MODELING STABLE ISOTYPE RATIOS IN NEAR SURFACE WATER VAPOR IN THE MEDITERRANEAN: AN EVALUATION OF THE CRAIG-GORDON MODEL

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Abstract
Stable isotope ratios in water vapor at Rehovot (Israel) are modeled with the help of the Craig-Gordon model, applied in a Lagrangian setup using backward trajectories. The comparison of the simulation results with measurements at Rehovot allows to infer about uncertain model parameters as the non-equilibrium fractionation factor. A new parameterization for this fractionation factor is suggested and applied in a first case study with a mesoscale dynamical model.

Keywords: Water Transport, Air-Sea Interactions

Introduction
Stable water isotopes are widely used as diagnostic tools for investigating the global water cycle. An important step in this cycle is the evaporation of water from the ocean. The concurrence of equilibrium and non-equilibrium processes complicates a quantitative description and parameterization of isotope fractionation during evaporation. A linear resistance model, as introduced by Craig and Gordon [1], is commonly applied for this parameterization. In such a model, the isotope ratio in the evaporation flux can be expressed as follows:

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

where \( R_L \) and \( R_A \) give the isotope ratios in the ocean and in atmospheric vapor, respectively; \( h \) denotes the relative humidity of the atmosphere, defined with respect to saturation at the sea surface; \( \alpha \) is the equilibrium fractionation factor between vapor and liquid at the surface, and finally \( k \) denotes a non-equilibrium (diffusive) fractionation factor. This non-equilibrium fractionation factor is usually expressed according to [2], but its formulation is hardly constrained by atmospheric observations.

Methodology
This study addresses this issue by combining a recently developed Lagrangian moisture source analysis [3] with a Craig-Gordon fractionation parameterization (equation 1) in order to model isotope ratios in near-surface water vapor [4]. This technique is applied to 45 days of isotope measurements in water vapor at Rehovot (Israel) during the years 2001 to 2006 [5]. Different parameterizations for the non-equilibrium fractionation factor are tested in this setup. Finally, the mesoscale dynamical COSMO model [6] is equipped with the most successful parameterization and applied for simulating the spatial distribution of deuterium excess in water vapor close to the surface.

Results and Discussion
A comparison of the simulated deuterium excess from the Lagrangian approach with the measurements shows that a much better agreement can be achieved using a wind speed independent formulation of \( k \) (correlation coefficient \( r=0.80 \), RMSE=4.6 permil) instead of the classical parameterization by Merlivat and Jouzel [2] \((r=0.53 \), RMSE=10.7 permil). The numerical values of \( k \) that lead to the best agreement of simulated and observed deuterium excess are \( k_{BG}=0.9925 \) and \( k_{BJ}=0.9961 \). These values are consistent with data from other studies. In future research, it should be tested if the empirically derived, wind speed independent parameterization also leads to an improvement of the performance of other models, including GCMs, in modeling deuterium excess. A first case study with the COSMO model verifies that the model is suitable for simulating spatial distributions of isotopes in water vapor in an event-based manner. The simulated deuterium excess compares well with results from a Lagrangian diagnostic [4], confirming the usefulness of the new parameterization.

References