# D2.2: Software implementation of new ice core and marine core relevant code in UKESM1 to enable testing against water isotope measurements

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## About this document

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# Summary for publication


Stable water isotope measurements from ice and marine cores are used to generate proxy climate data for past climates. For example, isotope measurements from Antarctic ice cores have been used to estimate temperatures over the last 800,000 years (Jouzel et al., 2007). However, there are uncertainties in the methods used to derive the proxy climate data (Sime et al., 2009). This can make it challenging to assess past climate model simulations using proxy data derived from ice and marine cores, as differences can be due to the model or the proxy data being incorrect. This difficulty can be reduced by modelling water isotopes in the past climate simulations and then directly comparing the modelled values with the measured core data. Work by EU-TiPES has shown the value of water isotope enabled models (Malmierca-Vallet et al., 2020; Goursaud et al., 2021; Oger et al., 2023).

As part of the EU-TiPES project, a major code development has been carried out in the UK Earth System Model (UKESM) towards modelling stable water isotopes in this state-of-the-art ESM. Code which adds water tracers (model fields that track water around the model's hydrological cycle) has been developed for the atmosphere and land components (McLaren et al., in prep). The addition of these water tracers is a necessary step for adding water isotopes to an ESM and requires the most effort overall: water isotopes are a particular (sub)type of water tracer. Our new water tracer code can track water starting from where it evaporates at the surface, through the cloud and transport processes of the model, to where it eventually falls back to the ground as precipitation. This new capability provides new information on the hydrological cycle in the model and aids understanding of how the model works in an integrated sense.

Alongside the basic UKESM tracer work, we developed novel water tracers that provide information on the surface evaporative properties. These were initially tested in the (simpler) atmosphere component of the Alfred-Wegener Institute ESM, jointly under EU-TiPES and EU-DEEPICE (Gao et al., 2023). We subsequently then implemented this novel type of tracer in the UKESM (solely under EU-TiPES).

Testing shows that results from the two models are broadly consistent. This provides evidence that both EU-TiPES code developments are working as expected. The test also uncovered interesting differences that indicate these novel tracers can be used to diagnose contrasting hydrological cycles in the two models over Greenland, Antarctica and South Asia (McLaren et al., in prep.).

A key objective of this code development work was to ensure the longevity of the new tracer capabilities in the UKESM. This has now been achieved by implementing the code in the main trunk of the models' code repositories. This required that our code passed through the required review and approval process. As a result, the new code now resides in the main source code for the UKESM and is accessible to UKESM collaborators via the Met Office Science Repository Service. In total, 23,000 lines of Fortran code have been added to the UKESM's atmosphere and land component.

The importance of this new water tracer capability is recognised through its further development planned under the three subsequent NERC projects (PRESCIENT, SURFEIT, and SWAIS-2C) with scientific uses being developed under two additional NERC projects (KANG-GLAC and EXTANT) which will help complete, maintain, and use the EU-TiPES water isotope development.

The water tracer software implementation is a EU-TiPES deliverable and this is a short accompanying report describing the code development.

# Work carried out

Water tracers are valuable diagnostic tools for understanding the model's hydrological cycle and have been used to find the source locations of precipitation in models. Stable water isotopes can be considered a special type of these water tracers. A water tracer follows (normal) water throughout the model; it undergoes the exact same processes and pathways. Our tracers are passive, in that they have no impact on the physics of the underlying model. In modelling terms, water isotopes are a water tracer that undergo isotopic fractionation during phase changes, but are still passive.

**Code Development**

The implementation of water isotopes in the UK Earth System Model (UKESM; Sellar et al., 2019) has been separated into two components:

1) the addition of an array of water tracers into the model;
2) the inclusion of isotopic fractionation processes which enable a water tracer to represent a water isotope.

The first task requires the largest effort (Noone and Sturm, 2010). The focus of the work has been on the atmosphere component (Met Office Unified Model, UM; Brown et al., 2012) and the land surface component (Joint UK Land Environment Simulator, JULES; Best et al., 2011; Clark et al., 2011), which are the two most time consuming model components for the implementation of water isotopes. The code development in the UM was carried out by the British Antarctic Survey (BAS) with a contribution from the National Centre of Atmospheric Science (under contract to BAS), whilst the work on JULES was started at the University of Bristol and then latterly continued by BAS.

The first stage of the water tracer implementation was largely technical and established the infrastructure for the tracers within the UM. This involved adding a water tracer array to the model prognostic variables (including the input and output files) and setting up user-defined controls on the number and types of water tracers.

Once the infrastructure was set up, the scientific code development began on the atmospheric model. This involved adding water tracers to all the model processes that impact water in the model *i.e.* surface evaporation, large-scale advection, boundary layer mixing, large-scale precipitation, cloud microphysics and convection. This was a major task particularly for the cloud microphysics and convection schemes where the water tracers were plumbed through these highly complex schemes to ensure that they tracked all water processes as precisely as possible.

The code development in the Land Environment Simulator JULES was progressed alongside the UM work. For JULES, the water tracers needed to be passed through the following schemes: surface exchange (*i.e.* calculation of the evaporative flux), snow scheme, hydrology and river routing. Adding water tracer to the surface exchange scheme proved to be very challenging due to the method used to calculate the implicit solution in JULES. However, a method has been developed and implemented for water tracers.

## Code Testing

Rigorous testing was carried out on the water tracer code to ensure that the following scientific conditions were met:

1) The tracers are passive - the presence of water tracers in the model had no impact on the evolution of the underlying model.
2) The tracers are accurate - the water tracers tracked water as precisely as possible.

The second condition here was particularly difficult. This was due to the complexity of the hydrological cycle in the UM. It was found that numerical error could build up very quickly and cause the water tracer to diverge from the model default water field. Other standard technical tests were carried out such as ensuring the results remained unchanged when using a different configuration of processers when running the model.

## Code Management

The code for the UM and JULES is managed by the Met Office and regular new versions are produced. Given that these are operational models, there are strict working practices for code development. When developing code for these models, a 'branch' is made from the base code (the code 'trunk') and the new code is added to the branch. After the code has been fully developed and tested, the work undergoes a review and approval process. This includes both a Scientific/Technical review and a Code/System review by relevant experts. The code is also required to be tested in a test suite of standard model configurations, which aims to highlight any problems or change in results. When the new branch has successfully gained full approval, the new code is added to the code trunk and is then included in the next code version.

A major aim for this work was to ensure the longevity of the new water tracer/isotope code. This requires getting the new code into the model code trunks for both the UM and JULES, so the code does not become outdated. It is also highly beneficial to have the code thoroughly reviewed and tested.

The water tracer model development is a large amount of code and it has been necessary to split the code into several branches to make the development and review process manageable. This is detailed in the next section. As the water tracers are a new scientific development, a test configuration was created and added to the official test suite for the UM, which means that all future developments are tested in a model run containing water tracers and any potential problems are flagged up during the approval phase. This further helps to ensure that the water tracer code continues to work as expected whilst the underlying model is continually developed.

# Main results achieved

**Water tracer code committed to the UM trunk:**

UM13.1 release (Nov 2022): Water tracer infrastructure branch

UM13.2 release (Mar 2023): Water tracer top level branch
Water tracer boundary layer branch
Water tracer microphysics branch
Water tracer convection branch
Water tracer large scale precipitation branch
Water tracer test configuration branch

UM13.3 release (Jul 2023): Water tracer technical improvements branch (a few minor improvements requested by Met Office)

Branches under development to be submitted to future releases:
Water tracer UM/JULES coupling

**Water tracer code committed to the JULES code trunk:**

JULES 7.4 release (Nov 2023): Water tracer surface exchange branch

JULES 7.5 release (early 2024): Water tracer snow branch is currently under review

Branches under development to be submitted for future releases:
Water tracer hydrology branch
Water tracer river routing branch
Water tracer infrastructure branch

A total of approximately 23,000 lines of Fortran code have been added to the UM and JULES during this development. Figure 1 shows the number of added lines for the different scientific areas. The UM and JULES code (including the committed water tracer code) is available to UKESM collaborators through the code repository (the Met Office Science Repository Service).

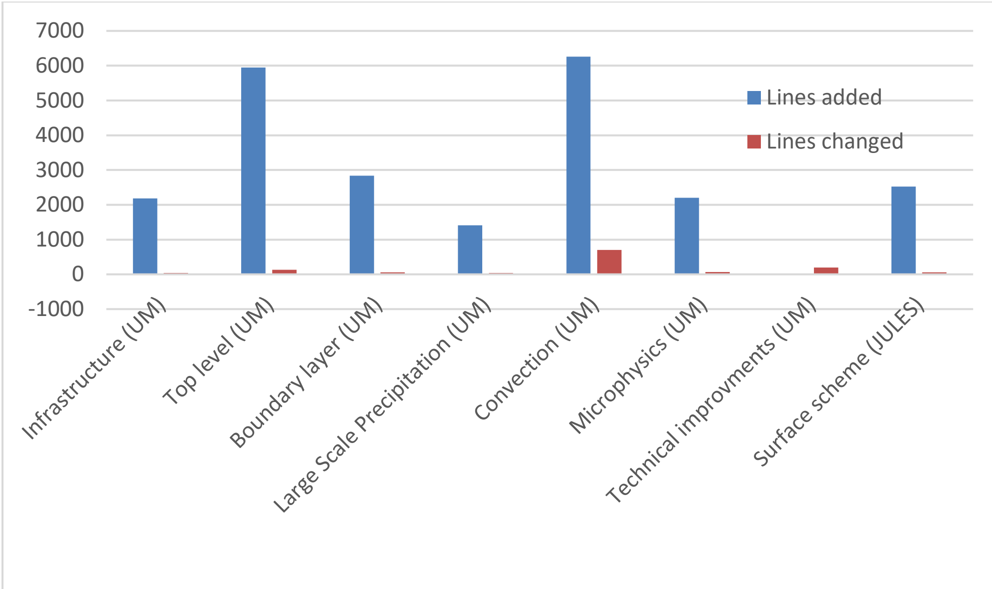


Figure 1: Number of lines of Fortran code added (blue bars) or changed (red bars) during the water tracer code development

# Progress beyond the state of the art

As well as implementing the code to the highest standard in the trunk, our new tracer capability has been further developed to track the pathways of water evaporating from the surface, together with the water's properties. Novel water tracers proposed by Fiorella et al. (2021) were further developed and initially tested in the ECHAM6 atmospheric model in collaboration with the EU-DEEPICE project (Gao et al, 2023). These tracers are named here as 'scaled-flux' tracers and efficiently provide the mass-weighted mean value of a source property of precipitation in the model (such as latitude or surface temperature). The same scaled-flux water tracers were then implemented in the UM as part of EU-TiPES, which allows direct comparison between the UM and ECHAM6. Standard water-tagging tracers (e.g. Koster et al., 1986; Werner et al., 2001) have also been added to the UM which track water evaporating from prescribed regions. Both types of water tracers can provide information on water pathways within the atmosphere that can help with interpreting ice core data.

For the first time, water tracers have been included in a historical simulation of the UM which was run for 35 years starting in 1979 (McLaren et al., in prep.). The results presented here are mean values for the 30-year period, 1985-2014. The simulation used: 1) water tagging tracers to separately track the water evaporated from land, open ocean and sea ice; and 2) scaled-flux water tracers to find the mass-weighted mean latitude and longitude of the *oceanic source* of precipitation. The water tracer results were compared to an ECHAM6 simulation run over the same period with identical forcing.

The results of the water tagging tracers show that the majority of precipitation is sourced directly from the ocean as expected (Figure 2). Water sourced from land evapotranspiration generally precipitates over land, however, there is some contribution to ocean precipitation (e.g. to the east of southern South America). Precipitation sourced from land has a strong seasonality with the largest values occurring in summer, particularly in the Northern Hemisphere, in agreement with other studies (Trenberth et al., 2007;

Dirmeyer and Brubaker, 2007). Sublimation from sea ice only contributes a small amount to precipitation locally over sea ice regions in spring and summer.

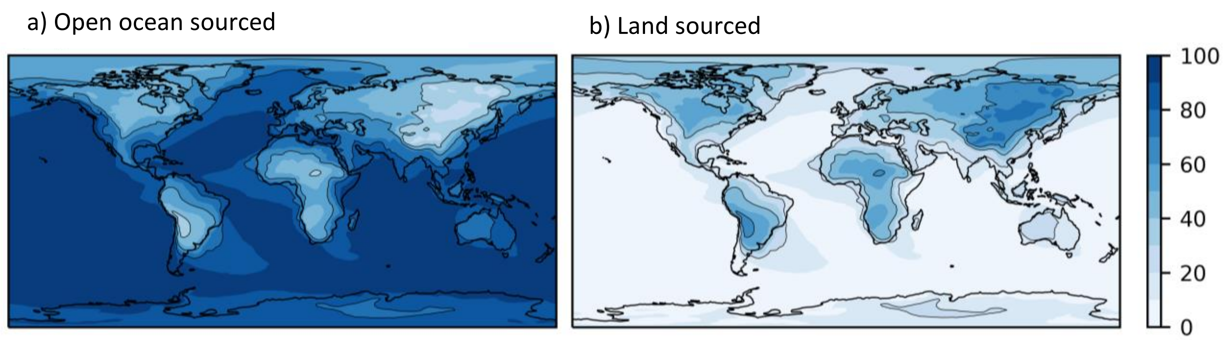


Figure 2: Percentage of annual mean precipitation from the 30-year UM simulation that has been sourced from: a) the open ocean; b) the land.

The comparison between the scaled-flux water tracers in the UM and ECHAM6 shows broad agreement in the results but with some interesting differences that will be explored in future work. For example, there is a difference in the ocean source latitude of the precipitation over South Asia (Figure 3). The UM sources ocean water from a more southerly location than ECHAM6. There are also differences over Greenland and Antarctic that warrant further investigation.

In conclusion, the water tracer results look sensible and are comparable to ECHAM6. This gives confidence that the new UM code is working correctly. The differences in the water tracers between the UM and ECHAM6 illustrate how useful the water tracers can be in investigating how the hydrological cycle contrasts between models.

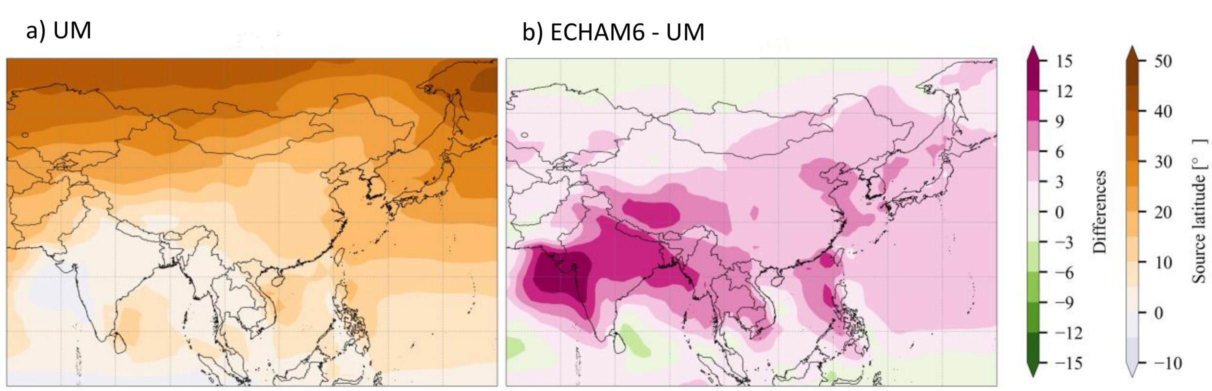


Figure 3. a) The mass-weighted mean source latitude of the annual mean (ocean sourced) precipitation falling over Asia for the 30-year UM simulation; b) the ECHAM6 – UM difference for the same field.

# Impact

## How has this work contributed to the expected impacts of TiPES?

The scientific achievements outlined in Section 1 will significantly contribute to the expected impacts formulated in the call:

| Expected impact | TiPES outcome/results | Contribution to expected impact |
|---|---|---|
| **"Supporting major international scientific assessments such as the IPCC"** | TiPES will put forward guidelines for improving the accuracy and reliability of climate models, model selection, and computation of TPs across the model hierarchy. Shortcomings in the present generation of earth system models will be investigated. New EMIC and ice sheet model parameterizations will be generated; the boundary conditions for TEs will be better defined for all models; and new ESM (isotope) code will be written to enable more appropriate model-data evaluations. (WP2-5/O1). | New water tracer code is now included in the UKESM atmosphere and land components as a result of TiPES. We chose to develop the new code ready for the 2nd version of the UKESM as this will be used in CMIP7.<br><br>Sime is the work group lead for the AR7 CMIP7-PMIP Interglacials group ([https://www.pmip-interglacials.de/overview/about-us/](https://www.pmip-interglacials.de/overview/about-us/)). This will ensure that all TiPES water tracer developments in UKESM will be used in the next PMIP. |
| **"increase confidence in climate change projections"** | TiPES will assess and improve the parameterisations of comprehensive ESMs (in particular EC-Earth, HadGEM3/UKESM, and CESM) of the CMIP-6 class to improve the representation of TEs in a collaborative effort of WPs 1-3 (O1). | TiPES has added a new hydrological diagnostic tool (water tracers) to the UKESM. This will allow improved understanding and assessment of the model's hydrological cycle, with the potential to improve parameterisations. (The water tracer code is accessible to UKESM collaborators via the Met Office Science Repository Service.) |
| | TiPES will give rigorous estimates of the relative impacts of uncertainties in the reliability of EWS, safe operating spaces, and TPs combined with political uncertainties. | The new TiPES water tracing capability in the UKESM will help identity which uncertainties are most important to improve reliability of the model's hydrological cycle. |
| | TiPES integrates EU leading climate science with novel approaches from non-equilibrium statistical mechanics, stochastic processes, time-series analysis, and dynamical systems theory that will be relevant to a much wider class of complex multi-scale systems. In particular, WP4 and WP5 strengthen the physico-mathematical basis of the study of TPs and the overall methodological underpinnings. | Sime has taught at two week-long EU-Beyond Epica summer schools which are training our next generation of PhD students. |
| | TiPES is strongly embedded in the climate science community, with PIs, Co-PIs and Steering Committee Members of projects such as PAGES, Past Earth Network, RISE actions, CMIPs and PMIPs (including the deep-time versions PlioMIP and DeepMIP), Copernicus Climate Services, CliMathNet, MCRN, SIAM MPE, CLIMCOR, EU-PolarNet, Blue Action, | This work has involved close collaboration with the EU DEEPICE project (see below for further details.)<br><br>Future work will involve using the new water tracer code in the following NERC projects: SURFEIT, SWAIS-2C, PRESCIENT, KANG-GLAC |

| | | |
|---|---|---|
| | CRESCENDO, East-GRIP, Oldest Ice, ITNs, ERC and other prestigious national and international grants. Among the TiPES team members there is a Lead Author of IPCC's AR3 and coordinating Lead Author of AR4, as well as two Lead Authors of IPCC's AR5, and five EGU medallists. | and EXTANT (see below for further details). |

*Table 4: TiPES expected impacts*

# Lessons learned and Links built

Links have been built with the following international projects and institutes:

- EU DEEPICE MSCA-ITN programme: Understanding Deep Ice Core Proxies to Infer Past Antarctic Climate Dynamics 15 PhD students. Sime leading one student project which has involved further development of water tracers in the atmospheric model ECHAM with close collaboration with the TiPES UM development detailed in this report. This has resulted in the TiPES publication, Gao et al. (2023).
- NERC's new National Capability International program (includes ~twenty EU partners). SURface FluxEs In AnTarctica: SURFEIT. UK NERC contribution is 2.5m (PI Sime).
- Ten nation drilling based project (including several EU nations): The Sensitivity of the West Antarctic Ice Sheet to +2C: SWAIS-2C. UK NERC contribution is 2.8m (CI Sime).
- Marin core and modelling project: "Assessing ocean-forced, marine-terminating glacier change in Greenland during climatic warm periods and its impact on marine productivity (KANG-GLAC)". UK NERC contribution is ~3m (CI Sime).
- NERC's new "Drivers and Impacts of Extreme Weather Events in Antarctica (ExtAnt)" program. UK NERC contribution is 2m (CI Sime). UK NERC contribution is ~3m (CI Sime).
- NERC's new National Capability Single Science (NCSS) "PRESCIENT: UK Polar Research Expertise for Science and Society". UK NERC contribution is ~5m (CI Sime).
- Alfred Wegener Institute (AWI): Productive collaboration with the water tracer/isotope modelling expert Martin Werner.
- Met Office: Successful working relationships established with the Simulation Systems and Deployment team and various scientific and technical experts involved in the code review process.

Lessons learnt include:

- The split of the model development between BAS and the University of Bristol worked well with excellent collaboration between the groups.
- The National Centre for Atmospheric Science (NCAS) was contracted by BAS for a period at the start of the project. This proved to be hugely beneficial to establish the technical infrastructure for the development and to provide technical support throughout the project.
- The original objective of this work was to implement water tracers, including isotopes, in the UKESM. This has proved to be extremely ambitious in the timeframe of the project. The most significant part of this work has been completed (i.e. adding water tracers). However, the work of adding water isotopes to all model components is still on-going. There are several reasons for this:

- The atmosphere and land components of the UKESM are very complex models. They are both used in a range of configurations (e.g. for weather forecasting). The hydrological cycle within the models is distributed across many different scientific areas, therefore, significant time was required to become familiar with the models and to plan the water tracer development.
- In order to achieve a high degree of accuracy for the water tracer tracking, it was necessary to plumb the water tracers fully through some of the complex atmosphere schemes (e.g. convection), rather than attempt to use diagnostic output from these schemes. This was time-consuming and was difficult to predict until the development was underway.
- The code review and approval process (described in 'Worked Carried Out') is a vital part of the model development process, which improves and thoroughly tests the new code and ensures the longevity of any development. However, this did increase the amount of time required for this development.
- Covid made it more challenging to start this code development through the effects on the hiring process and subsequently through a lack of in-person meetings.

## Relations to the TiPES crosscutting themes and objectives

The water tracer code development relates to TiPES Theme 1 'Tipping Elements in data and models' as it is a necessary (and the most labour intensive) step towards adding water isotopes to an ESM. Modelled water isotopes can be directly compared with measured values to evaluate the model's skill at simulating tipping elements in past climates.

The relevant TiPES Objective for this work is Objective 1, 'Identify tipping elements (TEs) and their interactions in models and data.' The ambitious aim for TiPES was to have water isotopes included in the UKESM and to use these to directly compare measured and modelled isotope values in past climates for model evaluation. The TiPES water tracer code development has made huge progress towards this goal, but the final aim of having isotopes in the model has not been achieved yet for reasons discussed above. However, the development of the water tracer code in the UKESM will be continued through the NERC projects SURFEIT, SWAIS-2C and PRESCIENT projects. This will help complete and maintain this important work, which will then enable output from simulations used to investigate tipping elements in the past, to be evaluated with marine and ice core data. TiPES will be acknowledged in any future relevant publications.

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# Dissemination and exploitation of TiPES results

## Dissemination activities

| Type of dissemination activity | Name of the scientist (institution), title of the presentation, event | Place and date of the event | Estimated budget | Type of Audience | Estimated number of persons reached | Link to Zenodo upload |
|---|---|---|---|---|---|---|
| Website | Louise Sime, BAS report on Antarctic Tipping Points | Online 01/06/2023 | | Scientific Community, Public | 1000s | Antarctic tipping points - British Antarctic Survey (bas.ac.uk) |
| Participation to a conference | Louise Sime (BAS), Dansgaard-Oescger events in models and reality (20 min talk), Willi Dansgaard Symposium | Copenhagen 02/09/2022 | | Scientific Community | 200 | |
| Participation to a workshop | Louise Sime (BAS), Overview of WP2 Tipping Events in Models (20 min talk & discussion), TiPES Workshop | Exeter 12/09/2022 | | Scientific Community | 100 | |
| Participation to a conference | Louise Sime (BAS), The Last Interglacial: Southern Ocean Warming (Poster), IPICS Open Science Conference | Crans-Montana, Switzerland 03/10/2022 | | Scientific Community | 500 | |
| Participation to an Event other than a Conference or a Workshop, | Louise Sime (BAS), Dansgaard-Oescger events in climate modetls (1hr invited seminar), National Oceanography Centre | Southampto n 20/10/22 | | Scientific Community | 150 | |
| Participation to an Event other than a Conference or a Workshop, | Louise Sime (BAS), The Last Interglacial: in Antarctic ice cores and models (1hr invited seminar), University of Victoria, NZ | Wellington, NZ 05/12/2022 | | Scientific Community | 40 | |
| Participation to an Event other than a Conference or a Workshop, | Louise Sime (BAS), The Last Interglacial: in Antarctic ice cores and models (1hr invited seminar), University of Dunedin | Dunedin, NZ 09/03/2023 | | Scientific Community | 50 | |
| Participation to a workshop | Louise Sime (BAS), The Last interglacial: in Antarctic ice cores and models (1st 30 min key note talk), GRISO Workshop | Bergen, Norway 19/04/2023 | | Scientific Community | 150 | |
| Participation to a workshop | Alison McLaren (BAS): The Introduction of Stable Water Isotopes to the UK Earth System Model (UKESM2) (Poster), Water Isotopes: 'From Weather to Climate' Workshop. | Online 15/11/2021 | | Scientific Community | 40 | |

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|---|---|---|---|---|---|---|
| Participation to a workshop | Merve Gorguner (U. Bristol): Stable Water Isotope Incorporation in the Joint UK Land Environment Simulator (JULES) Model (Poster), Water Isotopes: 'From Weather to Climate' Workshop. | Online 15/11/2021 | | Scientific Community | 40 | |
| Participation to a conference | Alison McLaren (BAS): The Introduction of Stable Water Isotopes to the UK Earth System Model (UKESM2) (Poster), IPICS Open Science Conference | Crans-Montana, Switzerland 02/10/22 | | Scientific Community | 500 | |

## Peer reviewed articles

| **Title** | **Authors** | **Publication** | **DOI** | **Is TiPES correctly acknowledged?** | **How much did you pay for the publication?** | **Status?** | **Open Access granted** |
|---|---|---|---|---|---|---|---|
| Sea ice feedbacks influence the isotopic signature of Greenland ice sheet elevation changes: Last interglacial HadCM3 simulations. | Malmierca-Vallet, I. , Sime, L. C. , Valdes, P. J. and Tindall, J. C. | Climate of the Past | https://doi.org/10.5194/cp-16-2485-2020 | Yes | Don't know | Published | Yes |
| Antarctic Ice Sheet elevation impacts on water isotope records during the Last Interglacial. | Goursaud, S., Holloway, M., Sime, L., Wolff, E., Valdes, P., Steig, E. J., and Pauling, A. | Geophysical Research Letters | https://doi.org/10.1029/2020GL091412 | Yes | Don't know | Published | Yes |
| Evaporative controls on Antarctic precipitation: An ECHAM6 model study using innovative water tracer diagnostics | Gao, Q., L. C. Sime, A. J. McLaren, T. J. Bracegirdle, E. Capron, R. H. Rhodes, H. C. Steen-Larsen, X. Shi, and M. Werner | The Cryosphere | https://doi.org/10.5194/egusphere-2023-1041 | Yes | Don't know | Accepted | Yes |

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| Decoupling of δ18O from surface temperature in Antarctica in an ensemble of Historical simulations | Oger, S., Sime, L., and Holloway, M. | EGUsphere (preprint) | https://doi.org/10.5194/egusphere-2023-2735. | Yes | Don't know | Submitted | Yes |
| Implementation of Water Tracers in the Met Office Unified Model | McLaren, A.J., L. C. Sime, S. Wilson, J. Ridley, Q. Gao, M. Gorguner, G. Line, M. Werner, P. Valdes. | | | | | In preparation | |

**Uptake by the targeted audiences**

As indicated in the Description of the Action, the audience for this deliverable is

| | |
|---|---|
| X | The general public (PU) is and is made available to the world via [CORDIS.](https://cordis.europa.eu) |
| | The project partners, including the Commission services (PP) |
| | A group specified by the consortium, including the Commission services (RE) |
| | This reports is confidential, only for members of the consortium, including the Commission services (CO) |

**This is how we are going to ensure the uptake of the deliverables by the targeted audiences:**

This work is a very large model development due to the complexity of the hydrological cycle and the UKESM. The importance of this new water tracer capability is recognised through its further development planned under the three subsequent NERC projects (PRESCIENT, SURFEIT, and SWAIS-2C) with scientific uses being developed under two additional NERC projects (KANG-GLAC and EXTANT) which will help complete, maintain, and use the EU-TiPES water isotope development. Future work will include publicising the new model development through published papers and presentations (which will acknowledge EU-TiPES funding) and supporting UKESM collaborators to use the new capability.