Improved High-Resolution Global and Regionalized Isoscapes of $\delta^{18}O$, $\delta^{2}H$, and *d*-Excess in Precipitation

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Abstract

Patterns of $\delta^{18}O$ and $\delta^{2}H$ in Earth's precipitation provide essential scientific data for use in hydrological, climatological, ecological and forensic research. Insufficient global spatial data coverage promulgated the use of gridded datasets employing geostatistical techniques (isoscapes) for spatiotemporally coherent isotope predictions. Cluster-based isoscape regionalization combines the advantages of local or regional prediction calibrations into a global framework. Here we present a revision of a Regionalized Cluster-Based Water Isotope Prediction model (RCWIP2) incorporating new isotope data having extensive spatial coverage and a wider array of predictor variables combined with high-resolution gridded climatic data. We introduced coupling of $\delta^{18}O$ and $\delta^{2}H$ (e.g. *d*-excess constrained) in the model predictions to prevent runaway isoscapes when each isotope is modelled separately. We validated RCWIP2 isoscape performance by cross-checking observed versus modelled *d*-excess values. We improved model error quantification by adopting full uncertainty propagation in all calculations. RCWIP2 improved the RMSE over previous isoscape models by ca. 0.6 ‰ for $\delta^{18}O$ and 5 ‰ for $\delta^{2}H$ with an uncertainty <1.0 ‰ for $\delta^{18}O$ and <8 ‰ for $\delta^{2}H$ for most regions of the world. The improved RCWIP2 isoscape grids and maps (season, monthly, annual, regional) are available for download at https://isotopehydrologynetwork.iaea.org.

Introduction

Distinctive and predictable long-term regional and continental-scale patterns of $^2H/H$ and $^{18}O/^{16}O$ ratios in global precipitation result from inter-related physicochemical factors controlling the isotopic composition of water in the terrestrial freshwater cycle, including evaporative conditions in water vapor source areas, temperature of condensation, elevation, seasonality, rainfall amount, and local versus distal moisture sources affected by climatic oscillations and atmospheric teleconnections. These coherent spatial isotopic patterns for global precipitation are revealed in long-term monthly precipitation collections taken at hundreds of meteorological stations around the world since the 1960s (Aggarwal et al., 2010; Craig, 1961; Dansgaard, 1964; Rozanski, Araguas-Araguas, & Gonfiantini, 1993; Terzer, Wassenaar, Araguás-Araguás, & Aggarwal, 2013). Currently, global precipitation δ^2H and $\delta^{18}O$ data are web-hosted by the IAEA *Global Network for Isotopes in Precipitation* (International Atomic Energy Agency, 2020) and in databases such as the *United States Network of Isotopes in Precipitation* (USNIP; Welker, 2000) or the *Austrian Network of Isotopes in Precipitation* (ANIP; Kralik et al. 2003).

Accurate predictions of δ^2H and $\delta^{18}O$ values for annual, seasonal, or month-specific precipitation inputs are often needed at sites, regions, or among watersheds to help inform isotope-based water resource assessments, water balance modelling, and for use in other interdisciplinary studies (Jespersen, Leffler, Oberbauer, & Welker, 2018; Klein, Nolan, Cable, Cherry, & Welker 2016; Welker 2012; Zeno et al. 2014). Moreover, in the past decade the need for point-based or regional predictions for the isotopic composition of precipitation are driven by disciplines outside of hydrology owing to the fact δ^2H and $\delta^{18}O$ in precipitation are mirrored and preserved in flora and fauna through water and food which is ultimately controlled by the isotopic composition of precipitation (Hobson & Wassenaar, 2008; Meier-Augenstein, 2011). Spatiotemporal δ^2H and $\delta^{18}O$ patterns driven by precipitation-biosphere isotopic connectivity have presented new opportunities for the application of isotope hydrology data into other disciplines like criminal forensics, commodity trading and food authenticity, archaeology and paleoecology, and migratory and wildlife studies (Bowen, 2010a,b; Camin et al., 2017; Cerling et al., 2016; Hobson & Wassenaar, 2018; Laffoon et al., 2017; Meier-Augenstein, 2011; O'Brien & Wooller, 2007; Van der Zanden et al. 2015; and others)

The paucity of station-based precipitation isotope data for many local and regional studies drove the need for predictive precipitation isotope models (e.g. isoscapes) to help scientists obtain accurate estimates for monthly, seasonal, or annual amount weighted precipitation isotopic composition inputs at their study site or regions of interest. The first δ^2H and δ^{18}O isoscape models used simple regression models based on a few geographical predictors (Bowen & Wilkinson, 2002) whereas advanced models use regression and/or interpolation models with multiple geographic and climatic predictor variables and interpolation of the residuals using sine or other custom fittings to optimize prediction outcomes (Allen et al., 2019; Terzer et al., 2013) to determine the isotope response variable. Owing to the strong covariance between δ^2H and δ^{18}O with mean annual air temperature (MAT) nearly all globally calibrated isoscape models predict reasonably well the mean-annual stable isotope compositions of precipitation where there is strong variability in air temperature; however these simplified parameterizations are inevitably inaccurate in many parts of the world (e.g. in the equatorial tropics) or break down entirely for monthly or seasonal predictions (Allen et al., 2019). This led to downscaling methods restricted to discrete geographical regions, adding more explanatory variables to help improve prediction accuracy (e.g. precipitation amount, vapour pressure, etc.), or by using fuzzy clustering with ecoclimatic zones as in the RCWIP model (Terzer et al., 2013). Some researchers focused detailed isoscape model predictions at their local or national scales (Delavau, Chun, Stadnyk, Birks, & Welker, 2015; Giustini, Brilli, & Patera, 2016; Hatvani, Erdelyi, Vreca, & Kern, 2020; Hollins, Hughes, Crawford, Cendon, & Meredith, 2018; Kaseke, Wang, Wanke, Turewicz, & Koeniger, 2016; Kern, Kohán, & Leuenberger, 2014; Stumpp, Klaus, & Stichler, 2014; Vachon, Welker, White, & Vaughn, 2010; Yamanaka et al., 2015; Zhao, Guo, She, & Tang, 2019). Downscaled isoscape models excel at smaller or regional scales but fail for the global scale predictions that are required for climatic and other large-scale interdisciplinary studies. The global RCWIP isoscape model (Terzer et al., 2013) was the first to use a wide suite of regression combinations for model consideration, with the best performing prediction model applied using fuzzification methods to weigh and merge many regionalized prediction outcomes into large global-scale prediction maps for both δ^{2}H and δ^{18}O. The regionalized RCWIP model outperformed earlier one-size-fits-all global models 67% of the time, and significantly improved the accuracy and uncertainty of the predicted results.

Here we describe RCWIP2 which significantly improves upon the original model and other global isoscape models in key areas. First, we expanded the foundational precipitation δ^{2}H and δ^{18}O datasets to 2016 (from 2009 previously) through improved spatial GNIP coverage by the addition of many new GNIP and USNIP stations (RCWIP covered 1960-2009, without USNIP). The original RCWIP model was data deficient for ~42% of the 36 climatic clusters needed for the application of full regression regionalization, and in these data deficient areas a globally parameterized model was used as substitute. Second, all previous isoscape models produce univariate maps (e.g. δ^{18}O or δ^{2}H) by modelling each stable isotope as a single response variable but without considering whether *coupled* H and O predictions reproduced the observed deuterium excess (*d*-excess) values. Previous univariate isoscape models often produced large *d*-excess discrepancies, particularly in areas near the boundaries of the spatial model domain, indicating that the predictions were incorrect for one or both isotopes. Third, with improved online geo-datasets our spatial resolution of prediction was improved 40-fold by using the newest high-resolution gridded climatic datasets (WorldClim 2, Fick & Hijmans 2017), which improved model isoscape predictions for areas of high topographic relief. We used supervised machine learning methods to examine the relative spatial importance of the key predictor variables to gain new insights into the importance each of these variables according to spatial and climatic patterns. Finally, the use of new explanatory regressors (e.g. continentality, land fraction, distance from coast) also improved the predictions for some global regions. The revised isoscape model RCWIP2, along with high resolution isoscape prediction maps and grids are available at (https://isotopehydrologynetwork.iaea.org).

Materials and Methods

The statistical approach and fuzzy clustering schema used in the original RCWIP isoscape model is fully described elsewhere (Terzer et al., 2013); here we report on the key differences, additional datasets, and technical improvements in RCWIP2 isoscape prediction model compared to the original RCWIP. All geospatial calculations were performed in R (R Core Team, 2018) using mainly the *rgdal* (Bivand, Keitt & Rowlingson, 2019) extension.

Global Precipitation Isotope Data

The precipitation isotope dataset used in RCWIP2 consisted of monthly composites of δ^2H and δ^{18}O data in precipitation from curated GNIP and USNIP databases (International Atomic Energy Agency, 2020; Welker, 2000), CNIP (Birks & Gibson, 2009) and other sources (e.g. Kralik, Papesch, & Stichler, 2003; Kurita & Ichiyanagi, 2008; Wang & Peng, 2001). Compared to RCWIP (Terzer et al., 2013) the temporal span of stable isotopic data used was enlarged by seven years to cover the time period 1960-2016. As before, stations with less than two full years of *coupled* δ^2H and δ^{18}O isotopic data were removed to improve the data quality (Terzer et al., 2013), resulting in a carefully curated dataset of 638 global stations (vs RCWIP: 576 stations). GNIP efforts over the past few years focused on improving coverage in data deficient regions (e.g. Africa), and hereby allowed for a full statistical treatment and regionalized regressions for 30 of the 36 global ecozone clusters (vs. 16 in RCWIP) and lowered the fraction of data-deficient clusters to 20% (from 42% in RCWIP).

All spatial covariates corresponding to the site data (latitude [LAT], longitude [LONG], and elevation [ALT]) were obtained from the GNIP, CNIP, or USNIP databases and from online digital elevation models (DEM). Few stations in the combined global precipitation isotope dataset spanned the entire observation period of 1960-2016, therefore temporal stationarity was assumed as falling within the uncertainty of the regressions. As noted by Terzer et al. (2013), caveats regarding time gaps in coverage and the unavoidable limitations in pooling non-contiguous decadal scale datasets also apply to RCWIP2 or to any other isoscape model (Aggarwal et al., 2010; Bowen, 2010a,b).

Regressor Datasets

The core climatic regressors (monthly precipitation amount [PP], air temperature in °C [AT], and water vapor pressure in hPa [VP]) were obtained from the GNIP, USNIP, and CNIP databases. Where these data were unavailable, averaged climate data (monthly, annual) was obtained from the nearest station in the Global Historical Climate Network (GHCN) (Peterson, Vose, Schmoyer, & Razuvaev, 1998) or interpolated from the NCEP reanalysis 30-year mean dataset (Kalnay et al., 1996). The NCEP dataset was used to extract the mean precipitable water rate [PW] variable as mm/s (transformed to mm/month), which was previously found as a predictor of isotopic composition in tropical regions (Aggarwal et al., 2012), and an extended set of regressors not used in RCWIP or any other isoscape models. These new regressors included Convective Precipitation intensity in mm/month (recalculated from mm s^{-1}) [CPN]; Latent Heat Flux [LHF], Net Longwave Radiation [NLR] and Outgoing Longwave Radiation [OLR] as W/m², and Wind Speed [WS] in ms^{-1}. The Conrad's continentality index ([CI], e.g. Clark & Fritz, 1997) variable was calculated from the temperature data above. Finally, we computed new derived geographic variables for other explanatory regressor consideration. These include "Weighted Latitude" ([wtLAT]; calculated as the absolute latitude weighted by the number of grid cells falling on land masses at the corresponding latitude; this adjusts latitude for the differential fractions of land area in the northern and southern hemispheres), as well as the loxodromic distance to the nearest coastline in km [DTC] and the land mass fraction in a 1000-km radius around the data point [LMF, dimensionless]. Further details can be found in online Supplementary Materials. The shapefiles for these variables were obtained from the Natural Earth web page (www.naturalearthdata.com).

The source of most regressor data was WorldClim 2 (Fick & Hijmans, 2017) which provided mean annual PP (mm), AT (°C), VP (scaled to hPa), and WS (ms^{-1}) data as well as elevational data at 30 arc-second resolution. Other regressor grids were derived at the same geometric resolution (CI, LAT, LONG) or calculated and extracted at lower geometric resolution and up-sampled, since our computational resources were limited to desktop computing.

Climatic Zone Clustering

Climatic zone membership in RCWIP2 was based on the original fuzzy clustering schema of RCWIP (Terzer et al., 2013, Figure 1a), which used 36 climatic clusters pre-defined by their location and meteorological and seasonality conditions. RCWIP2 included a new framework to incorporate the Antarctic clusters, but the isotope data deficiency there precluded the application of RCWIP2 (compared to Masson-Delmotte et al. 2008) and hence the former functional cut-off at 60°S was retained. For the few remaining data-deficient climatic clusters, in which regionalized regression models could not be obtained (e.g. clusters 8 or 15, Figure 1b), RCWIP2 reverted to a fallback model option of: i) an *extratropical model* for clusters outside the Tropics of Cancer/Capricorn, or ii) a *tropical model* (see Fig 1c), whereby each fallback model comprised all station-based observed data of the clusters falling within its domain and was subjected to the same regression selection algorithm described above. <INSERT FIGURE 1 AROUND HERE>

Geostatistical Analyses

To identify the best-fitted linear models with limited computational resources, we restricted the length of the candidate regression equations to six predictor variables. For candidate equations with only two regressors, all variable combinations were tested, whereas for candidate equations with n>2 variables only the best 10 combinations with n-1 variables (ranked by their R^2) were tested. Candidate equations with an R^2 <0.5, p-value >0.05 or regressors with a Variance Inflation Factor (VIF) > 5 were discarded from further assessment. With statistical significance and VIF testing as our new requirements for evaluating RCWIP2 performance, the minimum allowable ratio of explanatory variables over residual degrees of freedom (which RCWIP used as a surrogate) could be relaxed from 7.5 to 5.0.

Furthermore, in addition to the dual-isotope data input criterion, RCWIP2 linked the computation of the δ^{18}O and δ^2H isotopic regressions. Any regressor combination was rejected if it failed the test for either isotope, or if it had R^2 or *p*-values falling outside the 10% band of its complementary isotope value. The accepted regressor combination finally applied to both isotopes for each cluster was the one having the higher R^2 for either δ^{18}O or δ^2H. This stricter model performance criteria inevitably led to some spatial coverage reductions for some of the climatic clusters; however, these losses were few and offset by a significant improvement in dual-isotope prediction accuracy. We furthermore used model derived deuterium excess (d = δ^2H – 8 δ^{18}O, Dansgaard, 1964) to constrain runaway predictions for δ^{18}O or δ^2H (e.g. isoscape points producing unrealistic d-excess values) to ensure the credibility of the isoscape predictions for both isotopes.

Another RCWIP2 improvement was to eliminate the computationally intensive interpolations of the residuals. The original RCWIP (and most other isoscape models) use variograms to interpolate the unexplained variability of the regression model by applying kriging methods. However, we found that the resulting improvements to the prediction models by the incorporation of kriging was insignificant and often local in nature (we found kriging to be ineffective beyond ~50 km of the observed data points) and added unnecessary uncertainty to the results (see below). The lack of spatial autocorrelation between data point residuals led us to conclude the computationally intensive kriging step was detrimental rather than advantageous.

Uncertainty Assessment

Uncertainty assessments of isoscape prediction model outcomes have largely been ignored to date. RCWIP initially focused on kriging error; but it too ignored the overall combined uncertainty of the modelling results. Reasonable expectations for isoscape model uncertainty are subjective and inevitably differ among data-rich or data-poor regions or depending on the degree of uncertainty the practitioner deems as fit for purpose. An unrealistic expectation is that isoscape prediction uncertainty might be lower than analytical uncertainty for δ^{18}O or δ^2H. This expectation is unrealistic considering the diversity of original H and O isotope data sources, the many analytical methods and isotope instruments used over decades, and the seasonal amplitudes of precipitation isotopic composition (or time-trends embedded therein). Moreover, the natural variability for all covariates used at each site substantially exceeds any instrumental measurement error (e.g. SD of annual mean

δ^{18}O in Vienna is ~1 ‰ versus an analytical error of <0.08 ‰). Thus, for RCWIP2 we operationally adopted the 30-year SD of meteorological parameters (derived from the monthly NCEP datasets) as our uncertainty criteria and treated the geographical regressors (LAT, LONG, ALT, wtLAT, DTC, LMF and also CI) as fixed constants without any uncertainty. Using full error propagation techniques, we derived our error grids for δ^{18}O and δ^{2}H as follows:

$$u_{regr} = \sqrt{\left(\frac{u_{Var_1}}{Var_1}\right)^2 + \left(\frac{u_{Coeff_1}}{Coeff_1}\right)^2 + \ldots + \left(\frac{Var_2}{u_{Coeff_2}}\right)^2 + \ldots + u_{Intercept}{}^2} \qquad (1)$$

Where *Var_1* stands for a meteorological variable; u_{Var_1} is its uncertainty; *Coeff_1* is the regression coefficient of *Var_1* and u_{coeff_1} the uncertainty on *Coeff_1. Var_2* exemplifies a geographical variable; u_{Coeff_2} is the uncertainty on regression coefficient *Coeff_2*; $u_{Intercept}$ is the error on the intercept, and so on.

RESULTS AND DISCUSSION

Data and Map Products

RCWIP2 yielded global gridded annual mean δ^{18}O, δ^{2}H and d-excess prediction datasets at a 30 arc-second spatial resolution, as summarized in a new global map of mean annual δ^{18}O (Figure 2; world map in online Supplementary Material S3.1). To our knowledge, this is the first global precipitation isoscape map resolved to the sub-kilometre resolution and the first to depict *d*-excess at global levels in the cross-validation of δ^{18}O and δ^{2}H predictions (see Supporting Materials for full-size images). The gridded isoscape data (comprising a full-extent 360° x 180° GeoTIFF or tiles of 20° x 20°) are also available for download from the IAEA Isotope Hydrology Network website (https://isotopehydrologynetwork.iaea.org). <INSERT FIGURE 2 AROUND HERE>

Isoscape Coverage

The expanded isotope dataset with improved global spatial coverage and new statistical improvements allowed us to extend RCWIP2 model coverage from 21 to 32 regional clusters (see Supplemental Materials). The inclusion of USNIP resulted in substantive improvements in model predictions in North America with eight out of nine North American clusters covered with full regression models. Furthermore, five out of six clusters in Africa were improved using the regionalized RCWIP2 model. One South American cluster (cluster 29) which RCWIP previously met for δ^2H was now covered by both isotopes.

The overall improvement in accuracy and precision of the isoscape predictions affirmed that stricter selection of curated input isotope data and dual-isotope constrained regressions along with *d*-excess as a control justified the additional steps. We note that data coverage factors still need to be considered by isoscape users when comparing RCWIP2 to any other isoscape model, as GNIP data density and coverage remains globally non-uniform despite the substantive improvement over the decades. This underscores the need for the isotope community to continue filling in data gaps via long-term monthly sample collections at current and new GNIP stations and to help ensure robust time series by seeking new stations in data sparse or in montane regions.

Benchmarking RCWIP2 Performance

We compared RCWIP2 to RCWIP performance by the root mean squared error (RMSE) of regionalized predictions on a per-cluster level and against the global regression equation as applied to each cluster (Figure 3). The best fit RCWIP2 model had an improved RMSE for δ^{18}O of 0.96 ‰ (compared to 1.58 ‰ of RCWIP and 7.6 ‰ for δ^2H, versus RCWIP: 12.7 ‰). Marked improvements in RMSE outcomes were seen in the African (10-

14) and Australian (34-35) clusters due to recent data gathering efforts and for North American clusters (16-24) from the addition of the USNIP data. Several clusters remained difficult to predict, as exemplified by above-average RMSE values and/or as a result of poor isotope data coverage. Other reasons for underperformance include data paucity (e.g. clusters 15, 19 or 33) or the inability to construct suitable regression equations with the available data (e.g. 8: Himalayas and Tibet, 16-17: North American Arctic, or 34-35: Australia). As new isotope data accumulates, or if the inclusion of additional explanatory regressors does not improve predictions for under-performing clusters, a review of the clustering scheme may be warranted or to consider introduction of new clusters. New climatic clusters would be difficult to populate with isotope data in the short-term, hence that trade-off remains uncertain. <INSERT FIGURE 3 AROUND HERE>

Deuterium Excess

The predicted *d*-excess determinations were evaluated for point-based station data residuals as well as for global gridded data. RCWIP2 yielded an overall improved *d*-excess RMSE of 2.3 ‰ (compared to RCWIP: 4.4 ‰). Figure 4 shows a global map of predicted *d*-excess in comparison with station-based observations (long-term weighted mean *d*-excess). Purple circles indicate locations where the absolute value of the prediction bias exceeds two times the RMSE. Histograms of the *d*-excess residuals for RCWIP and RCWIP2 (Figure 5b) revealed narrower and more normally distributed patterns, indicating that the coupled isotope approach led to more reasonable predictive isoscape results. <INSERT FIGURE 4 AROUND HERE><INSERT FIGURE 5 AROUND HERE>

Regression Uncertainty Assessment

RCWIP2 produced gridded maps of $\delta^{18}O$ and $\delta^{2}H$ prediction uncertainty using error propagation methods based on the analytical and climatic data used (and static geographical regressors). For all climatic clusters except for two, the propagated isoscape prediction uncertainty was <1.5 ‰ for $\delta^{18}O$ and <10 ‰ for $\delta^{2}H$. For some areas, like cluster 14 (Sub-Saharan Africa) and 17 (North American Arctic and Greenland), higher uncertainties of up to ±3 ‰ for $\delta^{18}O$ and ±24 ‰ for $\delta^{2}H$ were obtained. These higher uncertainties stem from above-average variability in annual air temperature for these regions (e.g. if AT was the sole regressor). However, the regressions for cluster 14 fully met our model criteria but here 45% and 37% of the $\delta^{18}O$ and $\delta^{2}H$ variability was still left unexplained. Notably this approach to quantifying and depicting model prediction uncertainty is not helpful for *d*-excess, as the propagated uncertainty for this derivative was between ±12 ‰, and ±34 ‰, which is well beyond the inter-annual variability observed in *d*-excess for most stations. We compared the natural intra-annual variability of observed $\delta^{18}O$ (expressed as standard deviation of the annual weighted $\delta^{18}O$ means of 186 GNIP sites with ≥ 10 years of record) to the prediction uncertainty and found that the medians were 0.84 and 0.90 ‰, respectively, within an inter-quartile range (IQR) of 0.49 ‰ each. Global and regional maps of the spatial distribution of prediction errors for both isotopes are summarized in Figure S3.2 in the Supplemental Materials.

Selected Comparative Model Performance

We compared the isoscape predictions of RCWIP2 to our previous results for North America after the addition of the USNIP data, especially for western North American montane regions where the predictive capability of RCWIP was unsatisfactory. We did not undertake outcome comparisons where the data paucity did not improve upon RCWIP or other isoscape models (e.g. Namibia; Kaseke et al., 2016), or where a lack of predictive isoscape capability was well-known as a result of localized hydrological processes such as snowmelt biases influencing Baltic isoscapes (Raidla et al., 2016).

North America: The RCWIP2 isoscape for North America (25-90°N, 50-180°W) revealed a dramatic improvement over its predecessor, with the RMSE vs RCWIP reduced from 3.0 ‰ to 0.9 ‰ and 22.5 ‰ to 6.5 ‰ for δ^{18}O and δ^{2}H, respectively. To quantify how well the incorporation of USNIP and CNIP datasets improved our predictions, we extracted RCWIP δ values from the gridded product for sites added to RCWIP2. Using this approach, we were able to correct for the data paucity in RCWIP and found the RMSE for North America would have been 1.3 ‰ and 11.3 ‰ for δ^{18}O and δ^{2}H, respectively. Figure 6 depicts the improved distribution of the residuals for RCWIP and RCWIP2 for δ^{18}O for North America (NAM v1 and NAM v2, respectively). <INSERT FIGURE 6 AROUND HERE>

High topography regions: Several studies (Kern et al., 2014; Yamanaka et al., 2015) noted that RCWIP did not correctly predict the altitudinal lapse rates for some high-topography areas in Europe or Japan. We assumed that the RCWIP altitudinal model failure was from the low-resolution Digital Elevation Model (DEM) (10 arc-seconds) used. Hence, we extracted new δ^{18}O predictions from RCWIP and RCWIP2 along with the new underlying high-resolution DEM altitudes for the same station-based data in the European Alps (Kern et al., 2014), the Japanese Alps (Yamanaka et al., 2015) and in Italy (Giustini et al., 2016). A comparative summary of isoscape benchmark parameters for these high topographic relief datasets are found in Table 1. <INSERT TABLE 1 AROUND HERE>

In the case of the European Alps, RCWIP2 improved the outcomes across all prediction metrics. The RMSE was lowered from 1.76 to 1.49 (Figure 6) by using the data from Kern et al. (2014). However, the results revealed that for some regions of exceptionally rugged topography, elevational differences at the sub-grid geographical resolution biased the predictions in a systematic manner. We regressed the RCWIP2 δ^{18}O predictions against DEM altitude to obtain a new "local interpolation fitting" (Table 1). Surprisingly, the original RCWIP provided better results than RCWIP2 (RMSE 1.00 vs. 1.27‰ δ^{18}O). We assumed this was due to slight differences in the modelling of the altitudinal isotopic lapse rate; in this case RCWIP found a best-fit model for $\delta^{18}O$ (including both ALT and AT as regressors) whereas the RCWIP2 enforcement of suitable regressor combinations for dual isotopes and *d*-excess forced the use of AT alone to model the altitudinal lapse for this cluster.

For the Japanese Alps, we found the RMSE of RCWIP2 improved to 1.47 ‰ $\delta^{18}O$ compared to 2.27 ‰ in RCWIP (Figure 6). Although the median altitudinal bias did not change substantively (1 m compared to 33 m previously) a strong linear relationship of $\Delta\delta^{18}O_{RCWIP}$ and $\Delta\delta^{18}O_{RCWIP2}$ revealed a poor relationship between ALT_{RCWIP} and ALT_{RCWIP2}, which suggested our expanded set of regressors in RCWIP2 contributed to the improved isoscape prediction rather than simply the application of a higher resolution DEM. The predictive capabilities of the fully localized model described by Yamanaka et al. (2015, RMSE of 0.24 ‰ for $\delta^{18}O$) are unlikely to be matched using a global isoscape model even after applying customized local interpolation techniques. The RCWIP2 approach, however, reduced the spread of residuals, which suggested that observed biases were systematically related to the altitudinal lapse rate, whereas applying the same technique for RCWIP resulted in an unacceptable result (Table 1).

For the Italian montane data set, we found the RCWIP2 performance was comparable to the most parsimonious local regression model (Giustini et al., 2016) (Table 1). In comparison with RCWIP (Figure 6), we found only minor improvements despite the clusters in Italy are data-rich and the RMSE for clusters 1 and 10 did not change substantially (Figure 3).

Spatial Importance of the Predictor Variables

Beyond the depiction of global and regional H and O isoscape maps, we extracted the results of the RCWIP2 regression selection algorithms and spatially visualized the relative importance each predictor regressor for those clusters wherever the regional model was used. In this assessment, for each cluster and predictor variable we identified the fraction of statistically valid candidate regressions (as meeting the R-Squared, p-value and variance inflation targets; see “Materials and Methods”). Stacking these fuzzy cluster fractions allowed us to create new maps of the relative importance of those predictor variables most influencing the isotopic composition of precipitation (Figure 7), which was expected to be in line with the well-known isotopic effects like precipitation amount or air temperature (e.g. Dansgaard 1964, Rozanski et al. 1993) To our knowledge, mapping of the relative importance of the predictor variables on the isotopic composition of precipitation is done here for the first time, particularly for newly used relevant variables like precipitable water or convective precipitation rate or intensity, although caution should be used given some of the previously described spatial and data limitations (see Figure 1b). We caution that the relative preponderance of a regressor may be due to the lack of relevance of the other regressors, especially for areas where there were few candidate regression equations (Fig. 7h). <INSERT FIGURE 7 AROUND HERE>

Precipitation Amount: Figure 7a depicted the relative importance of precipitation amount as a predictor of precipitation δ^{18}O. For only three clusters was precipitation amount relevant for more than 30% of the candidate regression equations. Notably, these clusters were in arid or semi-arid regions of south western North America, central Africa and Central Asia, which also have strong seasonal rainfall curves. This pattern corroborated the spatial patterns of the R^2 of observed precipitation δ^{18}O against precipitation amount (i.e. reasonable R^2 is mainly observed in these regions).

Air Temperature: In Figure 7b, a contrasting pattern was revealed for the dependence of the isotopic composition of precipitation on air temperature, which affirmed expected patterns of a strong temperature influence in the temperate climates of the northern and southern hemispheres (some clusters were data deficient though). Surprisingly, the relative importance of air temperature for many of the North American clusters was not as strong as we anticipated. Air temperature was found to be an important regressor for one arid tropical cluster (14 – Sahelian Africa), which could be attributed to low temperature amplitudes co-evolving with the annual mean precipitation and isotope curves. Cluster 30 (warm-temperate to subtropical South America) also stood out in terms of air temperature importance, which may be representative of its seasonal gradient (amplitude of >16 °C monthly mean air temperatures at the index location of La Rioja, Argentina); however this cluster represents a complex geographical transition zone in many ways (e.g. lowland to Andean, tropical to temperate gradients).

Precipitable water (Fig. 7e) was especially relevant in the western and southeast parts of North America but also in equatorial Africa. This observation agreed with that of Aggarwal et al. 2012 in part; however, the comparability of the input datasets was limited and a further detailed breakdown into seasonal isotopic distributions is warranted. Our analysis identified a hotspot for the relative importance of convective precipitation in Southeast Asia (Fig.7e) but in no other tropical regions. In agreement with He, Goodkin, Kurita, Wang and Rubin (2018), *outgoing longwave radiation* ([OLR], Figure 7g) was an important predictor variable over large parts of Southeast Asia and the Pacific, but also for the Amazonian basin. The equatorial African tropics were assumed to be a secondary hotspot, yet this pattern may be blurred by relative data paucity and the climatic cluster structure for that region.

All other regressors fell into well-known and previously established patterns (Figure 7, Supplemental Figure S3.3). For example, altitude or continentality (Supplemental Figures S3.3ab) did not show preponderance of relative importance in relation to the other variables. Notably, mapping of covariate relative importance should be viewed with caution given these are based on six decades of non-contiguous averaged stable isotope data. Nevertheless, our depictions reveal how systematic and higher spatiotemporal frequency isotope data coupled with machine learning tools may eventually be used to map or predict differential effects of climatic and hydrological changes over space and time.

RCWIP2 caveats and issues

RCWIP2 is based on the WorldClim2 (WC2) and NCEP datasets, whereby the NCEP was resampled to meet the spatial resolution of WC2. Due to computational limitations several parameters were derivatives of the primary WC2 grids, such as cluster membership and the uncertainty of meteorological parameters, were also resampled. This artefact became visible for some of the grids and, although it did not degrade overall predictive performance of RCWIP2, it may appear aesthetically unacceptable when mapped. In case of doubt, RCWIP2 users should consider larger areas than their observation point or to cross-validate the isoscape predictions with data such as from nearby GNIP stations covering an expanded area, a verification practice that is generally encouraged. Furthermore, there were some zones (e.g. coastal fringes in the Arctic) where marked "steps" in temperature modelling inherent in the WC2 dataset used impacted the model outcome. Most of these caveats will eventually be overcome in time as newer and expanded online datasets become available.

Conclusions

With expanded foundation datasets and updates to the global precipitation isotope databases like GNIP, and using newly available high-resolution gridded climatic datasets, we demonstrated an improved RCWIP2 isoscape model with better regionalization coverage and higher spatial resolution for H and O isoscape maps and grid products. The coupling of δ^{18}O and δ^{2}H in geostatistical analyses resulted in accurate predictions of global *d*-excess patterns, which also helped to constrain H or O isoscape model predictions. We used innovative error uncertainty quantification in line with natural multi-annual variabilities, which could eventually lead to a universal approach for quantifying isoscape model performance against some key benchmarks, akin to laboratory proficiency testing (e.g. z- and ζ-scores for isoscapes). The improved isoscape modelling process in RCWIP2 rendered kriging procedures unnecessary, reducing the computational intensity and eliminating a major source of isoscape prediction error.

Despite improvements in isoscape mapping efforts over the years, we caution users to critically reflect upon the use of gridded data results prior to their use in practical applications, bearing in mind the limitations, deficiencies and underlying assumptions as detailed in this paper, including the stationarity assumption of multi-annual δ^{18}O and δ^{2}H time series, or unresolved particularities in elevational lapse rates amongst different topographic regions (e.g. no one-size-fits-all elevational model). RCWIP2 is a global prediction tool which attempts to combine the potential of regionalized predictions at the highest spatial resolution possible, but clearly it cannot compete with small-scale regionally optimized isoscapes, or may fail altogether where extreme hydrological processes alter the isotopic signature of rainfall (e.g. use isocapes with caution in highly arid regions).

RCWIP2 was used to create new seasonal isoscapes (annual, monthly, seasonal, and growing season) for δ^{18}O, δ^{2}H and d-excess. A full suite of these specialized grids and maps are available online but are not discussed in detail here. The progressive accumulation of new GNIP station isotope data with increasing spatial coverage and the use of machine learning tools will continue to improve prediction quality for currently limited clusters; however, if unsatisfactory regressions persist then new explanatory regressors may need to be considered, or the current clustering composition may need to be reconsidered. Components of the RCWIP2 regression selection algorithm can also be used to derive higher time resolution precipitation prediction mapping products (e.g. daily, event based predictions), provided sufficient high-resolution isotope and gridded meteorological data are made available and that the processes affecting the isotopic composition can be appropriately modelled over such short timeframes.

Data availability:

The gridded data are available from IAEA-IHN. Numerical GNIP data can be obtained from https://nucleus.iaea.org/wiser.

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