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DEVELOPMENT AND VERIFICATION OF A VERTICAL INTEGRATED TWO DIMENSIONAL WATER ISOTOPE CIRCULATION MODEL

By

Kei YOSHIMURA
Institute of Industrial Science, the University of Tokyo, Japan

Taikan OKI
Research Institute of Humanity and Nature, Japan

Nobuhito OHTE
Graduate School of Agriculture, Kyoto University, Japan

and

Masahiro KOIKE
Institute of Industrial Science, the University of Tokyo, Japan

SYNOPSIS

Large spatial and temporal variability of stable water isotopes (D and ^{18}O) in precipitation are widely used to trace the global hydrologic cycle. However, a primal factor in causing variability has not been quantitatively described by previous studies. In particular, the causes of short-term (less than 10 days) variability of precipitation isotopes remain unclear. Thus, in this study we developed a new isotope circulation model (ICM), which covers the global scale with higher spatial and temporal resolution ($1.25° \times 1.25°$) and daily time-scale than former isotope model studies. The ICM has only one vertical layer and includes a Rayleigh equation to simulate vertically integrated isotopic behavior. As a result, the ICM reproduced the daily variability of precipitation $\delta^{18}O$ in Chiangmai, Thailand with sufficient correlation (R=0.76), as well as the monthly $\delta^{18}O$ on the whole globe with a statistically significant level >99%. Findings (1) revealed the primal factor of the temporal and spatial isotope variability and (2) support the validity of the vertical one layer modeling in the ICM.

INTRODUCTION

How water circulates on the Earth in reality has been of great interest to many researchers. However, its query, such as from where and how rain today comes, is not yet understood clearly. The stable water isotopes, HDO and $H_2{}^{18}O$, can be useful tracers to these questions. Even though their total amounts on the earth are constant, there is great heterogeneity in the temporal and spatial distributions of stable water isotopes caused by phase changes of water (such as liquid to vapor, liquid to solid, etc.) as it transports. Investigation of the spatial and temporal distributions therefore helps us to understand the water circulation system of the earth.

The temporal and spatial variability of precipitation isotopes are remarkably large because of the atmospheric water circulation, which causes frequent and complicated water phase changes. Many previous studies including Clark and Fritz (1) have described the spatial and temporal characteristics of precipitation isotopes, such as elevation effect or the continental effect, etc. Few studies, however, have analyzed the atmospheric water circulation quantitatively to account for the isotopic variability succinctly. We have not yet gained a clear

understanding or the characteristics of these isotopes.

Since the 1980s, studies that incorporate the stable isotope physics in an atmospheric general circulation model (AGCM) have reasonably reproduced the major isotopic features in precipitation and revealed the large-scale characteristic of observed isotope-climate relationships. Such studies have been carried out by Jouzel et al. (2), Hoffmann et al. (3), Mathieu et al. (4), etc. AGCMs can account for the complexity of dynamical and atmospheric-micro-physical processes leading to the formation of precipitation, which seems to dominantly cause the spatial and temporal isotopic variability. However, their spatial resolutions are rather coarse as at most 2.8°×2.8°, and temporal resolutions are monthly or more. Mathieu et al. (4) indicates the necessity of validation in daily time-scale, and appeals the lack of the observations for their validation. In fact, Hoffmann et al. (5) notes that these AGCM studies cannot reproduce this short-term isotopic variability, perhaps because of spatial resolution limitations.

Therefore, the present study will develop a new model, namely, an isotope circulation model (ICM), which has finer temporal and spatial resolution than the previous isotope AGCM studies, as latitudinal 1.25° by longitudinal 1.25° and its outputs will be discussed on a daily time-scale. Unlike isotope-AGCMs, the new model incorporates external meteorological datasets that are based on observations, such as reanalyses that include long-term gridded global datasets of key variables constrained and assimilated by observations (6). Notice that the new model is designed to integrate all vertical atmospheric processes that influence isotope composition in each grid by the use of a Rayleigh equation. The Rayleigh equation describes an isotopic equilibrium relationship between water vapor and precipitation, regardless of any isotopic variability introduced by micro atmospheric processes (7). This is perhaps the distinctive originality of this model while the isotope-AGCMs attempt to incorporate these isotopic physics as precisely as possible. Thus, in the study we verify the ICM results with observations on monthly to daily scales. Finally, this study provides possible answers to (1) the primal factor of the temporal and spatial variability of precipitation isotopes; and (2) the validity of this vertical integrated modeling to analyze the atmospheric and isotopic circulation.

FUNDAMENTALS OF WATER ISOTOPES

Terminology

The stable water isotopes, D and ^{18}O, are measured in units of parts per thousand (‰) relative to a standard (SMOW: Standard Mean Ocean Water) composition. For example, δ^{18}O values are calculated by

$$\delta^{18}\mathrm{O} = ((R/R_S) - 1) \times 1000\ [‰] \tag{1}$$

where R and R_S denote the ratios of the heavy to light isotope (^{18}O/^{16}O) in the sample and standard, respectively.

Fractionation and Fractionation Factor

Because of their mass differences, H and D and ^{16}O and ^{18}O have slightly different chemical and physical properties. Such differences are manifested as a fractionation effect. Generally, when water changes from liquid to gas (solid to liquid) at near normal temperature, the heavy isotopes are enriched in the liquid (solid) than the gas (liquid). The fractionation can be expressed as the isotope fractionation factor α

$$\alpha = R_B/R_A \tag{2}$$

where R_A and R_B are the isotope ratios of phase A and phase B, respectively. When α is more than 1, the heavy isotopes are enriched in phase B, and vice versa.

Rayleigh Equation

As water changes phase, the evolution of the isotopic composition in the residual phase is described by

the Rayleigh equation as follows for ^{18}O,

$$\frac{R}{R_0} = \frac{1+10^{-3}\delta^{18}O}{1+10^{-3}\delta^{18}O_0} = \left(\frac{W}{W_0}\right)^{\alpha-1} \quad (3)$$

where R_0 and R are the initial and final isotope ratios and $\delta^{18}O_0$ and $\delta^{18}O$ are the respective δ values calculated by Eq.1, and W_0 and W are the initial and final amounts of water.

Daily Variability of Precipitation Isotope in Thailand

Since July 1998, we have collected daily precipitation samples in three places in Thailand (Bangkok, Sukhothai, and Chiangmai: see Fig.1), for the activity of GAME-T (GEWEX Asian Monsoon Experiment in Tropics; GEWEX: Global Energy and Water Cycle Experiment) project. Fig.2 and Fig.3 show the results of 1998 and 1999. They indicate that the isotope ratios in the three places deplete (lighten) from May to November, which correspond to the onset (beginning) and the withdrawal (end) of the rainy season, respectively. Furthermore, the figures indicate the large-scale (more than 10 ‰) fluctuations in the short-term (10-45 days) period. More significantly, the fluctuations seem to be very similar in the same year in all three places regardless of the distance as far as 600km. Ohte et al. (8) found that these spatially uniform temporal fluctuations show that the effect of the large scale atmospheric circulation behavior on precipitation isotope is somewhat greater than the various local scale rain-forming processes.

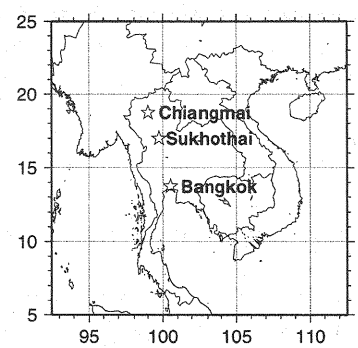

Fig.1 Location of the observation sites, Bangkok, Sukhothai, and Chiangmai, in Thailand.

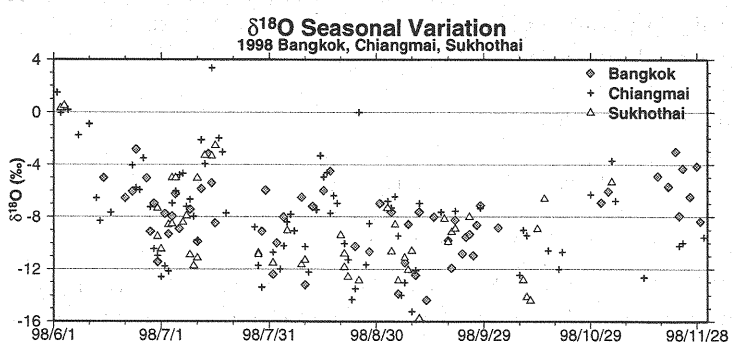

Fig.2 Daily variability of precipitation $\delta^{18}O$ in three places, Thailand (1998)

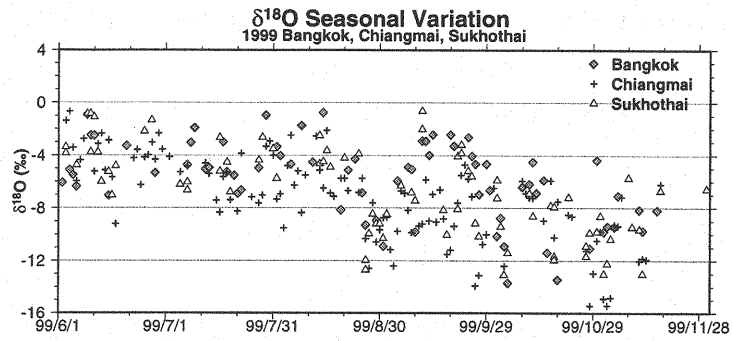

Fig.3 Daily variability of precipitation δ^{18}O in three places, Thailand (1999)

DESCRIPTION OF AN ISOTOPE CIRCULATION MODEL

Grid Modeling and Dataset

The grid size of the ICM is 1.25°×1.25° horizontally and one layer vertically. The area of each grid is approximated as a trapezoid drawn by the latitude and longitude lines. With great care on varieties of the area and the sides' lengths in each trapezoid, the atmospheric water budgets are calculated using the variables from GAME reanalysis (detailed in Yatagai et al. (9)) Ver.1.5 with two dimensional forecast. Used variables are precipitable water (total column water vapor), vertical integrated water vapor fluxes (zonal and meridional), evaporation, and precipitation. The temporal resolution of these variables is every six hours for the period of 1998/04/01/00:00UTC – 1998/10/31/18:00UTC.

Water and Isotope Circulation Modeling

The assumptions of ICM are described as follows:

(a) The water vapor and its isotope in each grid mix to uniform in an instant by the inflows in either vertical or horizontal direction.
(b) The horizontal transport of water vapor and evaporation do not cause the fractionation.
(c) In each time step in the model, precipitation occurs at the end, after evaporation and horizontal water vapor transport take places.
(d) The isotope fractionation derived from the difference of the diffusion velocity of each molecule (the kinetic fractionation) is not considered in the ICM.
(e) The isotope ratio in evaporation water stays at a constant whose value depends on the land or sea types.
(f) The fractionation by precipitation occurs in accordance with the Rayleigh equation.

Fig.4 shows the conceptual outline of the model processes.

Water Budget Equation in Each Grid

Precipitable water W at time t and $t + \Delta t$ are calculated by

$$W_{(t+\Delta t)} = W_{(t)} + Q_{Uin} - Q_{Uout} + Q_{Vin} - Q_{Vout} + E - P \qquad (4)$$

where Q denotes the water vapor flux for Δt, with suffixes *in* and *out* that indicate the inflow and the outflow of the zonal (U) and the meridional (V) directions, respectively; and E and P denote the amount of evaporation and precipitation for Δt, respectively.

Isotope Budget Equation in Each Grid

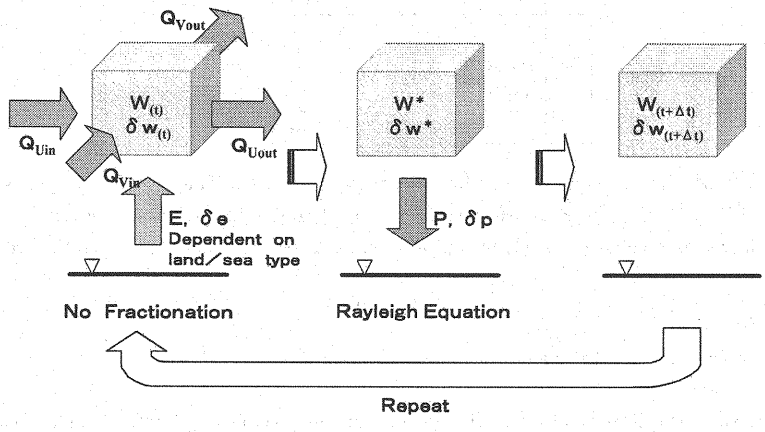

Fig.4 Outline of ICM processes in each timestep

Eq.4 is combined with the isotope-mass balance to form

$$\delta w_{(t+\Delta t)} W_{(t+\Delta t)} = \delta w_{(t)} W_{(t)} + Q_{Uin} \times \left(\delta w_{(t)}\right)_{\mathrm{lon}} + Q_{Vin} \times \left(\delta w_{(t)}\right)_{\mathrm{lat}} - (Q_{Uout} + Q_{Vout}) \times \delta w_{(t)} + \delta e E - \delta p P \tag{5}$$

where δw, δe and δp indicate the isotope ratios of W, E and P. Suffixes "lon" and "lat" denote either adjacent grid, which are determined by whether the value of the fluxes are positive or negative, in the zonal and the meridional directions, respectively.

Only precipitation causes isotope fractionation in accordance with the Rayleigh equation, so that Eq.3 can be modified as

$$\delta w = \left(\left(\frac{W}{W^*} \right)^{\alpha - 1} (1 + 10^{-3} \delta w^*) - 1 \right) \times 10^3 \tag{6}$$

where W and δw denote precipitable water and its isotope ratio, respectively; W^* and δw^* are those just before considering precipitation ($W = W^* - P$); and α is the fractionation factor. Thus, assuming the mass and the isotope balances are conserved, the isotope ratio of precipitation is calculated by

$$\delta w W = \delta w^* W^* - \delta p P$$

$$\delta p = \frac{\delta w^* - \delta w f}{1 - f} \tag{7}$$

where $f = W/W^*$. Finally, the weighted daily mean precipitation isotope ratio is calculated.

Parameterization

In this study, we manipulate the ICM for ^{18}O. The parameters are given as shown in Table1.
An initial δ-values of atmospheric water is set to 0 $\%_{00}$ at all grid points. The ICM runs for the first month (April 1998) to reach an isotopic steady state, and re-runs from 1 April with the δ-value on 30 April in the first run at each grid point.

Correcting Divergence Error of Precipitable Water

Because the water balance in each grid is not always closed when external meteorological data are used,

Table 1 The values of each parameter

α		1.0094 (25°C)(10)
δe	at sea	−9.4 (‰)
	on land (high* lat.)	−15 (‰)
	on land (low* lat.)	−10 (‰)
	* Both 40°N and 40°S are the borders	

precipitable water W diverge as ± 150 (mm/month) at the maximum. Thus, the ICM depends on the method that Eq.5 uses $W_{(t+\Delta t)}$ given by Eq.4. However, in the next time step, precipitable water on the right side of Eq.5 is taken from observed (reanalyzed) precipitable water instead of using $W_{(t+\Delta t)}$ in the previous time step.

RESULTS

Daily Validation in Indochina Peninsula

Fig.5–7 show the ICM results and the observations of precipitation δ^{18}O in three places in Thailand. These figures indicate that ICM reproduced accurately the daily and the seasonal variability of precipitation isotope. The correlation coefficients and RMSEs (root mean square error) are 0.76 and 4.23‰ at Chiangmai (18.8°N, 99.0°E), 0.72 and 4.10‰ at Sukhothai (17.0°N, 99.8°E), and 0.56 and 3.50‰ at Bangkok (13.8°N, 100.5°E), respectively. Note that the lines from the results of ICM in Fig.5–7 are almost continuous for all period, but the bars from observations are intermittent. It implies that the reanalysis generates rainfall almost everyday on these areas.

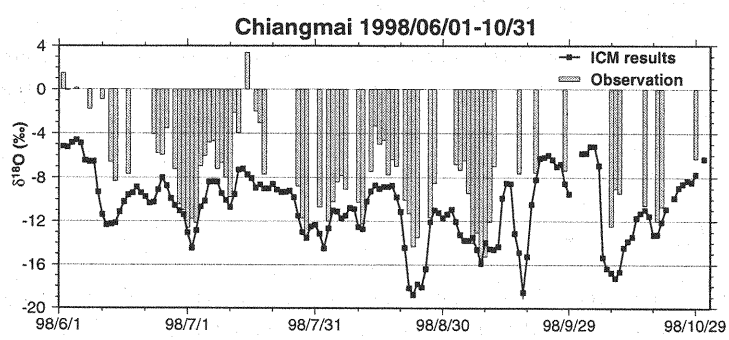

Fig.5 ICM result and the observation (Chiangmai)

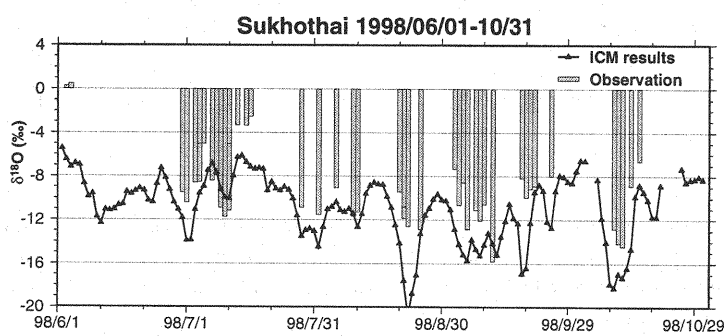

Fig.6 ICM result and the observation (Sukhothai)

Fig.8 shows the variability of the vapor δ^{18}O, the precipitation δ^{18}O, and precipitation amount in the

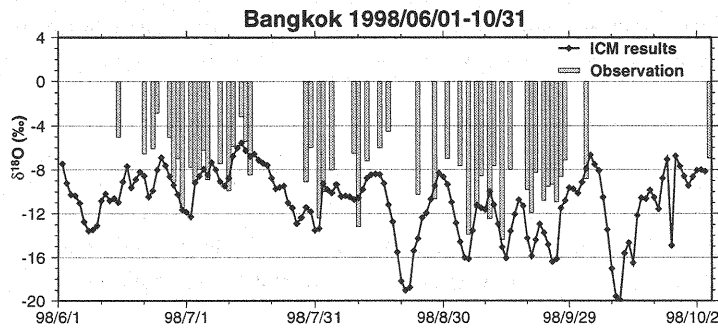

Fig.7 ICM result and the observation (Bangkok)

model. Fig.9 illustrates the relationship between the amount and δ^{18}O of precipitation in Chiangmai, likewise.

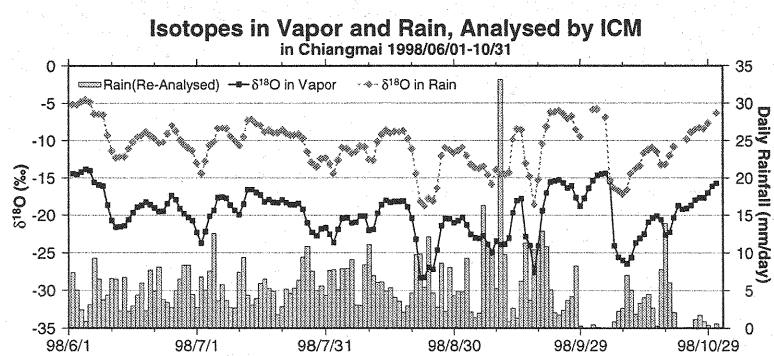

Fig.8 Vapor and rain δ^{18}O and rain amount (Chiangmai)

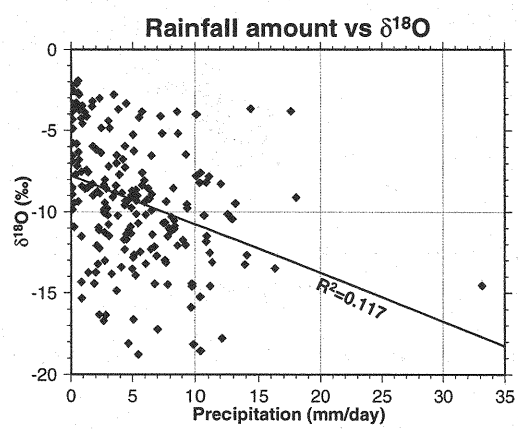

Fig.9 Relationship between daily rainfall amount and δ^{18}O (Chiangmai)

These figures lead us to the following findings:

(a) The fluctuation of precipitation isotope δp corresponds to that of the vapor isotope δq as $\delta p \simeq \delta w + 9$.

(b) There seems to be no close correlation between precipitation amount and its isotope ratio.

These statements possibly concludes that precipitation isotope ratio is affected by the vapor isotope ratio above the observational place, but not by the rainfall amount there. The histories of the vapor (e.g. where the vapor

is originated; how much rainfall it has generated; and which rate the vapor mixes to another vapor) are the primal factors of the precipitation isotope ratio.

Monthly Validation in the Globe

Fig.10 shows the comparison between the monthly precipitation isotope ratio of ICM and the monthly observations of GNIP (Global Network of Isotopes in Precipitation: (11)). Fig.11 is its scattergram. The GNIP data are the weighted monthly mean of precipitation in several years, but the inter-annual variability is not so large as the seasonal or the daily variability, so we used these values for comparison.

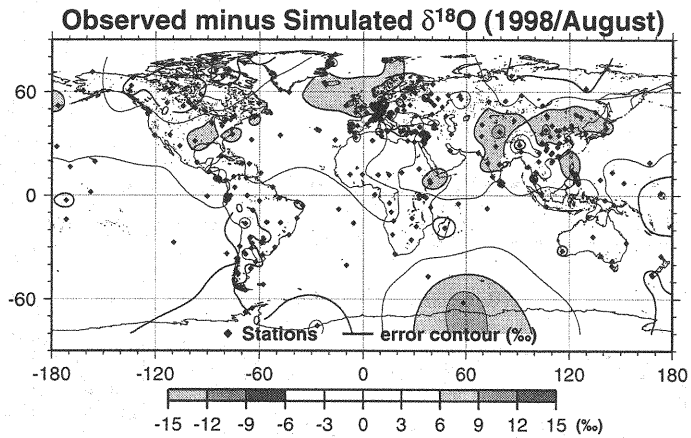

Fig.10 The global comparison between ICM and GNIP (1998 Aug.)

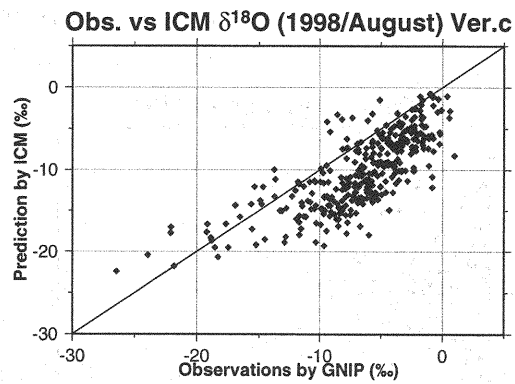

Fig.11 The scattergram of ICM and GNIP (1998 Aug.)

Fig.10 indicates ICM's good reproduction in the oceans, northern Eurasia, South America, Australia, Africa, and Southeast Asia, within 6 ‰ error range. Fig.11 indicates that ICM successfully traced the spatial characteristic on a global scale. The correlation coefficient was 0.76, with a significant level exceeding 99%, and the RMSE was 4.80 ‰. These values are not quantitatively comparable with previous isotope-AGCM studies, because few have verified by site-to-site comparison with observations. However, Vuille et al. (12) have recently reported such site-to-site correlation coefficients of four different model results compared with annual mean precipitation-weighted $\delta^{18}O$ of the 62 IAEA stations in the range of 0.44 to 0.79. Thus, the monthly global reproduction in this study is sufficiently accurate and comparable with other studies for a first order estimate.

However, the isotope ratios in many places are estimated lower than the observations, and these underestimates show the need to improve the ICM. Moreover, the observation sites of GNIP are only 389 and not dense enough to discuss thoroughly the global precipitation isotope distribution. The minimum temporal unit is as long as a month and monthly observation data are not always available. Thus, spatially and temporally denser observation data, such as the observation in Thailand shown in Fig.2 and Fig.3, are expected for the global validation.

DISCUSSION AND FUTURE WORKS

Main Mechanism of the Temporal and Spatial Fluctuation of $\delta^{18}O$

As aforementioned, this study revealed that precipitation isotope ratio is dependent on the isotope ratio of the vapor that generates the rainfall. The isotope ratio of the vapor is quantitatively calculable considering of the fractionation with the condensation and of the water and isotope transport horizontally and vertically on large scale. Moreover, the results quantitatively supported that precipitation isotope in Thailand is dominantly determined by the large-scale atmospheric water circulation processes rather than the local scale rain-forming processes. This description is only applicable in the area of Indochina Peninsula at the present stage. If daily observation increases, however, the validation will be implemented and this understanding, the dominance of the large-scale atmospheric circulation effect with the comparison of the local scale processes, might become popular.

Validity of the Vertical Integrated Modeling to Analyze the Atmospheric Circulation

The vertical profiles of the atmospheric water vapor, the temperature, etc. are not uniform. Nevertheless, the ICM assumes that the vertical atmospheric and isotopic physics are vertically integratable. It regards the atmospheric vapor in each grid as a single-layered uniform mass when the Rayleigh equation is applied for the fractionation. However, with the well reproduced results shown in the last section, the modeling seems to be adequate enough as the first order for the global scale atmospheric isotope circulation. In particular, the large convective rainfall amount in Thailand during the rainy season can support the validity of the vertical integrated model more rigidly. This validity of the vertical integration in the atmospheric and isotopic circulation can be regarded as a new knowledge of this research field. Without considering detailed atmospheric physics, this precipitation isotope reproduction can give us information about the possibility of the utilization of the vertical integration model and provides the reliability of tools that adopt this concept. Though, verification in various area, such as high-latitude or the winter hemisphere, which seem to have weak convective activities, are necessary.

Reliability of the Dataset

The rainy days by the reanalysis (shown as bars in Fig.8) and those by the observation (shown as bars in Fig.5) are very different. This implies the roughness of precipitation accuracy in the reanalysis. Because of the spatial distribution problem between the area-averaged data and the point data, the difference is considerable. Moreover, the horizontal atmospheric water transport surpass the vertical transport (e.g. precipitation and evaporation). Nevertheless, the results show good reproduction. This possibly implies that the reliability of the reanalyzed vertical integrated water vapor fluxes.

Improvement of ICM

The sensitivity analysis for the parameter α and δe will be held and more adequate parameters will be set in the future. Further, changing the model itself will be planned. For example, among the assumptions written in Model Description section, assumption (e) can be improved by incorporation of feedback mechanism

of precipitation isotopes to isotope ratio of evaporation, and assumption (d) can also be improved by taking into account of variety of fractionation factor α with ambient humidity and temperature.

CONCLUSION

This study has developed the vertical integrated two dimensional water isotope circulation model. Then, it verified its output with the daily observations of the precipitation isotope in Thailand and had a success to reproduce the daily precipitation isotope ratio in good correlation. Moreover, this study showed good results with the monthly global observation.

Our findings reveal that the precipitation isotope ratio is determined by the vapor isotope ratio above the observational place but not by the rainfall amount. Furthermore, the isotope ratio of the vapor can be calculated by quantitatively regarding the fractionation at its condensation and the water vapor transport.

Then, the vertical integrated modeling has been validated as adequate enough as the first approximation of the large-scale atmospheric isotope circulation. Consequently, with this imformation we are able to estimate the temporal and spatial fluctuations of the precipitation isotopes without considering the detailed atmospheric physics in the vertical direction.

Moreover, the model can also be used for the reliability test of the water vapor transport in a dataset. This knowledge can be applied to enhancing the reliability of new tools with the dataset to analyze the behavior of the atmospheric circulation. The trajectory analysis and the vapor tagging analysis can be used as a tool.

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APPENDIX - NOTATION

The following symbols are used in this paper:

E	=	evaporation
f	=	fraction of material remaining
P	=	precipitation
Q_{Uin}, Q_{Uout}	=	vertical integrated water vapor inflow and outflow in zonal direction
Q_{Vin}, Q_{Vout}	=	vertical integrated water vapor inflow and outflow in meridional direction
R	=	isotope ratio (the ratio of the heavy to light isotope concentration)
R_S	=	isotope ratio of the standard water
R_A, R_B	=	isotope ratios of water in phase A and B
R_0	=	isotope ratio of initial water before its amount changes by phase transition of water (such as evaporation, condensation, etc.)
t, Δt	=	time and time step in the model
W	=	precipitable water (total column water vapor)
W_0	=	initial amount of (precipitable) water before the amount changes by phase transition of water
$W_{(t)}$	=	precipitable water at any time, t
$W_{(t+\Delta t)}$	=	precipitable water at next time step, $t + \Delta t$
W^*	=	precipitable water just before precipitation (condensation) takes place
α	=	the isotope fractionation factor
$\delta^{18}\mathrm{O}$	=	oxygen isotope ratio relative to a standard in units of parts per thousand ($‰$), referred as delta-value in the manuscript
$\delta^{18}\mathrm{O}_0$	=	isotope delta-value of initial water before its amount changes by phase transition of water
δe	=	isotope delta-value of evaporated water
δp	=	isotope delta-value of precipitated water
δw	=	isotope delta-value of precipitable water
$\delta w_{(t)}$	=	isotope delta-value of precipitable water at any time, t
$\delta w_{(t+\Delta t)}$	=	isotope delta-value of precipitable water at next time step, $t + \Delta t$
$\left(\delta w_{(t)}\right)_{\mathrm{lon}}$	=	isotope delta-value of precipitable water on adjacent upstream grid in longitudinal direction at any time, t
$\left(\delta w_{(t)}\right)_{\mathrm{lat}}$	=	isotope delta-value of precipitable water on adjacent upstream grid in latitudinal direction at any time, t
δw^*	=	isotope delta-value of precipitable water just before precipitation (condensation) takes place

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