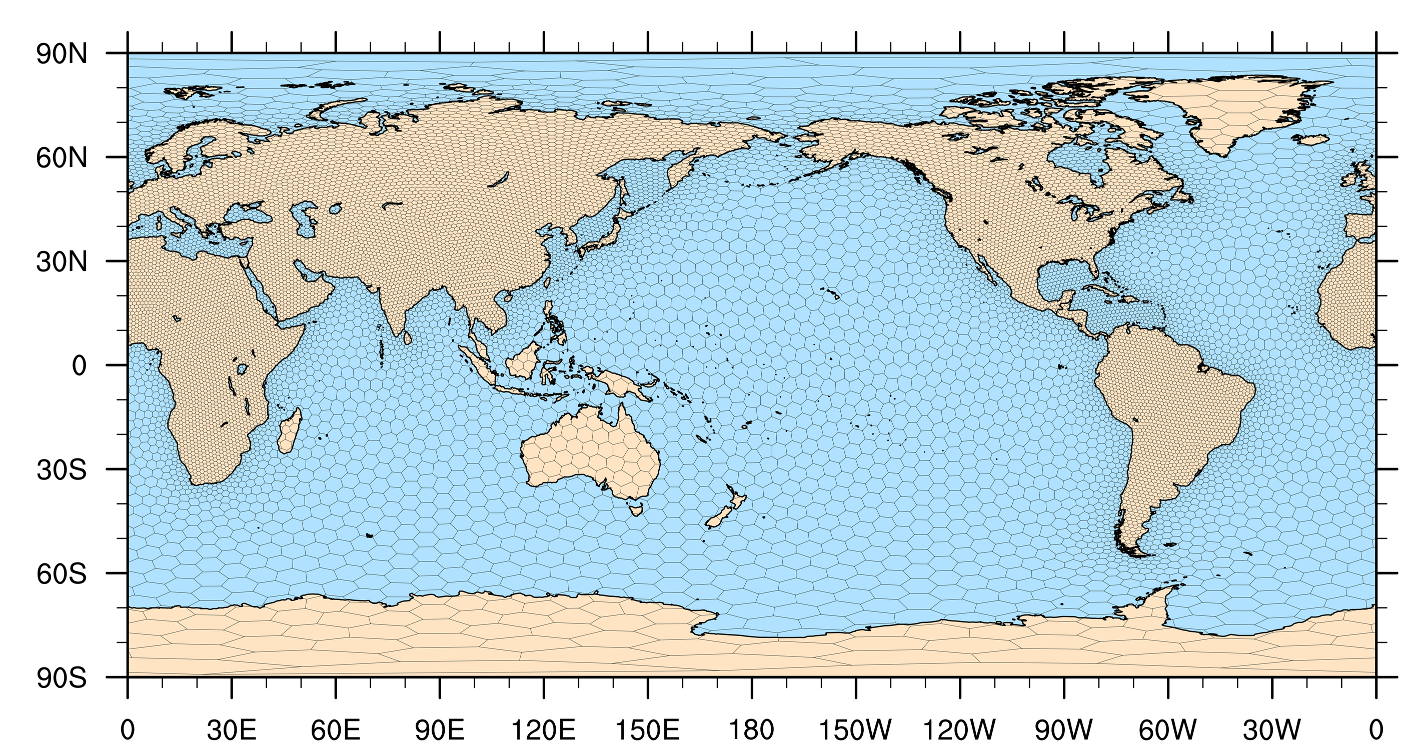


Figure 1. An MPAS-CO2 global variable resolution mesh ranging from 120km over most land regions to 480km over oceans

MPAS-CO_2 transport model (Zheng et al. 2021) is an online transport model with variable-resolution capability (Fig. 1). The transport of CO_2 is characterized by the continuity equation:

$$\frac{\partial(\tilde{\rho}\, q_{co_2})}{\partial t} = -(\nabla \cdot \tilde{\rho}\, q_{co_2} \mathbf{V})_\zeta + F_{bl} + F_{cu} \tag{1}$$

where q_{co_2} is CO_2 dry air mixing ratio, $\tilde{\rho} = \rho_d/(\partial\zeta/\partial z)$, ρ_d is the dry air density, ζ is the vertical coordinate, z is geometric height, t is time, $\mathbf{V} = (u, v, w)$ is the velocity vector, and F_{bl} and F_{cu} are CO_2 tendency from the boundary layer and convective transport schemes, respectively.

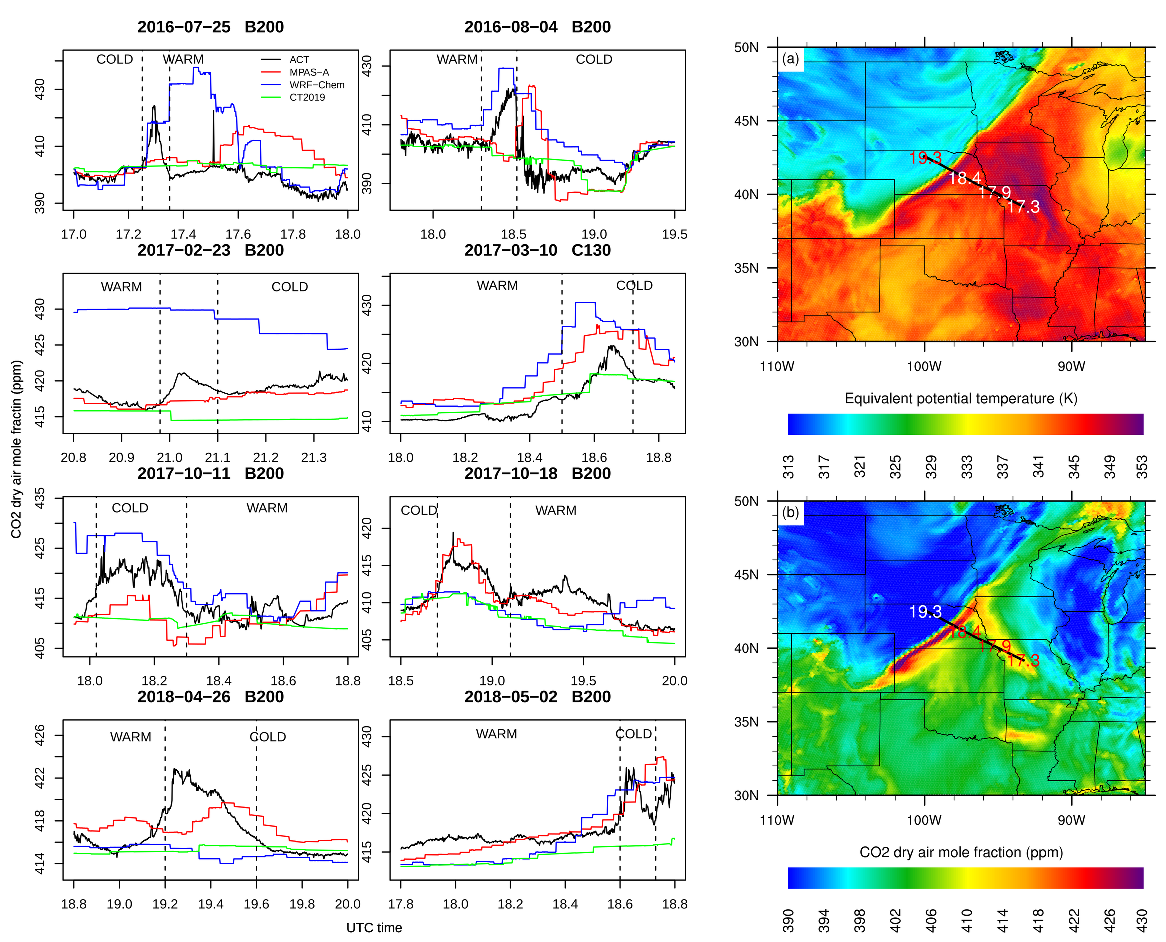


Figure 2. Validation of MPAS-CO2 simulated CO_2 mixing ratio against ACT-America airborne measurements and other model systems (WRF-Chem and Carbon Tracker). The dark line represents a flight track (about 400m above the surface) from ACT.

MPAS-CO_2 has been extensively evaluated using the airborne and near-surface (Fig. 2). The model is capable of achieving a comparable level of accuracy with high-resolution regional model WRF-Chem, CarbonTracker (CT) assimilation system and ECMWF IFS global modeling system. **With its variable-resolution capability and accurate online transport, MPAS-CO_2 serves as an ideal modeling tool for high-resolution carbon flux estimation.**

Development of TL model of MPAS-CO_2

The tangent linear (TL) model of the MPAS-CO_2 forward model can be symbolically expressed as the first derivative of the forward model:

$$\Delta\mathbf{x}_t = \mathbf{M}(\Delta\mathbf{x}_0, \Delta\mathbf{k}) \tag{2}$$

where $\mathbf{M}(\,)$ represents the MPAS-CO_2 TL model, $\Delta\mathbf{x}_0$ and $\Delta\mathbf{x}_t$ are the TL variable of CO_2 mixing ratio at the initial and forecast time, respectively, and $\Delta\mathbf{k}$ is the TL variable of the flux scaling factor $\mathbf{k}$. Eq. (2) shows that the TL model computes the perturbation in the forecast time CO_2 mixing ratio ($\Delta\mathbf{x}_t$), given the perturbation in the flux scaling factor ($\Delta\mathbf{k}$) and/or perturbation in the initial time CO_2 mixing ratio ($\Delta\mathbf{x}_0$). The adjoint model code was manually developed to avoid redundancies and improve computational efficiency.

Validation of the TL model

The correctness of the MPAS-CO_2 TL model is verified by checking whether Eq. (3) is satisfied.

$$\Phi(\alpha) = \frac{\parallel \mathcal{M}(\mathbf{x_0}, (1+\alpha)\mathbf{k}) - \mathcal{M}(\mathbf{x_0}, \mathbf{k}) \parallel}{\parallel \mathbf{M}(0,\ \alpha\mathbf{k}) \parallel} = 1 \tag{3}$$

where $\mathbf{M}()$ is the MPAS-CO_2 TL model, $\mathcal{M}()$ is the MPAS-CO_2 forward model, k is the CO_2 flux scaling factor, and α is a scalar.

α	$\parallel \mathcal{M}(\mathbf{x}_0, (1+\alpha)\mathbf{k}) - \mathcal{M}(\mathbf{x}_0, \mathbf{k}) \parallel$	$\parallel \mathbf{M}(0, \alpha\mathbf{k}) \parallel$	ratio
1.0×10^2	$2.07316571683768 \times 10^{-1}$	$2.07316571683768 \times 10^{-1}$	1.0
1.0×10^1	$2.07316571683768 \times 10^{-3}$	$2.07316571683768 \times 10^{-3}$	1.0
1.0	$2.07316571683769 \times 10^{-5}$	$2.07316571683768 \times 10^{-5}$	1.0
1.0×10^{-1}	$2.07316571683765 \times 10^{-7}$	$2.07316571683768 \times 10^{-7}$	0.99999999999998
1.0×10^{-2}	$2.07316571683799 \times 10^{-9}$	$2.07316571683768 \times 10^{-9}$	1.00000000000015

Table 1. Results of the correctness check for the newly-developed MPAS-CO_2 TL. The results are from 1-month integration (from 2018-10-01 00:00 UTC to 2018-11-01 00:00 UTC) of the forward and tangent linear models using the 120-480 km global variable-resolution mesh (Fig. 1). The terms in the table refer to Eq. (3).

Development of adjoint model of MPAS-CO_2

An adjoint model is an essential component of a variational data assimilation system and is very useful for adjoint sensitivity analysis. Symbolically, the MPAS-CO_2 adjoint model can be expressed as:

$$(\Delta\hat{\mathbf{x}}_0, \Delta\hat{\mathbf{k}}) = \mathbf{M}^T(\Delta\hat{\mathbf{x}}_t), \tag{4}$$

where $\mathbf{M}^T(\,)$ is the MPAS-CO_2 adjoint model, $\Delta\hat{\mathbf{k}}$ is the adjoint variable of the flux scaling factor, and $\Delta\hat{\mathbf{x}}_0$ and $\Delta\hat{\mathbf{x}}_t$ are the adjoint variables of CO_2 mixing ratio at the initial and forecast time, respectively. Eq. (4) demonstrates that starting with $\Delta\hat{\mathbf{x}}_t$ at the forecast time, the MPAS-CO_2 adjoint model runs backward in time to the initial time, resulting in the adjoint variable of CO_2 mixing ratio at the initial time ($\Delta\hat{\mathbf{x}}_0$), and the adjoint variable of the flux scaling factor ($\Delta\hat{\mathbf{k}}$).

Validation of MPAS-CO_2 adjoint model

We validated the newly developed MPAS-CO_2 adjoint model using Eq. (5)

$$\langle \Delta\mathbf{x}, \mathbf{M}(0, \Delta\mathbf{k}) \rangle = \langle \mathbf{M}^T(\Delta\mathbf{x}), \Delta\mathbf{k} \rangle \tag{5}$$

where $\langle\ \rangle$ represents the inner product operator, $\Delta\mathbf{x}$ is a perturbation of CO_2 mixing ratio and $\Delta\mathbf{k}$ is a perturbation of CO_2 flux scaling factor.

Integration length	LHS	RHS	(LHS-RHS)/LHS
$\Delta\mathbf{k} = 10^{-1}\mathbf{1}$ and $\Delta\mathbf{x} = \mathbf{M}(0, \Delta\mathbf{k})$			
7-day	$1.436630106778291 \times 10^{-7}$	$1.436630106778298 \times 10^{-7}$	$-5.158974640379662 \times 10^{-15}$
31-day	$2.073165716837682 \times 10^{-7}$	$2.073165716837683 \times 10^{-7}$	$-2.553561385538706 \times 10^{-16}$

Table 2. Results of the correctness check for the newly-developed adjoint model of MPAS-CO_2. The LHS and RHS in the table refer to Eq. (5).

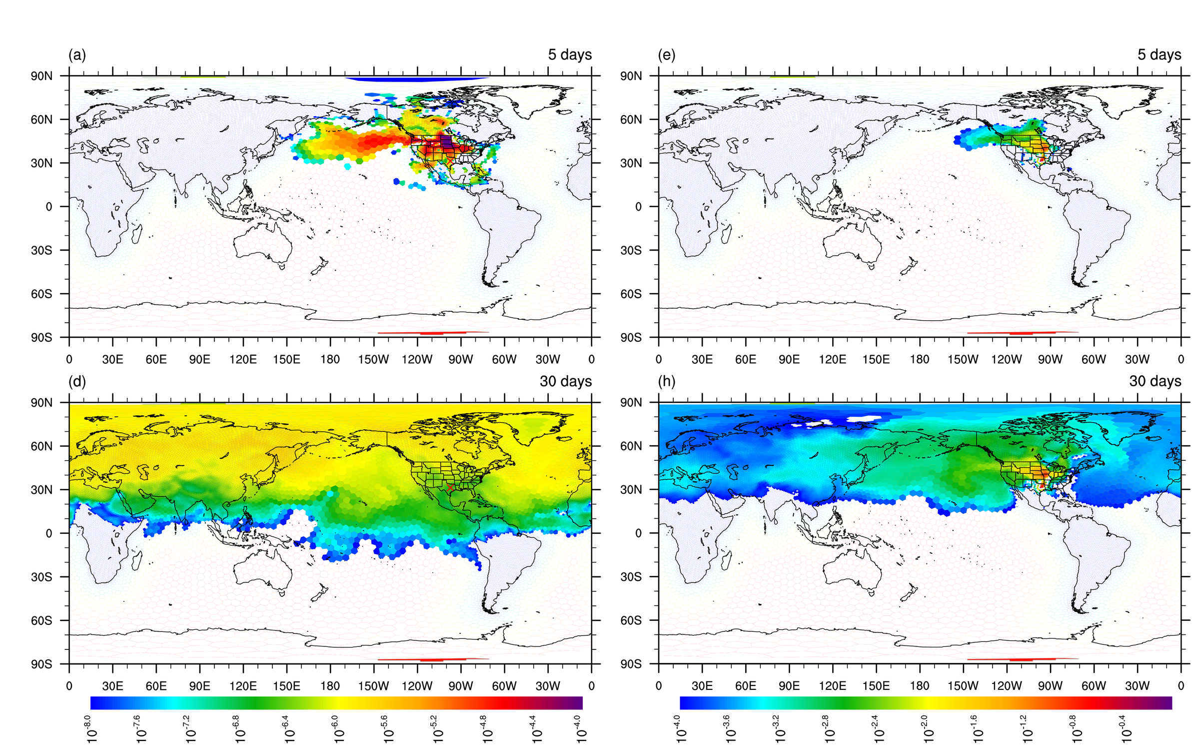


Figure 3. The column average of sensitivity of CO_2 at the WKT tower at 00:00 UTC on March 31, 2018 to CO_2 mixing ratio (units: ppm/ppm, left column) and CO_2 flux scaling factor (footprint, units:ppm/μmol m^{-2} s^{-1}, right column) at 5 and 30 days backward in time.

Computational cost

Model	Resolution (km)	Cost (min)	Time step (second)
Forward Model	120	45	720
	120-480	20	720
TL model	120	48	720
	120-480	22	720
Adjoint Model	120	48	720
	120-480	22	720

Table 3. The computational costs for a 30-day simulation of MPAS-CO_2 at 120km quasi-uniform resolution and at the 120-480km variable-resolution meshes. All simulations are conducted using 128 AMD EPYC 7H12 2.595 GHz processors running in parallel.

Adjoint sensitivity analysis

In addition to being a key component of variational assimilation systems, MPAS-CO_2 adjoint model is a powerful tool for sensitivity analysis. We use the newly developed MPAS-CO_2 adjoint model to calculate the footprints of CO_2 observations from towers and OCO2 X_{CO_2}. We compared MPAS-CO_2 adjoint model calculated footprint with those from the Carbon Tracker-Lagrange (CT-L) footprints (Fig. 4). We found that the two systems yield similar results for the 10-day backward footprints in general although some differences exist. In addition, the CT-L footprints, due to their regional domain limitation, miss a substantial portion of the influence area.

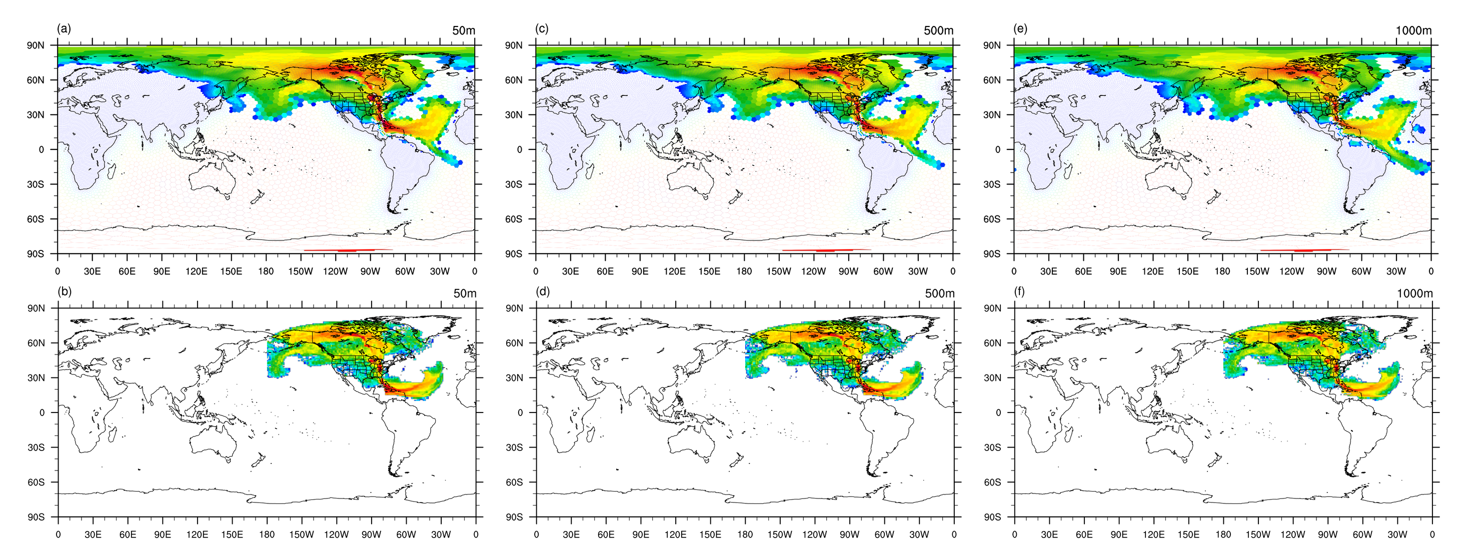
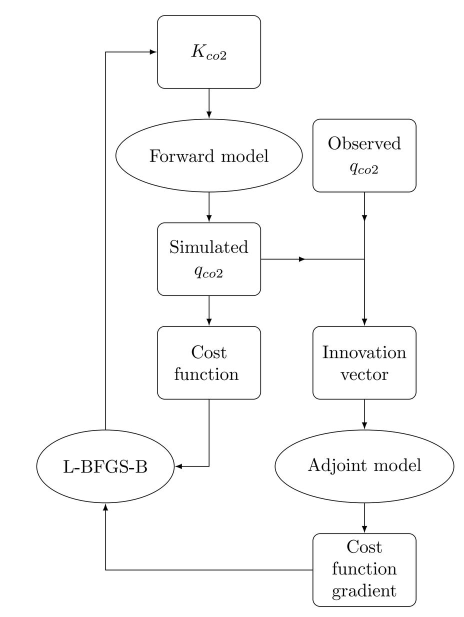


Figure 4. Comparison of OCO-2 footprints calculated by MPAS-CO_2 adjoint model (top panel) and Carbon Tracker-Lagrange (CT-L, bottom panel). All footprints are 10-days backward in time.

The next step: MPAS-CO_2 4D-Variational data assimilation system



We have successfully developed and validated the global online chemical transport model MPAS-CO_2, including its forward (Zheng et al. 2021) and TL and adjoint models (Zheng et al. 2023). Presently we are working on the integration of the forward, TL, and adjoint models into a 4D-Variational data assimilation system MPAS-CO2 4DVar. The 4D-Var data assimilation system is a super structure that includes MPAS-CO_2 forward and adjoint model, observational operators, and their adjoints, and an optimization algorithm. The flowchart to the left is from the WRF-CO_2 4D-Var data assimilation system (Zheng et al. 2018). While WRF-CO_2 4DVar is a regional assimilation system, the MPAS-CO_2 4DVar will be a global assimilation system that does not have the artificial chemical lateral boundary problem of the regional system.

Acknowlegment

This research has been supported by the NASA Carbon Monitoring System (CMS) grant no. 80HQTR21T0069.PI: Sha Feng, PNNL.

References

[Zheng et al.(2021)Zheng, Feng, Davis, Pal, and Morguí] Tao. Zheng, S. Feng, K. J. Davis, S. Pal, and J.A. Morguí. Development and evaluation of co_2 transport in mpas-a v6.3. *Geoscientific Model Development*, 14(5):3037–3066, 2021. doi: 10.5194/gmd-14-3037-2021.

[Zheng et al.(2023)Zheng, Feng, Stewart, Tian, and Baxter] Tao. Zheng, S. Feng, J. Stewart, X. Tian, and M. Baxter. Development of the tangent linear and adjoint models of the global online chemical transport model mpas-co2 v7.3. *Under Review at Geoscientific Model Development*, 2023.

[Zheng et al.(2018)Zheng, French, and Baxter] Tao Zheng, Nancy H. F. French, and Martin Baxter. Development of the WRF-CO_2 4D-Var assimilation system v1.0. *Geoscientific Model Development*, 11(5):1725–1752, MAY 4 2018. doi: 10.5194/gmd-11-1725-2018.