Modeling stable isotopes in near surface water vapor

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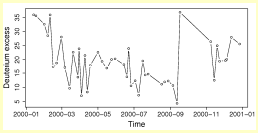
Motivation

- Stable water isotopes are widely used as diagnostic tools in climatology, hydrology etc.
- There are still many open questions related to the processes determining isotope variability in atmospheric waters, in particular with regard to short-term variations and non-equilibrium fractionation.
- One important and critical aspect in many isotope models is the parameterization of fractionation during the evaporation of water from the ocean.
- In the Craig-Gordon model (which is commonly applied for this parameterization), important parameters, specifically the non-equilibrium fractionation factor, are hardly constrained by atmospheric observations.
- Our approach: implement a Craig-Gordon parameterization in a Lagrangian and an Eulerian model and perform a direct, event-based evaluation of model results with measurements.

Isotope data

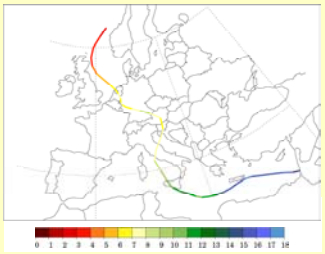
- measurements of $\delta^{18}O$ and $\delta^{2}H$ in water vapor at Rehovot, Israel (*Angert et al.,* 2008)
- vapor was gathered for approximately 8 hours and analyzed in a mass spectrometer
- period 2000 - 2006, measurements ca. twice a week
- altogether 270 measurements available



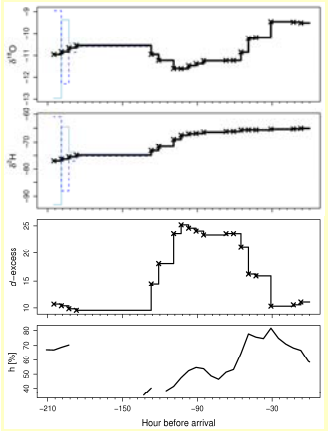
example time series of deuterium excess (*d*-excess) for the year 2000

Lagrangian isotope simulation approach

- Backward trajectories are calculated from ECMWF analysis data, started at Rehovot.
- Trajectories are clipped to exclude clouds and rain from above.
- Locations in the oceanic boundary layer where the specific humidity increases along the trajectory are identified as evaporation sources.



Example 10-day backward trajectory, started from Rehovot at 12 UTC, 10.8.2005. Colors give the specific humidity in g/kg.



Simulated isotope ratios ($\delta^{18}O$, $\delta^{2}H$ and *d*-excess) in water vapor and diagnosed relative humidity h (on the lowest atmospheric model level, calculated relative to SST) along the example trajectory. h is only shown over the ocean. Black crosses denote diagnosed evaporation locations where the Craig-Gordon model has been applied. The blue lines show the sensitivity to changes in initial conditions.

- At every evaporation location, the Craig-Gordon model is applied to parameterize isotope fractionation:

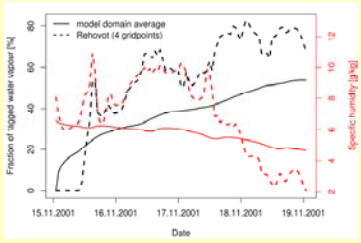
$$R_E = k \cdot \frac{\alpha R_L - h R_A}{1 - h}$$

R: isotopic ratio in {*E*: evaporation flux, *A*: atmosphere, *L*: ocean}; *k*, α: (non-)equilibrium fractionation factor; *h*: relative humidity

- The isotopic composition of atmospheric water vapor along the trajectory and at Rehovot is calculated from previous evaporation events (weighted with the specific moisture contributions).
- Measured and simulated *d*-excess are compared for different settings of the fractionation parameterization, in particular with respect to the non-equilibrium fractionation factor *k*.

Stable water isotopes in the COSMO model

- The mesoscale, limited-area COSMO model is extended in order to simulate water isotope physics.
- first step: introduction of tracers for water species; prognostic water fields in the model: vapor, cloud water, cloud ice, rain, snow
- water is tagged during evaporation from the ocean and subsequently traced through the atmospheric water cycle up to precipitation



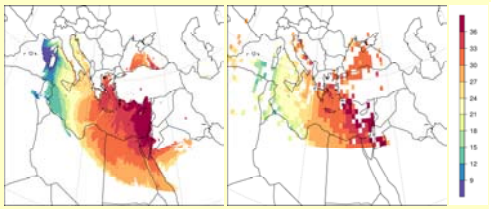
Water vapor on lowest COSMO model level from 4-day model simulation, started at 00 UTC, 15.11.2001. The red curves show the specific humidity, the black curves give the fraction of tagged vapor, both for the whole COSMO model domain and the location of Rehovot.

- second step: parameterization of isotope fractionation during evaporation from the sea, using the Craig-Gordon model and the new form of *k*

Deuterium excess in near surface water vapor at 12 UTC, 18.11.2001.

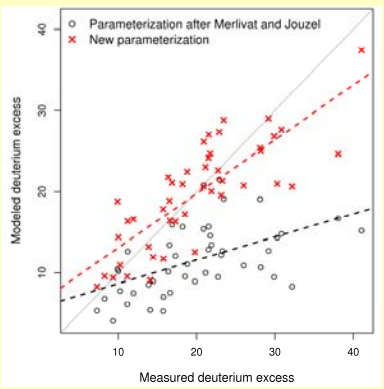
left: result from COSMO simulation (only shown where fraction of tagged water vapor is larger than 60%)

right: result from Lagrangian diagnostic (*Pfahl and Wernli*, 2008)



Results from Lagrangian simulations

- relatively poor agreement between measurements and model results obtained with the classical parameterization of *k* after *Merlivat and Jouzel* (1979); correlation coefficient r = 0.53, RMSE = 10.7; underestimation of non-equilibrium fractionation
- much better agreement with new, wind speed independent parameterization (constant *k*); r = 0.80, RMSE = 4.6



- compared to the same measurements, a historical GCM simulation (*Yoshimura et al.,* 2008) also underestimates *d*-excess; r = 0.49
- numerical values of *k* obtained here are in agreement with data from other studies (e.g. *Uemura et al.*, 2008)
- limitations of the approach: cloud processes and sea spray evaporation are not taken into account
- but: equilibrium fractionation does not affect general conclusion

Conclusions

- A new Lagrangian simulation approach allows a direct, event-based evaluation of the Craig-Gordon model with atmospheric isotope data.
- A wind speed independent parameterization of the non-equilibrium fractionation factor leads to better results than the widely used parameterization by *Merlivat and Jouzel (*1979).
- The success of the Lagrangian method corroborates that the physical fractionation processes during water evaporation from the ocean are properly described by the Craig-Gordon model.
- The implementation of isotope physics in the limited-area COSMO model sets up a framework for comprehensively simulating many atmospheric processes leading to isotope fractionation.
- With the help of a tagging approach, event-based simulations and comparisons to measurements are possible. First tests show that a substantial amount of water at a specific location is traceable within a regional model simulation.
- A Craig-Gordon parameterization has been successfully implemented in the COSMO model. Other fractionation parameterizations will follow.

Pfahl and Wernli (JGR, in press): *Lagrangian simulations of stable isotopes in water vapor - an evaluation of non-equilibrium fractionation in the Craig-Gordon model.*

Angert et al. (Tellus, 2008): *Seasonal variations in the isotopic composition of near surface water vapor in the Eastern-Mediterranean.*

Pfahl and Wernli (JGR, 2008): *Air parcel trajectory analysis of stable isotopes in water vapor in the Eastern Mediterranean.*

Merlivat and Jouzel (JGR, 1979): *Global climatic interpretation of the deuterium-oxygen 18 relationship for precipitation.*

Yoshimura et al. (JGR, 2008): *Historical isotope simulation using reanalysis atmospheric data.*

Uemura et al. (JGR, 2008): *Evidence of deuterium excess in water vapor as an indicator of ocean surface conditions.*

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