Simulations of the stable isotope composition (ratio of HDO or $\text{H}_2^{18}\text{O}$ to $\text{H}_2\text{O}$) of water reservoirs and fluxes in climate models can be used to help diagnose which aspects of the model hydrologic cycle and clouds are accurately represented, and which are not. Early global isotope models used bulk exchange schemes to represent the isotopic changes during condensation and evaporation, which was of a similar level of complexity to the underlying cloud parameterizations (e.g., Noone and Simmonds, 2002). With the advent of more elaborate cloud schemes and the inclusion of multiple water phases, a new strategy for simulating isotopes that is of comparable complexity is required. Such a scheme has been added to the NCAR Community Atmosphere Model Version 3. Nonetheless, simulated isotopic distributions from climate models, although credible, can be compared with observations (from satellite, aircraft and surface sampling) only in a statistical manner since the model’s atmospheric circulation does not match the observed, and thereby their practical use is limited. Specifically, diagnosing shortcomings in cloud parameterizations with isotopes is presently confounded by the lack of sufficient observational data for meaningful statistical comparison, while data is available for case studies.

To simulate isotopic composition that matches the synoptic conditions, a scheme is developed by which the atmospheric circulation is constrained by reanalysis data, while the hydrology is free to evolve as governed by the model’s parameterizations. The constrained simulation proceeds as follows: 1) A global prediction is made for $\Delta t=6$ hours, when reanalysis data is next available; and 2) the predicted horizontal velocity and temperature are corrected by relaxing to the Reanalysis with an adjustment of the form

$$\hat{T} = T + \eta \frac{\Delta t}{\tau} (T_{\text{NCEP}} - T)$$

and similarly for $u$ and $v$ wind components. The relaxation time scale is set uniformly as $\tau = 24$ hours, which is typical for adjustment to geostrophic flow in midlatitudes. The factor $\eta$ varies vertically from unity above $\sigma=0.850$, and reduces linearly to zero at and below $\sigma=0.950$, such that there is no adjustment performed near the surface - the rationale being that boundary layer conditions are strongly dependent on the specific physical parameterizations. The 6 hour predictions and corrections are continued until a simulation of desired length is achieved. In practice it is convenient to configure CAM to use the same 28 $\sigma$ levels as the NCEP Reanalysis, while the NCEP Reanalysis is first truncated to T42 spherical harmonic resolution, and the topography from the NCEP Reanalysis is used to minimize possible mismatch. Although this simple scheme conserves neither momentum nor energy, the results are remarkably satisfying, largely because the 6 hour forecasts are reasonably accurate. Figure 1a shows that differences in surface pressure between 6 hour predictions and Reanalysis is typically less than 1 hPa. Given
the horizontal resolution, the predicted water vapor fields match the Reanalysis well in the midlatitudes, while in the tropics greater difference is attributed to the stronger dependence on the details of the cloud parameterization (Fig. 1b). Further, a limitation of this scheme is that by adjusting the temperature, there is a thermodynamic inconsistency between the water vapor and temperature fields, which can lead to spurious condensation events in the tropics. This is partially due to the selection of a uniform $\tau$ based on midlatitude considerations. One strength of the scheme is that both total mass and water vapor mass are conserved, which is necessary for accurate isotope simulations. Successful isotopic simulations are evidence that the dynamically constrained hydrology is performing well (Fig. 1c). Indeed, since the water vapor and isotopic fields are not adjusted, the predicted precipitation fields are free from some of the known biases in the Reanalysis associated with assimilation of radiosonde moisture profiles. As such, the isotopic simulations can be reliably compared to available observations to diagnose which aspects of the model hydrology do not perform as desired.

Figure 1: Constrained simulation results from 1200 UTC 1 June 2004 for a region of the southern hemisphere. a) Surface pressure (bold), and difference between 6 hour prediction and NCEP Reanalysis (contour interval is 0.2 hPa). b) Specific humidity at 850 hPa from T42 simulation (bold) and T63 NCEP Reanalysis (dashed). c) Simulated HDO isotope composition (as $\delta^18D$, contour interval is 20 permil) at 850 hPa shows depletion in the wake of cold fronts in the Southern Ocean, and in association with tropical disturbances.