

CARBON ATMOSPHERIC TRACER RESEARCH TO IMPROVE NUMERICAL SCHEMES AND EVALUATION



CATRINE

Carbon Atmospheric Tracer
Research to Improve
Numerics and Evaluation

D2.1 IFS tracer advection scheme with improved properties for accurate estimation of emissions in CO2MVS

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1 Executive Summary

The CATRINE project evaluates and improves numerical schemes for tracer transport in the new Copernicus anthropogenic CO₂ emissions Monitoring and Verification Support capacity (CO2MVS), and more broadly within the Copernicus Atmosphere Monitoring Service (CAMS). This report refines and extends the developments proposed in CATRINE deliverable D1.2 (Malardel et al., 2025), which were based on the analysis, findings, and recommendations presented in deliverable D1.1 (Diamantakis et al., 2025). The latest developments provide substantial gains in the mass conservation and transport accuracy of the IFS, resulting in an improved advection scheme for the global CO2MVS model that will support more accurate estimates of greenhouse gas emissions. The report concludes with specific recommendations for the IFS advection scheme to improve the accuracy of both CO2MVS inversions and CAMS forecasts.

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2 Introduction

2.1 Background

Work packages 1 and 2 of the CATRINE project, WP1 and WP2 respectively, focus on improving the conservation properties and accuracy of numerical algorithms for solving the transport equations in the IFS model. The semi-Lagrangian (SL) advection scheme is a numerical discretisation method for solving the partial differential equations (PDEs) that describe the resolved, non-parametrized component of atmospheric transport driven by atmospheric dynamics. While the SL method is accurate, monotonic, and positive-definite, it does not inherently conserve mass except under idealised conditions that are rarely met in practice. As a result, it can introduce mass conservation errors. These errors are particularly relevant in atmospheric composition and climate simulations where conservation is critical.

To address this issue, IFS includes mass-fixer algorithms that adjust tracer concentrations after advection to restore global mass conservation. These methods have evolved from early two-dimensional approaches (Bermejo and Conde, 2002) to more advanced three-dimensional implementations (Diamantakis and Agusti-Panareda, 2017). The fixers preserve monotonicity and positive-definiteness and have been shown to improve greenhouse gas (GHG) simulations and the water and energy balance and the skill of high-resolution Ensemble (probabilistic) forecasts (Rackow et al, 2025). However, these corrections are applied independently of the governing equations, and they can be large in certain situations, such as plume tracer transport. Additionally, as the mass fixer corrects the global mass error, in situations where the global mass conservation error is large, there is a risk that the mass fixer correction may also affect regions without error. This risk is limited by the weighted approach adopted by the Diamantakis and Agusti-Panareda, 2017 mass fixer algorithm but it is not perfect. Therefore, for these reasons it is desirable to reduce the need for mass fixing by limiting conservation errors during the advection process itself. This should improve both the advection scheme and the estimation of surface fluxes.

Substantial progress on this problem was made in CATRINE WP1. WP2 extends this work, with further improvements in the conservation properties and overall accuracy of IFS. These developments support more accurate estimation of greenhouse gas emissions, which is a key objective of CO2MVS. The following sections outline the recent progress, its implications for CO2MVS and CAMS, and the resulting recommendations for the model configuration to be used in both services.

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverable

The objective of this deliverable is to finalise numerical method developments related to the IFS advection scheme that were initiated in CATRINE WP1 and summarised in deliverable D1.2 (Malardel et al., 2025). These developments improve the mass conservation properties and overall transport accuracy of the global CO2MVS model, IFS and are gradually released in IFS model cycles 50 and 51. They have been tested using realistic CO₂ flux protocols defined in WP5 and WP8. In addition, an alternative formulation of the continuity equation in terms of dry air is tested and a preliminary evaluation of the impact of the newly developed schemes is conducted using an experimental OSSE inversion system. Recommendations for further integration of these developments into CO2MVS are made.

2.2.2 Work performed in this deliverable

This deliverable report builds on work presented in the two previous CATRINE deliverables D1.1 (Diamantakis et al., 2025) and D1.2 (Malardel et al., 2025). Hereafter, these will be referred to as D1.1 and D1.2, respectively.

A major conclusion of D1.1 was that the interpolation limiter, which filters physically unrealistic tracer concentrations that the IFS advection scheme may occasionally produce, has a major impact on the mass conservation properties of IFS. D1.1 therefore identified this as a critical area for improvement. The challenge was to provide an alternative limiter with better conservation properties without degrading accuracy. In this context, a new limiter, LQM3DCONS, was presented in D1.2. For plume-type simulations, this limiter reduces the conservation error by a factor of 4 to 5 while maintaining the overall accuracy of IFS. This report takes a further step by extending the scheme within the more sophisticated three-dimensional ILMC algorithm of Sørensen et al. (2013). In plume cases, this reduces the conservation error of the original scheme by up to two orders of magnitude and achieves a nearly conservative advection scheme, for which mass fixer corrections are very small.

The development of the sweep-interpolation SL scheme of Mortezaazadeh et al. (2024) has also been completed. Simulations using WP5 and WP8 flux protocols show that both developments, which can be combined, reduce biases and the standard deviation of errors while substantially improving the conservation properties of the IFS advection scheme. In addition, the tangent-linear and adjoint counterparts of the mass fixer used in IFS to keep the global mass of tracers constant during advection have been developed, together with the tangent-linear and adjoint versions of the sweep semi-Lagrangian interpolation scheme. These developments have enabled tests using the OSSE system described in D1.1 to help establish an optimal configuration for an inversion system. Work has also progressed on alternative forms of the continuity equation that can conserve the dry mass of air and impose a more physically consistent mass-conservation constraint, enabling improved seasonal variability of atmospheric mass and a more accurate representation of tracer mixing ratios consistent with satellite observations.

As presented in the following sections, the latest results indicate substantial improvements in IFS mass conservation and transport accuracy, exceeding those achieved in Task 1.2 of WP1 and were summarized in D1.2. These results allow concrete recommendations to be made on the most suitable options for CO2MVS and CAMS atmospheric composition forecasts.

2.2.3 Deviations and counter measures

None.

2.3 Project partners:

Partners	
EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS	ECMWF
COMMISSARIAT A L ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES	CEA
METEO-FRANCE	METEO-FRANCE
WAGENINGEN UNIVERSITY	WU
KARLSRUHER INSTITUT FUER TECHNOLOGIE	KIT
HELSINGIN YLIOPISTO	UH
UNIVERSITE DE REIMS CHAMPAGNE-ARDENNE	URCA
ALBERT-LUDWIGS-UNIVERSITAET FREIBURG	UFR

3 Implementation into IFS of the SWEEP interpolation for SL advection

The tracer advection problem in IFS is defined by the equation (see D1.1 for further details):

$$\frac{D\phi}{Dt} = S \quad (3.1)$$

where, ϕ is a scalar quantity, namely the mixing or specific mixing ratio measured in kg of tracer per kg of air, and S is a source or sink term, for example representing emissions or absorption from biogenic processes. For $S=0$, the advection problem becomes globally conservative which means that advection does not change the global tracer mass. D is the “material” or “Lagrangian” derivative operator which is defined as $D/Dt = \partial/\partial t + \vec{V} \cdot \nabla$, where ∇ is the 3D nabla (gradient) operator applied in spherical coordinates and $\vec{V}$ is the wind vector that advects a tracer ϕ . The IFS SL advection scheme first computes the upstream departure points and then interpolates each advected variable such as temperature, wind components, and all atmospheric tracers (see Diamantakis and Vana, 2022). To obtain satisfactory accuracy a cubic-Lagrange interpolation method is used. This could be either the standard cubic-Lagrange or its COMAD variant (Malardel and Ricard, 2015) which improves the conservation of the advection scheme.

Mortezazadeh et al., 2024, proposed a quadratic instead of cubic interpolation method which alternates between two different interpolation stencils pairing a quadratic backward with a quadratic forward interpolation across two-time steps, achieving the same order of accuracy with the centred cubic-Lagrange interpolation polynomials through cancellation of truncation errors. Implementation of this method started in WP1 of CATRINE and has been finalised in WP2. This new option will be incorporated in a later release of the IFS software. Testing SWEEP has shown advantages which makes it very attractive for CO2MVS, CAMS but also NWP forecasts providing a unified and consistent method for advecting all atmospheric tracers. The benefits are:

1. **Improved computational efficiency.** For simulations involving many tracers (e.g. 100 or more), the cost of interpolation at the departure points (a big part of the cost of the SL scheme) is reduced by around 30%.
2. **Improved forecast skill.** In 4D-Var experiments with SWEEP applied to NWP water tracer variables and ozone, total-column ozone Root-Mean-Square-Error (RMSE) and standard-deviation-of-errors (STDE) was reduced by up to 10% at medium range as shown in Fig. 3.1. Meteorological skill remained neutral, while small (0.5%–1%) but consistent improvements were obtained across a wide range of observations and against ECMWF analyses.
3. **Improved CAMS forecasts.** SWEEP improves mass conservation (see D1.2) and furthermore, according to Chabrilat et al, 2024 (personal communication), it introduces other beneficial changes such as: it reduces stratospheric ozone biases, it improves tracer gradients and lifetimes, it makes aerosol and ozone-transport estimates more realistic and improves the representation of polar ozone holes. Tropospheric ozone improves slightly, with smaller free-tropospheric biases, while impacts on surface ozone and aerosols remain modest but generally positive. As we will see in section 6, it is also beneficial for greenhouse gases, reducing bias, STDE and RMSE against TTCON observations.

The development of a combined SWEEP-COMAD scheme has also been pursued during this period i.e. using sweep-quadratic interpolation and adding the COMAD perturbation in the quadratic method interpolation coefficients testing if conservation properties of the original SWEEP scheme can be further improved. However, testing on different CATRINE case

studies has shown that the COMAD perturbations on sweep-quadratic are not giving any additional benefit, the results are very similar unlike the linear and cubic-Lagrange interpolation case where COMAD is genuinely improving conservation properties. However, combining SWEEP with either of the new limiters, LQM3DCONS or ILMC, leads to a much stronger reduction in conservation error as confirmed by different tracer tests shown in the next sections.

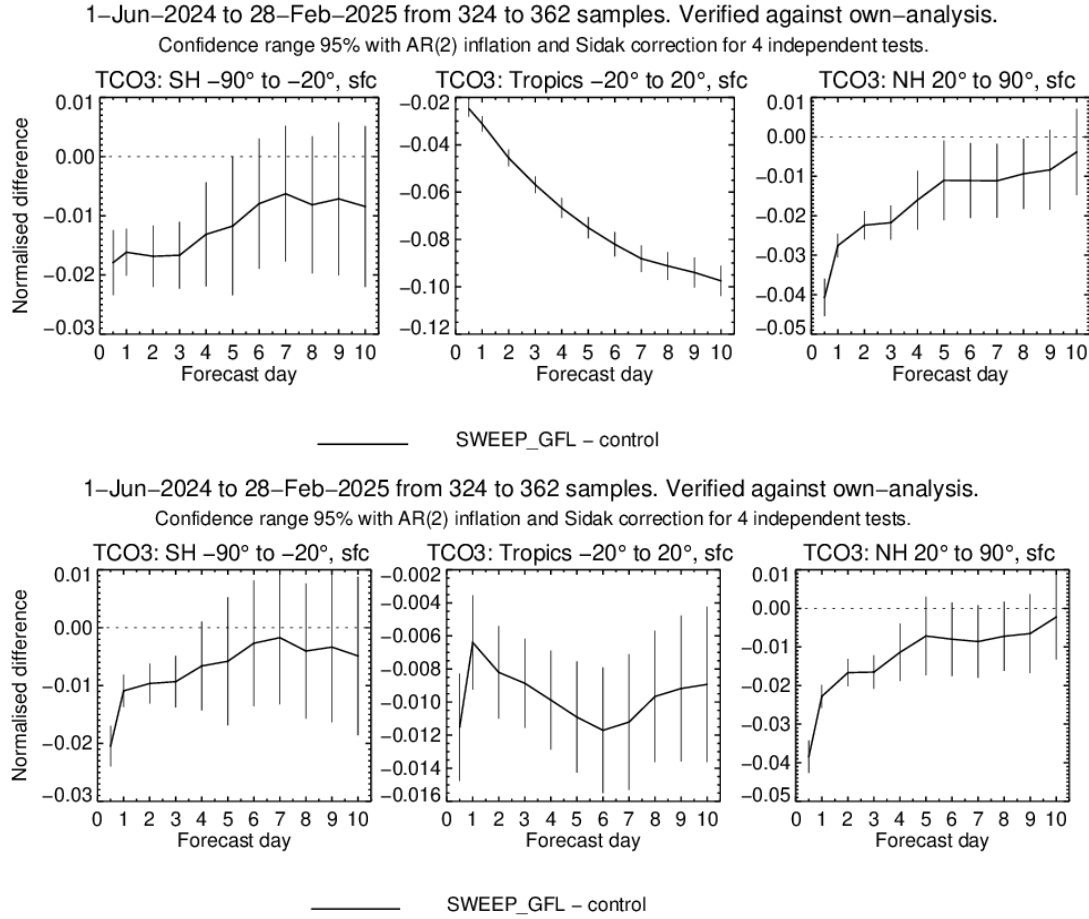


Figure 3.1. Change of RMSE (top plot) and STDE (bottom plot) for total-column ozone (TCO3) in combined 4D-Var experiments covering three winter months and three summer months. SWEEP is activated for all NWP tracers, namely water tracers and ozone. The change is shown relative to a control forecast using the standard cubic-Lagrange interpolation method in SL advection. Negative values imply reduction in the forecast error.

4 Implementation into IFS of a locally conservative limiter for SL advection

In deliverable D1.2, we described the implementation of a new limiter, LQM3DCONS, which reduced the mass conservation error by a factor of 4–5 in the most severe CATRINE tests, representing idealised plume tracers in realistic atmospheric flows. This new limiter was thoroughly tested on a range of tracers, including realistic GHG simulations, and showed improved conservation properties while maintaining the accuracy and high computational efficiency of the IFS advection scheme. However, the analysis in D1.1 suggested that substantially larger reductions in tracer mass conservation errors could be achieved if the limiter ensured monotonicity without changing the local or global tracer mass after SL advection. This is the aim of the ILMC limiter of Sørensen et al. (2013), which we have developed during the first nine months of WP2 with support from ECMWF core scientists. We have tested it within the IFS system by repeating the CATRINE WP1 experiments and by applying it to water tracers in weather forecast experiments. The ILMC limiter extends LQM3DCONS by correcting the advected field fully locally in three-dimensional space and, as shown below, yields impressive results.

As highlighted in Section 5 of D1.2, the main hurdles to implementing ILMC were integrating the algorithm into the mature IFS code, which relies on a specific blocked memory-access pattern for efficiency; managing its computational cost; and addressing its lack of reproducibility in parallel processing. While the computational cost remains a challenge, the other technical issues have now been resolved. The cost increase, estimated at 20–30% (depending on whether one or more iterations are used) at approximately 28 km grid spacing on the TCo399 IFS grid used for the CATRINE intercomparison tests and representative of the resolution at which CO2MVS will operate, may be a limiting factor. The results suggest that most of the conservation benefits can be achieved with a single iteration, while further work is ongoing to reduce the computational overhead.

The impact of ILMC in mass conservation error growth is clearly demonstrated in Fig. 4.1 where it has been applied in the plume tracer case from WP1 which is described in section 5.1 of D1.1. The formula used for computing the global mass of a tracer, the global atmospheric mass and the mass conservation errors are given in section 3 of D1.1. We have previously seen that in this case the IFS advection scheme without mass fixer produces a systematic error growth which is very sensitive to the choice of limiter. When the tracer is initialized near the surface, LQM3DCONS reduces the conservation error by more than 4, while with ILMC it is reduced by up to 2 orders of magnitude achieving a forecast which is nearly conserving. It produces similar conservation error with the SL scheme without a limiter but avoids negative unphysical values and violations of monotonicity. These conclusions are valid either with COMAD or SWEEP interpolation. The impact of these new limiters on SWEEP can also be seen in Fig. 4.2 where the total column mass of three tracers after 8 days of simulation is plotted. When the ILMC limiter is used, the mass fixer correction is very small given that the conservation error drastically reduces. There is a very small difference when ILMC uses 1 or 2 iterations with the latter producing slightly smaller conservation error. The first iteration distributes locally the clipped mass from the limiter at neighbouring points. If these points do not have the capacity of receiving this excess or balancing the deficit then the residual mass will be distributed to the next nearest neighbouring points at the following iteration (implementation details can be found in Sørensen et al, 2013). Large reduction of the conservation error with the ILMC limiter is also achieved when the tracer is initialized in the stratosphere or in the upper troposphere as shown in Fig. 4.1.

Consistent and substantial, at all geographical locations, reduction of the conservation error is achieved for the single-point source emission tests described in section 5.2 of D1.1 in which

a tracer with initial concentration 0 is increased by a fixed single-point emission equal to 0.5 kg/kg at each time-step. Given that the time-step is 900s and the grid-length is approximately 28km, this is equivalent with a very strong volcanic emission and is a test designed to stress test the IFS SL scheme conservation properties. The outcome of this test is illustrated in Fig. 4.3. We notice that when COMAD or SWEEP interpolation is combined with the ILMC limiter the conservation error almost vanishes. Furthermore, we see the reduction in conservation error that different developments undertaken in the CATRINE project bring, for example SWEEP interpolation reduces the conservation error compared with COMAD, the LQM3DCONS brings a large reduction but is superseded by ILMC.

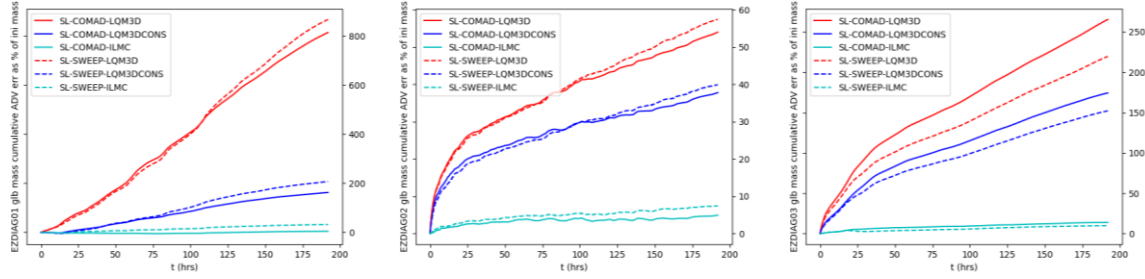


Figure 4.1. Mass conservation error growth, expressed as a percentage of initial tracer mass, for the WP1 plume tracer passive advection test case described in Section 5.1 of D1.1. The test uses a single-level $4^\circ \times 5^\circ$ rectangular tracer centred at 113E, 37.5N. From left to right, the tracer is initialised near the east coast of China at: (i) a near-surface atmospheric level; (ii) a model level near 30 hPa; and (iii) a model level in the upper troposphere near 260 hPa. All tests use the SL advection scheme without the mass fixer, with either cubic-Lagrange COMAD interpolation in the horizontal or SWEEP quadratic interpolation, and with different limiters: the operational CAMS quasi-monotone limiter LQM3D, the new LQM3DCONS limiter and the ILMC limiter with two iterations, both developed in CATRINE WP1 and WP2.

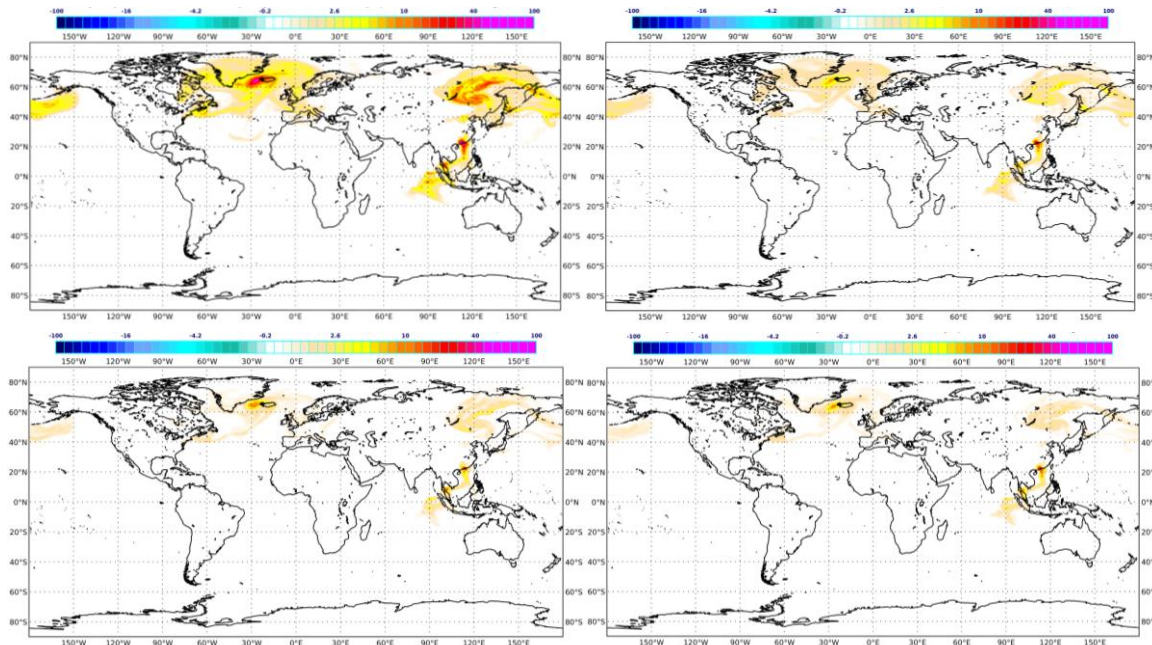


Figure 4.2. Total column mass in kg/m² of the plume tracer of Fig. 4.1 at t+8 days of simulation. Top row: SWEEP interpolation with LQM3D and LQM3DCONS limiter and without the IFS mass fixer. Bottom row: SWEEP interpolation with ILMC limiter without the mass fixer (left) and with the mass fixer (right).

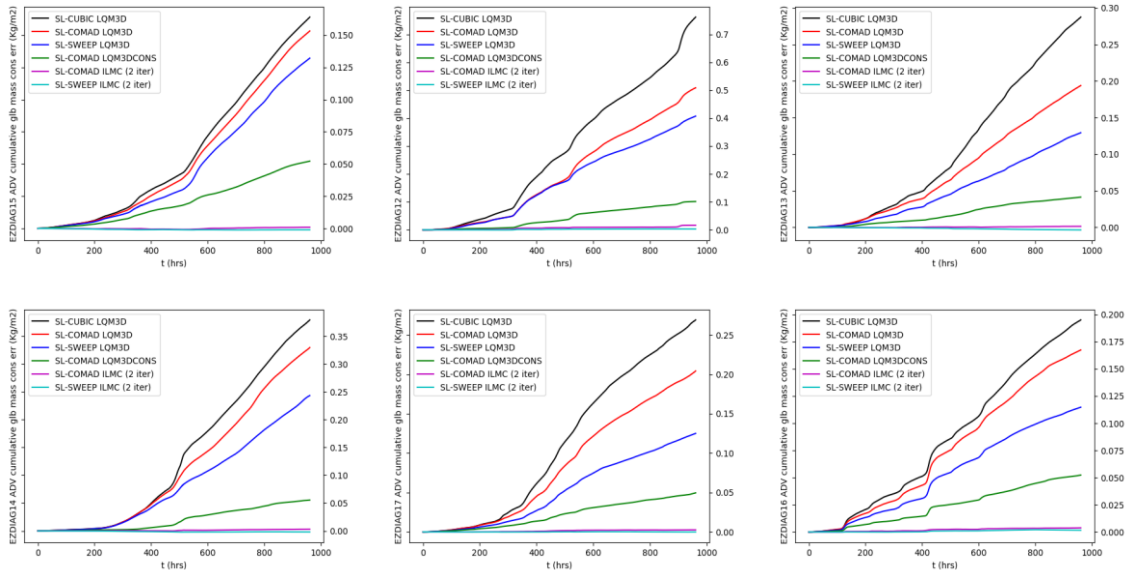


Figure 4.3. Mass conservation error growth (kg/m^2) for the WP1 single-point emission tracer passive advection test case described in Section 5.2 of D1.1. **Top** left to right: the emission point is at the known Nord Stream gas leak geographical location ($15.7\text{E}, 55.53\text{N}$), near the east coast of China ($113\text{E}, 37.5\text{N}$) and in Indonesia ($113\text{E}, 7.5\text{S}$). **Bottom** left to right: emission point at the east coast of the USA ($77\text{W}, 40.5\text{N}$), near Johannesburg ($28.04\text{E}, 26.2\text{S}$) and in Barrow Island in Australia ($115.4\text{E}, -20.8\text{S}$).

A further test demonstrating the effectiveness of the ILMC limiter is the warm-bubble tracer test case from WP1. Here, we have repeated the test described in Section 4.2 of D1.2. This idealised test case exposes a weakness of non-flux-form schemes such as SL schemes, which can result in systematic mass growth and unphysical behaviour near the surface i.e. the warm bubble does not detach from the boundary filling gradually the column as it rises. This behaviour is also known as the “infinite-fountain” effect. The SL scheme with COMAD and the ILMC limiter shows impressive behaviour in this case, resembling an Eulerian flux-form scheme, as shown in Fig. 4.4. Diagnostics of the accumulated ILMC correction help explain this behaviour: they show that ILMC systematically removes mass from the rising column, where the pointwise SL transport and lower boundary treatment would otherwise produce persistent accumulation. By redistributing the clipped by the limiter mass locally, ILMC prevents the column from being continually replenished, allowing the bubble to detach from the surface and almost eliminating the infinite-fountain effect.

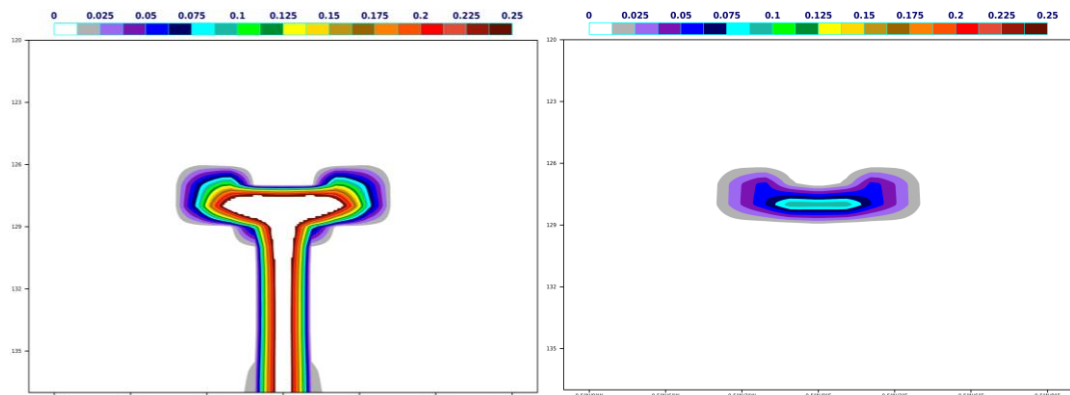


Figure 4.4. Semi-Lagrangian advection of a tracer embedded in a warm bubble. The tracer is initialised to 1 at the lowest three levels. Left: near equator 18 degrees wide East-West cross-section of the tracer concentration at $t=120\text{hrs}$ from initial time with COMAD-cubic-Lagrange and LQM3D limiter. Right: same as the left panel but using ILMC limiter. In both plots the vertical axis shows the lowest 17 vertical levels. Values exceeding 0.25 are in white.

5 Tangent linear and adjoint developments and OSSE testing

The tangent-linear (TL) model and its adjoint (AD) are essential components of the IFS 4D-Var data assimilation system (Rabier et al, 2000). They are used to compute both the value of the objective function and its gradient during the minimization, thereby ensuring an optimal fit between the model trajectory and the available observations. Because the CO2MVS inversions are based on 4D-Var, it is crucial that all relevant model components and algorithms have a complete and accurate TL/AD representation.

The TL/AD of the COMAD interpolation scheme was finalised in WP1. In WP2, the following developments were completed:

- The TL/AD of the new LQM3DCONS limiter was completed and has entered IFS cycle 50.
- The TL/AD of the tracer mass fixer was completed and has entered IFS cycle 50. This was a substantial development because of its complexity and non-linear nature.
- The TL/AD of the SWEEP interpolation algorithm was completed and will be included in a future IFS release.

With these developments in place, all key components of the transport dynamics now have tangent-linear and adjoint (TL/AD) counterparts. This makes it possible to assess the complete transport system within the experimental OSSE framework introduced in Deliverable D1.1. Building on the initial assessment presented there, this report extends the investigation of the IFS advection scheme and its impact on atmospheric emission inversions using an Ensemble Data Assimilation (EDA)-based Observing System Simulation Experiment (OSSE) framework. Deliverable D1.1 introduced an idealised methane inversion system based on synthetic observations to examine the sensitivity of emission estimates to key components of the advection scheme, including interpolation methods, monotone limiters, mass-fixer algorithms and their TL/AD counterparts. These initial experiments demonstrated that inversion performance is sensitive to several aspects of the transport formulation, while also highlighting limitations of the prototype system and the need for further investigation. The work presented here builds on these findings by extending the OSSE framework, incorporating the TL/AD implementations of the newly developed transport options, including the mass fixer, and providing a more comprehensive assessment of their impact on inversion accuracy and robustness.

A new round of OSSE experiments, based on a single observation located at the location of the point-source and a consistent use of the new Object-Oriented Prediction System (OOPS) in both the trajectory and the minimisation, identified some limitations of the inversion framework that may have impacted the results discussed in deliverable D1.1. In particular, methane concentrations were found to be highly sensitive to the meteorological initial conditions, with the assimilation of NWP observations degrading the fit to the synthetic methane observations. Although additional 4D-Var minimisations partly compensated for this degradation, they occasionally increased the bias of the analysis ensemble, while optimising emissions did not consistently improve the fit to the observations. Error reductions in emission space were generally larger and fit to observations better when NWP observations were not assimilated. The experiments further showed that the prescribed observation error (2 ppb, i.e. similar to the value used in operation) was too large relative to the (relatively small) ensemble spread, resulting in only modest error reductions and indicating that the inversion system would benefit from a larger representation of uncertainty. Additionally, the results exhibited a noticeable sensitivity to daily weather and random sampling variability. To further address some of these limitations, the OSSE framework was therefore adjusted by reducing the observation uncertainty to 0.5 ppb, and by omitting the assimilation of NWP observations,

while strengthening by a factor 10 the emission source. This revised setup provides a more robust framework for evaluating the WP2 transport developments, allowing their impact on atmospheric emission inversions to be assessed more clearly. Note that both the period chosen for the simulations (02-06 June 2022) and the location of the point source (38N, 113E) are the same as those described in deliverable D1.1. The benefits are demonstrated in Fig. 5.1 where it is shown that the minimisation procedure improves the fit to the assimilated observations in all EDA members in an experiment based on the new setting (bottom panel) compared to the previous configuration (top panel).

Using the revised OSSE system described above, a preliminary assessment involved the inclusion of the TL/AD versions of the mass fixer. For this purpose, the control experiment listed in Table 5.1, in which the mass fixer was active only in the nonlinear model and trajectory integrations, was repeated with the mass fixer TL/AD also activated during the minimisation. The results were sensitive to the formulation of the mass-fixer TL/AD. In the most complete configuration, which applies a formal linearisation of the nonlinear mass fixer algorithm without simplification or regularisation, the emission space uncertainty estimates deteriorated and occasional instabilities occurred. Simplifying the TL/AD formulation tends to improve its behaviour but provides no benefit relative to the control experiment. This behaviour is attributed to the switches and other nonlinearities within the mass fixer. The min/max operations and conditional tests make the algorithm non-differentiable at switching points and only piecewise differentiable elsewhere. Consequently, the TL approximation can behave spuriously when a finite perturbation causes the perturbed nonlinear solution to follow a different branch from that selected by the reference trajectory and result in unbound growth of error (see also Holdaway and Kent, 2015). Such problems are commonly mitigated by simplifying or regularising the linearised formulation. However, in the present experiments, such attempts did not improve the results relative to the control. We therefore conclude that, for the present OSSE configuration, the preferred option is to exclude the mass fixer from the TL/AD model. This is a slightly disappointing result given the effort required to develop a TL/AD for the mass fixer, however, it is a useful conclusion.

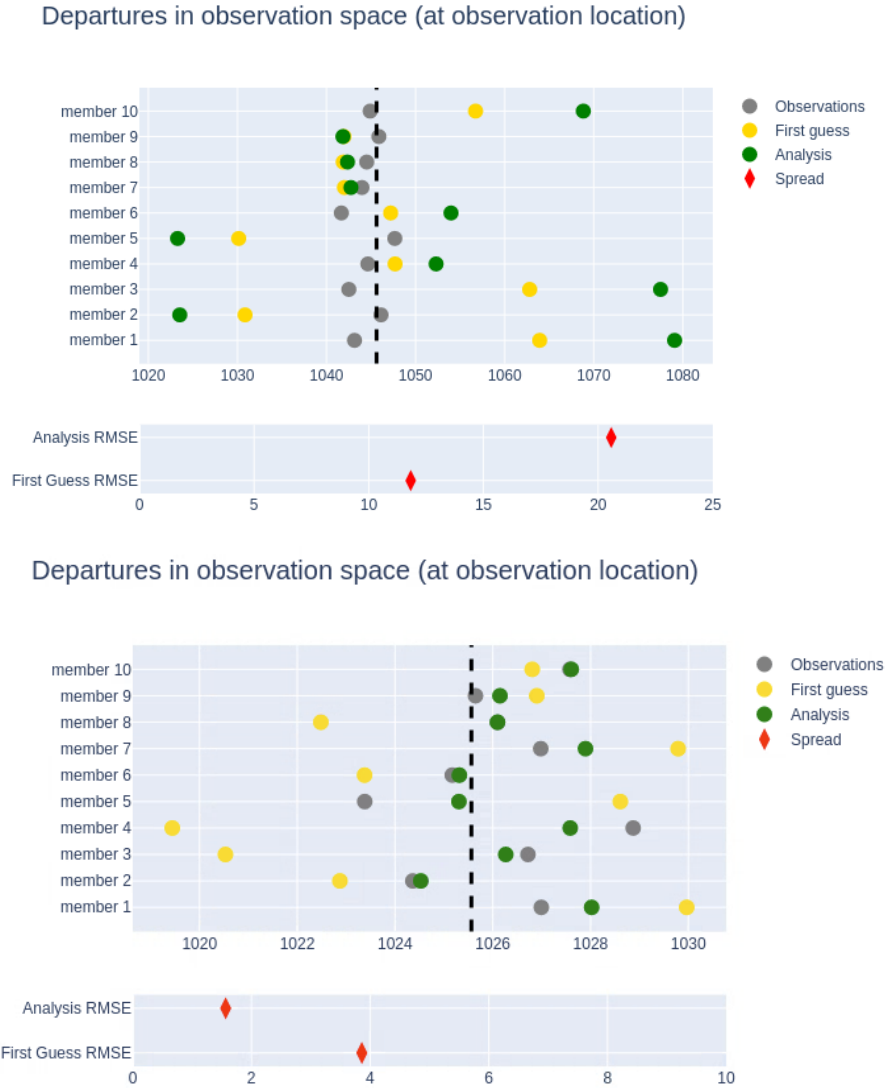


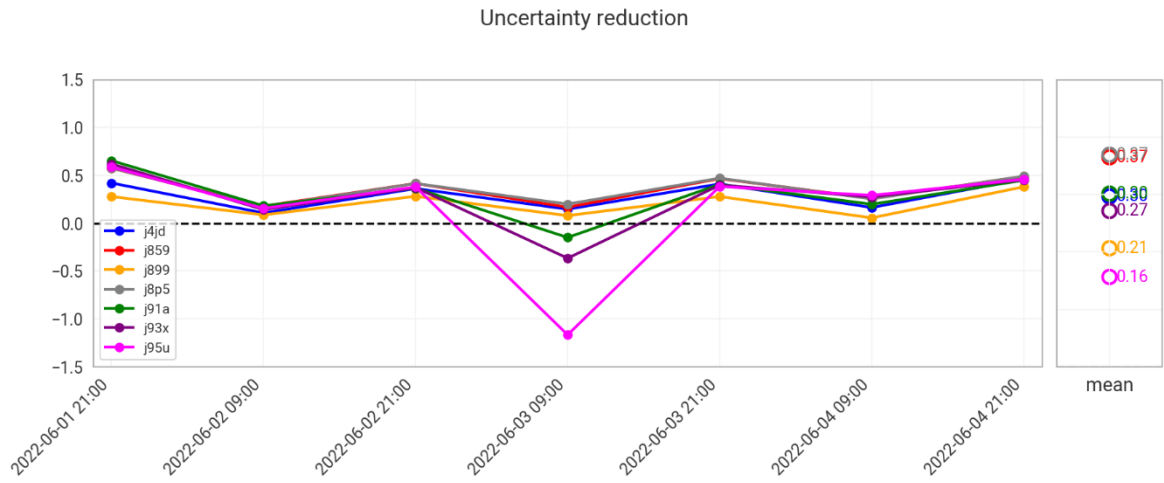
Figure 5.1. First guess (yellow dots), analysis (green dots) and observations (grey dots) values at the point-source location before (top) and after (bottom) the modifications to the original OSSE system, for two different experiments. The impact of the meteorology increments and inconsistency in the use of OOPS between trajectory and minimisation in the 4D-Var were producing a degradation of the fit to observations. The plot at the bottom refers to the control experiment.

Subsequently, further experiments were conducted to assess the impact of different limiters (LQM3D, LQM3DCONS, ILMC), advection schemes (COMAD, SWEEP) as well as the use of the mass fixer. The experiments analysed in this section are reported in Table 5.1 below. Fig. 5.2(a) shows the time series of the error reduction in emission space throughout the simulations, while Fig. 5.2(b) reports the time series of the root mean squared error (departure from observations) for the analysis (dashed lines) and the first guess (solid lines). As in Section 8.2 of D1.1, the emission error reduction is defined as $err = 1 - \sigma_{pos}/\sigma_{pri}$ where, σ denotes the RMSE of the scaling factor ensemble relative to the control member before (σ_{pri}) and after (σ_{pos}) the inversion. Positive values therefore indicate that the inversion reduces the emission space error, and negative values indicate that the error increases after the inversion.

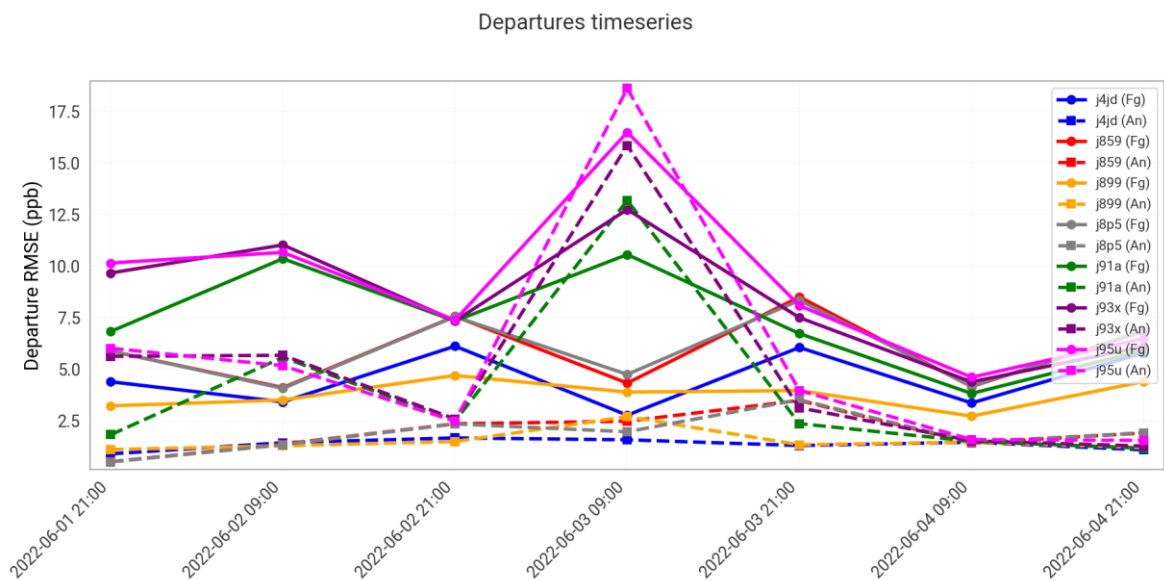
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ExpID	COMAD	SWEEP	Limiter	Mass Fixer
j4jd (control experiment)	Model	Off	LQM3D (model + TL/AD)	On (model)
j859	Model + TL/AD	Off	LQM3DCONS (model)	On (model)
j8p5	Model + TL/AD	Off	LQM3DCONS (model + TL/AD)	On (model)
j899	Off	On	LQM3D (model + TL/AD)	On (model)
j91a	Off	On	ILMC (model)	On (model)
j93x	Off	On	ILMC (model)	Off
j95u	Model + TL/AD	Off	ILMC (model)	On (model)

Table 5.1. List of OSSE experiments.



(a)



(b)

Figure 5.2. (a): Time series of the error reduction in emission space for the experiments listed in Table 5.1. (b): root mean squared analysis departures (dashed lines) and first guess departures (solid lines).

Overall, none of the configurations tested provides a consistent improvement over the control while some of them seem to perform worse than the control, both in terms of observation departures (both before and after the assimilation) and in terms of error reduction in emission space. At first sight, this contrasts with other results of forward model tests in this report which showed that these new developments benefit mass conservation and overall transport

accuracy (see also next section). However, the two findings are not necessarily inconsistent. Because each configuration in the OSSE system generates its own synthetic observations, differences in the overall OSSE performance mainly indicate how successfully 4D-Var adjusts the emissions and the concentrations in each EDA member to converge towards the observed plume, rather than which nonlinear transport scheme is the most accurate.

In particular, the experiments with the ILMC limiter (green, magenta and purple lines in Fig. 5.2b) show larger departures from the observations across most of the simulation period and they are all displaying larger analysis than first-guess departures in the fourth assimilation window (nighttime at this location), which also leads to an increase in the error in emission space (Fig. 5.2a). A closer look at these simulations (not shown) shows larger concentration values at the point-source location as well as larger ensemble spread than the experiments without the ILMC limiter. Analysing the concentration increments at the observation time for these simulations (not shown), a tendency for the 4D-Var to ‘overcorrect’ is apparent, i.e. more mass than required to match the observed value is added or removed at the point-source location. Separate model experiments using the mass fixer and comparing ILMC with LQM3D configurations reveal (not shown here) that the mass fixer correction near the source is much more aggressive with LQM3D because of the large mass growth which occurs with this limiter in the presence of a large gradient in the vicinity of the source. This results in a strongly damped plume. A plausible interpretation is that this damping reduces the sensitivity of the system to the perturbed emissions and produces smaller ensemble spread and analysis increments. Because all experiments generate their own observations, the experiment with LQM3D and mass fixer is not penalised for this damping, on the contrary it is given an advantage.

Moreover, the experiment using SWEEP interpolation and the original LQM3D limiter (solid orange line in Fig. 5.2b) has on average smaller first guess departures than the control experiment. However, as previously stated, because the SWEEP experiment also generates its own synthetic observations, this result should not be over-interpreted as direct evidence that SWEEP represents the physical plume more accurately. Instead, it indicates that with SWEEP the background trajectories remain closer to the corresponding control trajectory or are less sensitive to the EDA perturbations. The smaller first guess departures do not translate into smaller analysis departures (dashed orange line) than the control experiment but are similar in magnitude. The analysis remains close to the control trajectory throughout the simulation and the error reduction achieved is modest.

The experiments using the LQM3DCONS limiter (grey and red lines in Fig. 5.2) find themselves in the middle of the pack in terms of observations departures: they have larger first guess departures (and larger spread) than the control experiment, but less than the experiments using the ILMC limiter (solid lines). On the other hand, their analysis departures (dashed lines) are still closer to those of the control experiment, resulting in larger values of error reduction in emission space (Fig. 5.2a). Comparing the two LQM3DCONS configurations also indicates that including the LQM3DCONS limiter in the TL/AD has little effect using the OSSE system examined here.

These results should be interpreted as a test of the inversion problem under a self-consistent transport model, rather than as a direct test of which nonlinear transport formulation is most physically accurate. This is because every tested configuration generated its own synthetic observations using the unperturbed control member forecast model, therefore, forward transport errors are incorporated into that configuration's observations. The experiments nevertheless reveal some properties of the inversion system: limiter TL/AD appears to contribute little; activating the mass fixer TL/AD can degrade results leading to instability; and the nonlinear mass fixer can alter the response of the model near the source. The benefits of

SWEEP and improved conservation limiters (ILMC, LQM3DCONS) may become more visible in real-observation inversions, where transport error can no longer be absorbed into the “synthetic” observations. It is therefore **recommended** to test the new limiters and the SWEEP scheme in the actual inversion system where real observations are used and to verify them against independent observations.

6 Impact of new advection algorithms on the simulation of GHG using optimized flux protocols from WP8 and WP5

The overall quality of the new advection options developed in WP1 and WP2 has been evaluated through long GHG simulations covering the periods 2016-2017 and 2022-2023. These simulations use the optimised CO₂ fluxes from WP8, and their results can be compared against observations, thereby enabling an assessment of the overall accuracy of the IFS transport scheme and of the impact of the numerical developments introduced in CATRINE. In addition, the simulations allow an analysis of the effects of the new advection options on mass conservation under realistic conditions. The period 2022-2023 was already investigated in WP1 of CATRINE, and the corresponding results were documented in D1.1 and D1.2. Building on this existing experience, the present work extends the analysis to the SWEEP interpolation scheme and the ILMC limiter.

The impact of the CATRINE developments on mass conservation is illustrated in Fig. 6.1. The figure shows the global mass-fixer correction per time step for the anthropogenic CO₂ tracer, CO2APF, expressed as a percentage of the global tracer mass. Results are shown for the first day of the simulation and for a day six months later. A notable feature is the strong reduction in the magnitude of the mass fixer correction as the simulation progresses. As explained in D1.1, this is because CO2APF is initially zero everywhere, with no background CO2APF at the start of the simulation, and only gradually builds up through emissions. As a result, its initial behaviour is similar to the plume cases discussed in Section 5 of this report. As the simulation progresses and CO2APF mixes with the background air, the SL mass-conservation error decreases substantially. The strong impact of the ILMC limiter is evident in Fig. 6.1, particularly in the left-hand panel for the first simulation day, confirming its superiority in reducing conservation errors in plume-type cases. Even at the beginning of the simulation, when the emitted tracer has not yet mixed with the background air and very strong tracer gradients are present — conditions that can produce large conservation errors in SL advection — ILMC substantially reduces the mass conservation error, resulting in small mass fixer corrections. Later in the simulation, ILMC remains the most effective method, reducing the conservation error by a further factor of four compared with LQM3DCONS. The SWEEP interpolation scheme is only slightly more effective than COMAD when both use the LQM3D limiter, which is currently used operationally in CAMS. The apparent oscillation in the mass fixer correction is a feature of the SWEEP scheme and is reported in the original article by Mortezaadeh et al. (2024). Quoting the authors, “an oscillation in mass error, calculated by SWEEP interpolation, comes from the inherent behaviour of SWEEP interpolation to control the growth of numerical error over two successive time steps”.

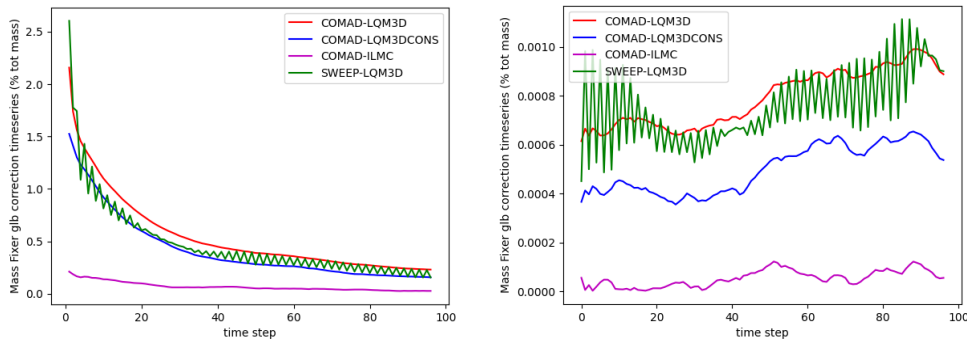


Figure 6.1. Mass fixer correction for CO2APF on the 1st day of the simulation (01-12-2021) and six months later (01-06-2022). The performance of the COMAD scheme in terms of mass conservation is assessed when three different limiters are used (LQM3D, LQM3DCONS, ILMC) and compared against the SWEEP interpolation scheme with the default limiter LQM3D.

The results from the 2022-2023 simulations for CO₂ have been analysed and compared against the available TCCON observations. As an illustration, time series from the IFS simulations for the two well-established sites of Paris and Pasadena, both located near anthropogenic emission sources, are compared with observations in Fig. 6.2. At both sites, the use of either the ILMC limiter or the SWEEP interpolation scheme combined with the LQM3D limiter leads to a noticeable reduction in bias and a small reduction in the standard deviation of the errors compared with the operational setup COMAD with LQM3D limiter. For Pasadena, the impact appears stronger, with a larger reduction in the errors obtained with these two new methods, especially ILMC, together with an increase in the correlation coefficient r with the observations. The overall impact on CO₂ across the TCCON stations is shown in Table 6.1. Across all metrics, the ILMC limiter combined with COMAD appears to produce the best results, followed by SWEEP, which, although associated with a small increase in bias, reduces the STDE and RMSE. Experiments with the LQM3DCONS limiter have the second smallest bias, but they are outperformed by SWEEP on the other error metrics.

Label	mean(δ)	mean($ \delta $)	mean(stde)	mean(rmse)	mean(r)
COMAD-ILMC	1.43e-01 (-23.53%)	3.50e-01 (-10.26%)	7.65e-01 (-4.49%)	8.66e-01 (-6.28%)	8.99e-01 (+0.90%)
COMAD-LQM3DCONS	1.87e-01 (+0.00%)	3.90e-01 (+0.00%)	8.01e-01 (+0.00%)	9.24e-01 (+0.00%)	8.91e-01 (+0.00%)
COMAD-LQM3D	2.01e-01 (+7.49%)	4.10e-01 (+5.13%)	8.02e-01 (+0.12%)	9.32e-01 (+0.87%)	8.91e-01 (+0.00%)
SWEEP-LQM3D	2.10e-01 (+12.30%)	4.15e-01 (+6.41%)	7.75e-01 (-3.25%)	9.07e-01 (-1.84%)	8.99e-01 (+0.90%)

Table 6.1. Mean bias (δ), mean absolute bias, standard deviation or errors, RMSE and correlation coefficient r metrics against TCCON observation sites for experiments run in the 2022-2023 period using the different transport options developed within CATRINE. Values in parentheses indicate the relative change with respect to COMAD with LQM3DCONS limiter and mass fixer which was identified in D1.2 as the reference configuration owing to its good performance for GHG transport.

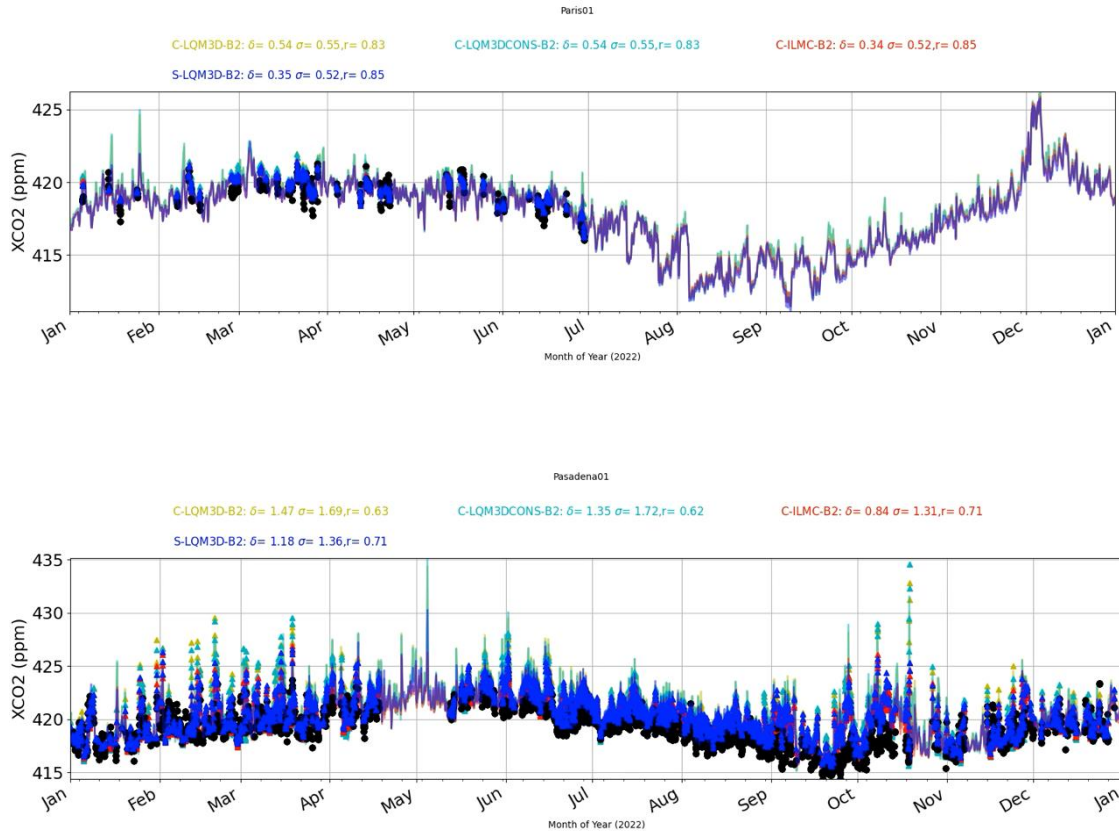


Figure 6.2. Time series (January 2022-January 2023) of daily average XCO₂ compared to TCCON observations at two city sites: Paris and Pasadena, California. In each plot the bias, standard deviation of errors and correlation coefficient is written at the top for each simulation. The letter **C** indicates COMAD scheme, **S** the SWEEP scheme where each is combined with a limiter and the default mass fixer e.g. C-ILMC-B2 implies COMAD with ILMC limiter with beta mass fixer parameter set to 2 (see D1.1).

Tests using the WP8 protocols were also extended over the period 2016-2017. Three tests were performed without the IFS tracer mass fixer: two separate ones using the COMAD scheme combined with either the LQM3D or ILMC limiter, and one using the SWEEP scheme with the ILMC limiter. In addition, five tests were performed with the tracer mass fixer, using different combinations of schemes and limiters: two simulations with COMAD combined with the new LQM3DCONS and ILMC limiters, and three simulations with the SWEEP scheme combined with the LQM3D, LQM3DCONS and ILMC limiters.

Global mass diagnostics for the CO₂APF, CO₂ and CH₄ tracers, and for these different options tested during 2016-2017, are shown in Fig. 6.3. These diagnostics complement the error metrics presented previously and assess whether it is acceptable to remove the mass fixer in a setup using ILMC, which has been shown to substantially reduce conservation errors and produce a nearly conserving simulation. In each left-hand panel of Fig. 6.3, the global mass of each tracer is shown for the different experiments. In the right-hand panels, results are shown relative to a control experiment, defined as the COMAD scheme combined with the LQM3DCONS limiter, since this was adopted in D1.2 as the best configuration. The experiment that stands out for all tracers is COMAD with the LQM3D limiter and no mass fixer, which produces noticeably larger total tracer mass because conservation errors introduced by the advection scheme are not corrected. Both COMAD and SWEEP, when combined with ILMC, nearly converge towards the experiments using the IFS mass fixer. However, as shown in the right-hand panels, noticeable differences remain, indicating that without the mass fixer the total tracer mass may drift slightly during long simulations. Once the mass fixer is applied,

the global tracer mass converges to nearly the same value regardless of the transport scheme. The largest difference is observed for CH_4 , although it remains very small, with the global mass differing by only approximately 0.03% between COMAD and SWEEP after two years of simulation. For the SWEEP experiments using different limiters, the differences in global mass are a further order of magnitude smaller. Overall, these differences are very small, related to slightly different responses of the model physical and land surface processes when the transport scheme changes, providing confidence in the robustness of the results.

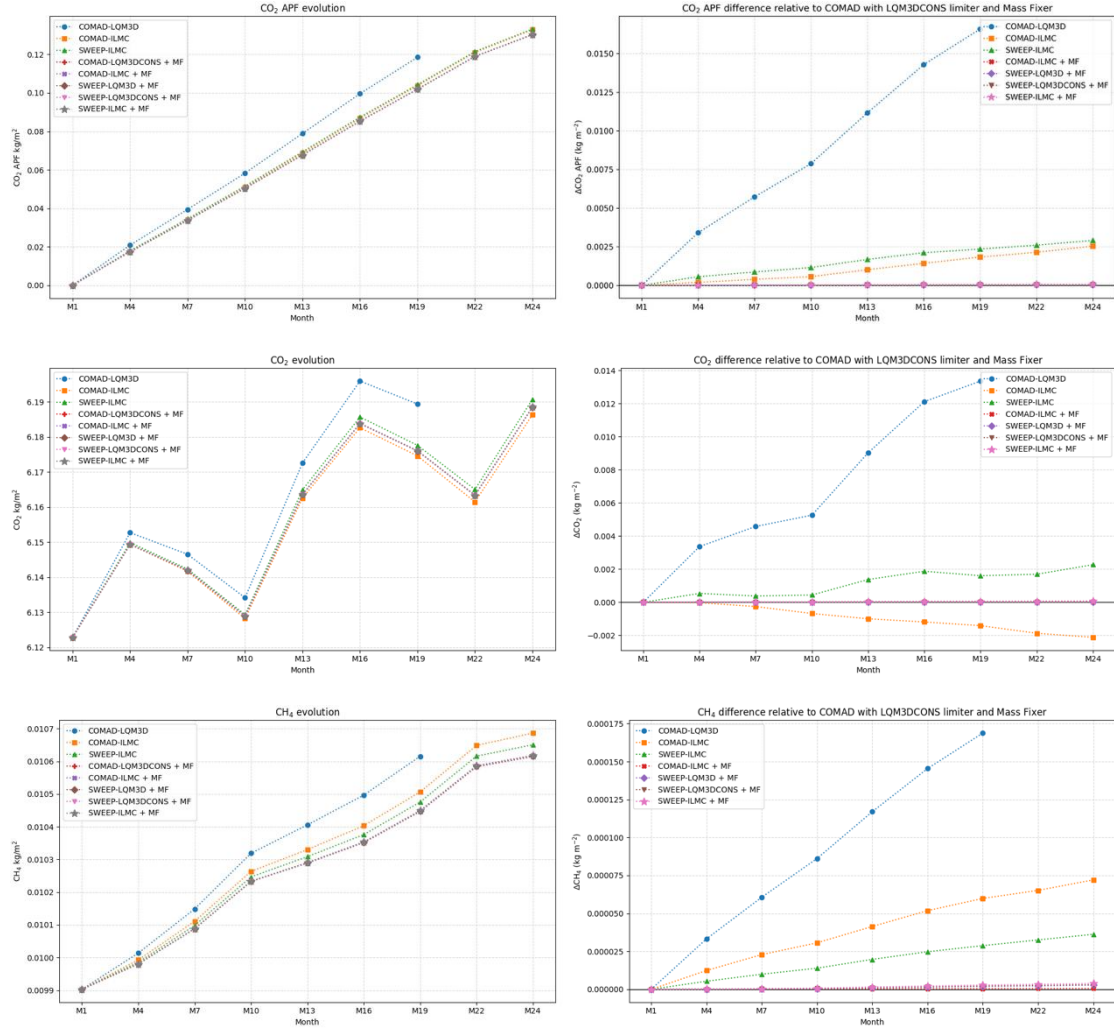


Figure 6.3. Global mass evolution during the 2016-2017 period for CO_2APF , CO_2 and CH_4 for different advection schemes. Left: global mean mass expressed in kg/m^2 . Right: global mean mass change relative to COMAD scheme with LQM3DCONS with mass fixer, expressed in kg/m^2 .

The 2016–2017 experiments have also been compared against TCCON CO_2 observations and are summarised in Table 6.2. Without the mass fixer, COMAD with LQM3D shows a very large increase in all error metrics. A striking outcome is that COMAD with ILMC gives the best results in terms of bias and RMSE, even compared with experiments that use the mass fixer. This is also evident in the scorecard shown in Fig. 6.4, where bias improvements can be seen across all atmospheric layers and geographical regions, together with improvements in both horizontal and vertical gradients across most regions and layers. With the mass fixer active, COMAD produces slightly better results with LQM3DCONS than with ILMC. Furthermore, the

SWEEP scheme produces the smallest standard deviations and the highest correlation with observations, even with the operational LQM3D limiter. This agrees with the 2022–2023 results in Table 6.1, where SWEEP was shown to be competitive with, and sometimes better than, COMAD with LQM3DCONS. Clearly, the mass fixer is very beneficial when the underlying scheme produces large mass-conservation errors; however, when the scheme is nearly conservative, for example COMAD with ILMC, its main benefit is to prevent slowly evolving mass drift in long simulations, as shown in Fig. 6.3. There is an important difference between the two sets of simulations, corresponding to the 2016–2017 and 2022–2023 periods: accurate tracer injection heights were specified in the 2016–2017 simulations, whereas in 2022–2023 the injection occurred at the lowest model level. It was shown in D1.1 and D1.2 that, when emissions originate from the near-surface level, mass conservation errors can increase considerably because of the way the SL advection scheme boundary conditions are specified. When emissions occur at higher levels, the mass fixer corrections are much smaller; in other words, ILMC has more impact in near-surface emission cases, where error growth is larger which explains why it appears better in the 2022–2023 period. Again, the differences in the error metrics are small when the mass fixer is used.

Scheme	mean(δ)	mean($ \delta $)	mean(σ)	Mean(rmse)	Mean(R)
COMAD-ILMC	2.13e-01 (-11.62%)	3.76e-01 (-3.59%)	7.18e-01 (+0.42%)	8.56e-01 (-1.15%)	9.04e-01 (-0.11%)
COMAD-LQM3DCONS MF	2.41e-01 (+0.00%)	3.90e-01 (+0.00%)	7.15e-01 (+0.00%)	8.66e-01 (+0.00%)	9.05e-01 (+0.00%)
COMAD-ILMC MF	2.53e-01 (+4.98%)	3.98e-01 (+2.05%)	7.19e-01 (+0.56%)	8.67e-01 (+0.12%)	9.04e-01 (-0.11%)
SWEEP-LQM3D MF	2.58e-01 (+7.05%)	4.03e-01 (+3.33%)	7.13e-01 (-0.28%)	8.67e-01 (+0.12%)	9.07e-01 (+0.22%)
SWEEP-LQM3DCONS MF	2.73e-01 (+13.28%)	4.07e-01 (+4.36%)	7.13e-01 (-0.28%)	8.70e-01 (+0.46%)	9.06e-01 (+0.11%)
SWEEP-ILMC MF	2.76e-01 (+14.52%)	4.07e-01 (+4.36%)	7.13e-01 (-0.28%)	8.71e-01 (+0.58%)	9.05e-01 (+0.00%)
SWEEP-ILMC	3.26e-01 (+35.27%)	4.41e-01 (+13.08%)	7.12e-01 (-0.42%)	8.87e-01 (+2.42%)	9.06e-01 (+0.11%)
COMAD-LQM3D	6.61e-01 (+174.27%)	7.03e-01 (+80.26%)	7.34e-01 (+2.66%)	1.05e+00 (+21.25%)	9.03e-01 (-0.22%)

Table 6.2. Same as in Table 6.1 but for experiments run in the 2016–2017 period.

In Table 6.3, the 2016–2017 experiments have been compared against TCCON CH₄ observations. It is noticeable that the bias and the remaining error metrics are all larger than the corresponding ones for CO₂. The reason for that is that protocols from WP5 are used for CH₄ which have not optimized fluxes. The rows are placed in ascending order of the magnitude of the mean bias which is positive for all stations. The outlook here is slightly different from CO₂. The top three schemes in the table overall seem to have the best performance against all metrics. The SWEEP scheme with LQM3D is the best in terms of bias. There is little

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difference with the remaining two schemes, COMAD with LQM3DCONS and COMAD with ILMC. Large degradations are observed when the mass fixer is switched off. In this case, either SWEEP or COMAD with the ILMC limiter is clearly the best but not competitive with experiments that are using the mass fixer.

Label	mean(δ)	mean(σ)	mean(rmse)	mean(r)
SWEEP-LQM3D MF	2.14e+01 (-0.93%)	1.80e+01 (+2.86%)	2.89e+01 (+1.05%)	7.61e-01 (+0.79%)
COMAD-LQM3DCONS MF	2.16e+01 (+0.00%)	1.75e+01 (+0.00%)	2.86e+01 (+0.00%)	7.55e-01 (+0.00%)
COMAD-ILMC MF	2.17e+01 (+0.46%)	1.75e+01 (+0.00%)	2.88e+01 (+0.70%)	7.55e-01 (+0.00%)
SWEEP-LQM3DCONS MF	2.19e+01 (+1.39%)	1.79e+01 (+2.29%)	2.92e+01 (+2.10%)	7.60e-01 (+0.66%)
SWEEP-ILMC MF	2.19e+01 (+1.39%)	1.81e+01 (+3.43%)	2.93e+01 (+2.45%)	7.60e-01 (+0.66%)
SWEEP-ILMC	2.41e+01 (+11.57%)	1.88e+01 (+7.43%)	3.15e+01 (+10.14%)	7.53e-01 (-0.26%)
COMAD-ILMC	2.67e+01 (+23.61%)	1.92e+01 (+9.71%)	3.37e+01 (+17.83%)	7.40e-01 (-1.99%)
COMAD-LQM3D	3.51e+01 (+62.50%)	2.25e+01 (+28.57%)	4.25e+01 (+48.60%)	7.20e-01 (-4.64%)

Table 6.3. Bias (δ), standard deviation or errors, RMSE and correlation coefficient r against CH_4 TCCON observation sites for experiments run in the 2016-2017 period using the different transport options developed within CATRINE. Values in parentheses indicate the relative change with respect to COMAD with LQM3DCONS limiter and mass fixer which was identified in D1.2 as the reference configuration owing to its superior performance for GHG transport.

CO ₂ seasonal scorecard difference (COMADH+ILMC_noMF vs COMADH+LQM3D_noMF) - JJA						
A. Bias						
	SH HighLat(60-90S)	SH MidLat(30-60S)	SH Tropics(30S-0)	NH Tropics(0-30N)	NH MidLat(30-60N)	NH HighLat(60-90N)
Stratosphere	▼ -0.22	▼ -0.17	▼ -0.38	▼ -0.41	▼ -0.42	▼ -0.28
Upper FT: 5km-tropz	▼ -0.2	▼ -0.26	▼ -0.39	▼ -0.42	▼ -0.41	▼ -0.39
Lower FT: 2-5km	▼ -0.23	▼ -0.25	▼ -0.36	▼ -0.43	▼ -0.46	▼ -0.39
PBL: 0-2km	▼ -0.22	▼ -0.26	▼ -0.35	▼ -0.45	▼ -0.43	▼ -0.37
Total Column	▼ -0.22	▼ -0.24	▼ -0.37	▼ -0.43	▼ -0.43	▼ -0.37
B. Vertical gradient						
	SH HighLat(60-90S)	SH MidLat(30-60S)	SH Tropics(30S-0)	NH Tropics(0-30N)	NH MidLat(30-60N)	NH HighLat(60-90N)
UTLS (tropopause)	▼ -0.02	▲ 0.09	▲ 0.01	0.0	▼ -0.01	▲ 0.11
LFT-UFT (5km)	▲ 0.03	▼ -0.01	▼ -0.03	▲ 0.01	▲ 0.05	-0.0
PBL-LFT (2km)	▼ -0.01	▲ 0.01	▼ -0.02	▲ 0.02	▼ -0.03	▼ -0.02
STD_Column	▼ -0.01	▼ -0.03	▼ -0.01	▲ 0.01	▼ -0.01	▼ -0.02
C. Horizontal gradient						
	STD_Lat	SH MidLat-HighLat	SH Tropics-MidLat	NH-SH Tropics	NH MidLat-Tropics	NH HighLat-MidLat
Stratosphere	▼ -0.06	▲ 0.05	▼ -0.21	▼ -0.04	▼ -0.01	▲ 0.14
Upper FT: 5km-tropz	▼ -0.05	▼ -0.06	▼ -0.13	▼ -0.03	▲ 0.01	▲ 0.02
Lower FT: 2-5km	▼ -0.03	▼ -0.02	▼ -0.11	▼ -0.07	▼ -0.03	▲ 0.07
PBL: 0-2km	▼ -0.03	▼ -0.04	▼ -0.08	▼ -0.1	▲ 0.02	▲ 0.06
Total Column	▼ -0.05	▼ -0.02	▼ -0.13	▼ -0.06	-0.0	▲ 0.05

Figure 6.4. Evaluation of COMAD with two different limiters: LQM3D and the newly developed ILMC using scorecards developed in WP8 of CATRINE.

The conclusions from this experimentation are:

1. For CO₂ COMAD usually produces better results than SWEEP. COMAD combined with ILMC and without the mass fixer gave slightly better results than any other combination. This is an impressive outcome because D1.1 had previously shown that results degrade without the mass fixer. The improvement is largely due to the good conservation properties of the SL scheme combined with the ILMC limiter.
2. For CH₄, combinations of SWEEP interpolation seem to perform slightly better than COMAD. An interesting aspect of this testing is that SWEEP performs very well with the default limiter LQM3D and shows little sensitivity with respect to the limiter choice when the mass fixer is active.
3. Using the mass fixer avoids mass drifts in long simulations. The global tracer mass remains the same regardless which scheme is used when the mass fixer is active. Using the mass fixer also reduces the sensitivity with respect to the choice of SL advection option and quasi-monotone limiter.

7 Alternative dry mass conserving forms for the continuity equation

The mass continuity equation of the IFS (see ECMWF, 2024) conserves the total atmospheric mass which includes water vapour and other water tracers (cloud liquid, cloud ice, rain and snow). This equation is correct in the adiabatic model (the dynamics) but it becomes approximate when the dynamics is coupled to the physics parametrization package where vertical sub-grid transport of water mass must also be accounted for. One of the consequences of the simplification of the coupling of the continuity equation with the physics parametrizations is that the global amount of dry air mass, which should be constant in nature, varies to compensate for the global variation of atmospheric water mass due to variations in precipitation and evaporation from the surface. More locally, at the scale of an IFS grid box, the evolution of the hydrostatic moist pressure doesn't include the correct (small) mass change due to the precipitation and moist vertical diffusion. But in practice this approximation has little impact on weather forecast accuracy and additionally it is convenient as it simplifies the implementation of hydrostatic models with pressure based vertical coordinates such as the IFS.

However, the assumption of total atmospheric mass conservation used in the IFS continuity equation has been shown to be problematic for GHG tracers when dry mixing ratio observations are converted into the specific ratios used by the IFS. Table 7.1 summarizes the problem using a simplified set of equations that compare the dry mass conservation law in the IFS with that in nature. In both cases, the water mass in a Lagrangian parcel changes because of the divergence of vertical sub-grid precipitation and evaporation fluxes, as shown in the first line of Table 7.1a. In nature, the dry mass m_d is conserved in a Lagrangian parcel. In the IFS, however, it is the sum of dry mass and water mass m_v that is conserved, as shown in the second and third lines of Table 7.1a. Consequently, the dry mass varies to compensate for changes in water content. This dry mass change is associated with unphysical vertical fluxes of dry air in atmospheric columns (gain of dry air to compensate for precipitation and loss of dry air to compensate for surface evaporation and vertical turbulent transport of water vapour).

In practice, the mass of a tracer t is known as a concentration with respect to dry mass (mixing ratio $r_t = m_t/m_d$) or with respect to the total mass of air (specific ratio $q_t = m_t/m_{tot}$). Table 7.1b shows the consequences of the IFS continuity equation on the concentration equations. The mixing ratios should in nature vary only because the tracer mass varies. But in the IFS, they vary also when the water mass varies in the parcel, thus creating an unphysical correlation between the tracer and the water mass evolution. This is why it is advised not to convert the current IFS specific ratios which vary only because of changes in tracer mass (blue equation on Table 7.1b) into mixing ratios.

	"Nature"	Current IFS
Water vapour	$\frac{Dm_v}{Dt} = -\frac{\partial F_{\varphi}}{\partial z}$	$\frac{Dm_v}{Dt} = -\frac{\partial F_{\varphi}}{\partial z}$
Dry air	$\frac{Dm_d}{Dt} = 0$	$\frac{Dm_d}{Dt} = -\frac{Dm_v}{Dt}$
Total mass	$\frac{Dm_{tot}}{Dt} = \frac{Dm_v}{Dt}$	$\frac{Dm_{tot}}{Dt} = 0$

(a)

$$\frac{Dr_t}{Dt} = \frac{1}{m_d} \frac{Dm_t}{Dt} - \frac{m_t}{m_d^2} \frac{Dm_d}{Dt} \quad \frac{Dq_t}{Dt} = \frac{1}{m_{tot}} \frac{Dm_t}{Dt} - \frac{m_t}{m_{tot}^2} \frac{Dm_{tot}}{Dt}$$

	"Nature"	Current IFS
mixing ratio	$\frac{Dr_t}{Dt} = \frac{1}{m_d} \frac{Dm_t}{Dt}$	$\frac{Dr_t}{Dt} = \frac{1}{m_d} \frac{Dm_t}{Dt} + \frac{m_t}{m_d^2} \frac{Dm_v}{Dt}$
specific ratio	$\frac{Dq_t}{Dt} = \frac{1}{m_{tot}} \frac{Dm_t}{Dt} + \frac{m_t}{m_{tot}^2} \frac{Dm_v}{Dt}$	$\frac{Dq_t}{Dt} = \frac{1}{m_{tot}} \frac{Dm_t}{Dt}$

(b)

Table 7.1. (a): simplified set of equations for the water mass (simplified as water vapour here), the dry air mass and total mass, both in nature and in the current IFS. (b): equation for the mixing ratio or the specific ratio of a tracer t in nature and in the current IFS. The flux term $\partial F_{\varphi}/\partial z$ represents precipitation/evaporation sources.

An alternative continuity formulation which conserves dry mass of air by coupling the continuity equation with water sources and sinks from the physics parametrizations is also available in the IFS and is described in the ECMWF tech memo by Malardel et al, 2019. This formulation is known as NODRYFLX or LNODRYFLX if referring to the corresponding IFS code option. An obstacle in using NODRYFLX was highlighted in Malardel et al, 2019, where it is explained that the implementation of individual constituent mass fixers becomes more complicated because the dry mass, which is the conservative quantity needs to be deduced from two independently advected non-conservative quantities, the total mass and the total water. As they interact it becomes more problematic to fix them simultaneously and maintain the correct balance between the total air, dry air and moist species (water vapour, cloud fields, rain, snow) mass. This problem has been addressed in CATRINE WP2 and it is possible to use the mass fixer with this alternative form of the continuity equation which does not allow a compensating flux of dry air to keep the total mass constant but instead keeps the dry mass constant.

The solution to the above problem is also linked with the details of the IFS time-stepping. In the IFS, the SL advection is coupled with a semi-implicit (SI) time-stepping scheme. After the advection and physics parametrizations are computed, the SI solver computes a final correction solving an elliptic Helmholtz equation which uses the continuity equation to produce a balanced model state at the end of the time-step. Finally, the pressure fixer is applied to ensure that the total model atmospheric mass is equal to its initial value as the continuity equation dictates but fails to achieve fully due to numerical errors. These surface pressure changes, which occur after the update of tracers by the advection scheme and the physical parametrizations, imply that the tracer specific ratio has changed slightly because the background air density has changed. To close fully the budget, a tracer correction is needed. This final correction is different for the default continuity and the LNODRYFLX option and is explained in the two subsections below.

7.1 Final tracer correction when the default continuity is applied

The tracer transport equation in IFS is:

$$\frac{Dq_t}{Dt} = S_t$$

where q_t, ρ_t are respectively the specific ratio and density of atmospheric tracer t and S_t is a term which represents sources or sinks of this tracer. Let p, ρ be the pressure and density of the moist air mass. The sequence of operations within a time-step that alter these variables is sketched below (in this diagram ADV includes also mass fixer application).

$$\text{ADV } (q_t^+, p^+) \rightarrow \text{PHYS } (q_t^{++}, p^+) \rightarrow \text{SI } (q_t^{++}, p^{(n+1)*}) \rightarrow \text{MASCOR } (q_t^{n+1}, p^{n+1})$$

where MASCOR involves application of a pressure fixer algorithm which ensures that the global mass of air remains constant as explained previously. From the specific ratio definition and the hydrostatic relationship:

$$q_t = \frac{\rho_t}{\rho}, \quad dp = -\rho g dz \Rightarrow -\frac{q_t dp}{g} = \rho_t dz$$

After advection and after the physical parametrizations have been applied, there is no further mass transport in a grid-box neither source nor sink, therefore we can assume that the tracer mass per unit horizontal area (kg m^{-2}) remains unchanged. Since neither the horizontal grid area nor the tracer mass contained within the grid box changes, conservation requires:

$$q_t^{n+1} dp^{n+1} = q_t^{++} dp^+.$$

Therefore,

$$q_t^{n+1} = q_t^{++} \frac{dp^+}{dp^{n+1}} \quad (7.1).$$

If the model performs only passive advection ($q_t^{++} = q_t^+$), equation (7.1) guarantees that the tracer mass remains constant throughout the entire forecast. The same result should hold whenever the physics parametrizations conserve and there are no sink/source terms present. The proposed adjustment removes a small residual error while it has no impact on model forecast accuracy as it has been verified experimentally.

7.2 Final tracer correction when NODRYFLX continuity is applied

In the NODRYFLX continuity formulation the tracer transport equation is modified (see Eq. (39) in TM849 Malardel et al., 2019) to

$$\frac{Dq_t}{Dt} = -q_t S_w + S_t$$

where

- S_t is the tracer source (or sink) term arising from physics,
- S_w is the total-water tendency.

An explicit time discretization gives:

$$q_t^* = q_{t,D}^n + \Delta t S_t - q_t^{++} \Delta t S_w,$$

where $+$, $+$, $+$ denote the states after dynamics (advection) and physics respectively and $q_{t,D}^n$ is the tracer field t interpolated at the upstream departure points D at time-step n .

Since,

$$q_t^{++} \equiv q_t^{phys} = q_{t,D}^n + \Delta t S_t,$$

The update can therefore be written as:

$$q_t^* = (1 - \Delta t S_w) q_t^{++} \quad (7.2)$$

An alternative, more implicit discretization is

$$q_t^* = q_{t,D}^n + \Delta t S_t - q_t^* \Delta t S_w$$

which gives

$$q_t^* = \frac{q_t^{++}}{1 + \Delta t S_w} \quad (7.3)$$

The sequence of operations within one IFS time-step then becomes:

$$\text{ADV } (q_t^+, p^+) \rightarrow \text{PHYS } (q_t^{++}, p^+) \rightarrow \text{NODRYFLX } (q_t^*, p^*) \rightarrow \text{SI } (q_t^*, p^{(n+1)*}) \rightarrow \text{MASCOR } (q_t^{n+1}, p^{n+1})$$

The pressure p^* introduced by the NODRYFLX adjustment is temporary. It is not passed to the SI solver. Its only purpose is to ensure that the tracer budget remains internally consistent. Conservation between the NODRYFLX adjustment and the final corrected state requires

$$q_t^{n+1} dp^{n+1} = q_t^* dp^*$$

or,

$$q_t^{n+1} = q_t^* \frac{dp^*}{dp^{n+1}} \quad (7.4).$$

As previously, we assume that the tracer mass per unit horizontal area remains constant between the physics, NODRYFLX, and SI/MASCOR steps. Therefore,

$$q_t^* dp^* = q_t^{++} dp^+.$$

Using equation (7.2) gives

$$dp^* = \frac{dp^+}{1 - \Delta t S_w}.$$

Substituting this expression into (7.4) yields:

$$q_t^{n+1} = \frac{q_t^*}{1 - \Delta t S_w} \frac{dp^+}{dp^{n+1}}. \quad (7.5)$$

With the correction introduced by equation (7.5), the time-stepping scheme can use the tracer values updated by the NODRYFLX formulation while preserving the tracer budget across the subsequent SI and mass correction steps. If the more implicit update given by (7.3) is used instead of (7.2), the corresponding adjustment becomes:

$$q_t^{n+1} = q_t^* (1 + \Delta t S_w) \frac{dp^+}{dp^{n+1}} \quad (7.6).$$

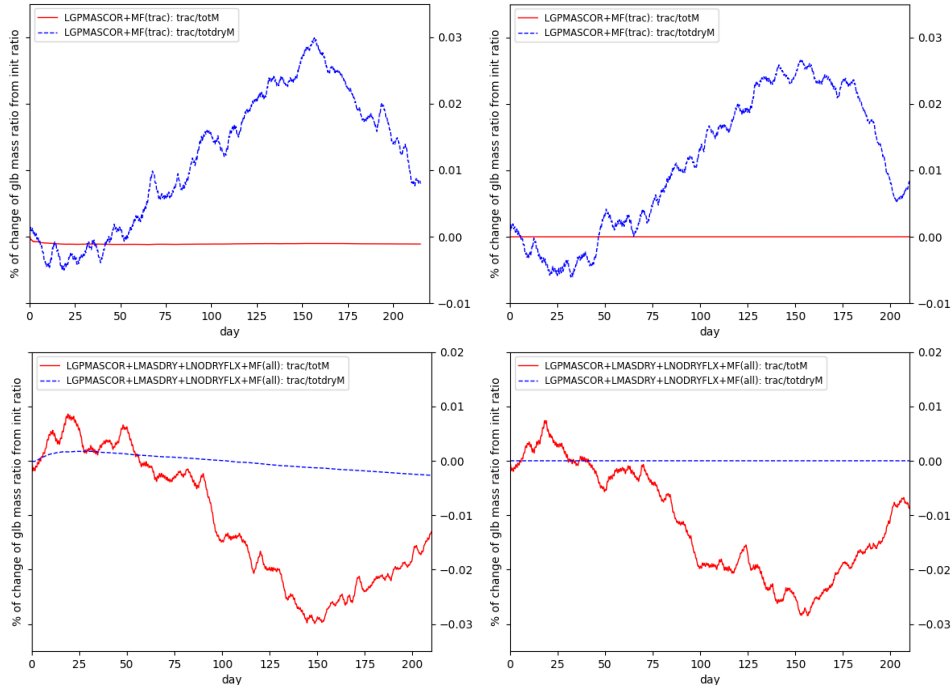


Figure 7.1. Percentage change in the ratio of the total tracer mass (trac) versus the total atmospheric mass (totM) or the total dry mass (totdryM) with respect to their initial value (red and blue lines respectively). **Top row:** the default continuity formulation is used which keeps total mass constant while the dry air mass varies according to the water content of the atmosphere. **Bottom row:** the alternative NODRYFLX continuity formulation is used which keeps the dry mass constant while the total air mass follows the variations of the total water content. **Left column:** no adjustment of specific ratios after SI

solver. **Right column:** adjustment (7.1) and (7.5) is applied for the default (top) and NODRYFLX (bottom) continuity respectively.

The two update methods, (7.5) and (7.6) give very similar results. The method adopted in the IFS is (7.5). The impact of these changes is shown in Fig. 7.1 using a passive tracer advection test at TCo399 resolution. The tracer has a CO₂-like spatial distribution, with a high-concentration plume embedded within it, initialized at the surface level as defined in Fig. 4.1. Applying either (7.1) for the default continuity formulation, which conserves moist air mass, or (7.5) for the NODRYFLX formulation, which conserves dry air mass, corrects a small mass drift.

7.3 Enforcing global conservation of mass in NODRYFLX

Given the above analysis, the steps taken to enforce dry mass conservation and tracer mass conservation when the LNODRYFLX IFS option is used are:

1. Activate the tracer mass fixer for water tracers and for surface pressure. This ensures that both the advected total mass and total wet mass of the atmosphere remain constant which implies that the dry mass of air is constant during the advection step.
2. After the surface pressure modification due to the semi-implicit correction and the final conservative adjustment of dry pressure, all tracers are adjusted locally (re-scaled) using (7.5) to ensure that their mass within a grid box does not change from these two processes which do not transport new mass in a grid box.
3. With the above corrections in place a tracer which is passively advected keeps its mass constant through a simulation at near machine precision (for double precision simulations) while the dry mass remains nearly constant with an oscillation of magnitude 1E-5% of its initial mass being observed. This is negligible but can be eliminated through an iterative procedure where the dry pressure fixer and the tracer adjustment mentioned above are iterated as illustrated in Fig. 7.2.

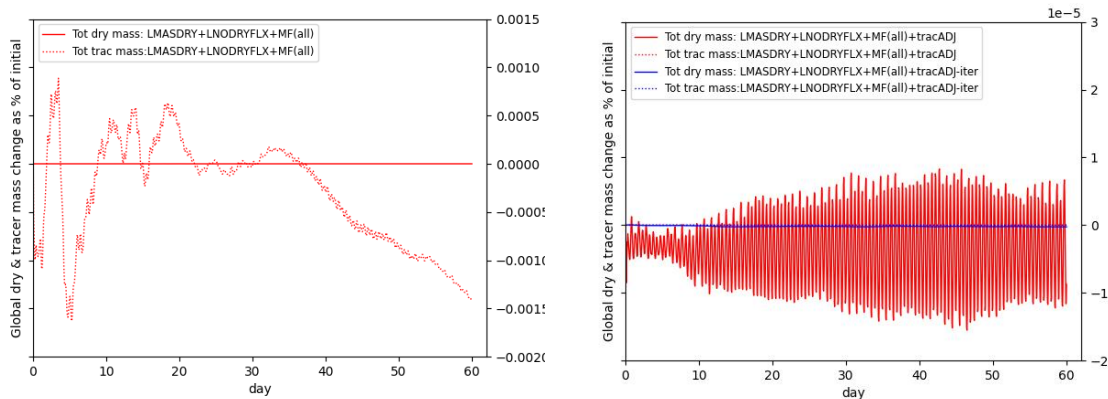


Figure 7.2. Passive advection of a tracer with characteristics of CO₂ in a model run which conserves the dry mass of air. The IFS experiment horizontal resolution is TCo79 (130km) with 137 vertical levels and runs for two months. **Left:** the dry air mass seems constant (thick red line) throughout the forecast but there is a small fluctuation of the tracer mass of the order of 0.001% (dotted red line). **Right:** using the local adjustment specified by Eq. (7.5) a constant tracer mass is obtained throughout the forecast (dotted red line has 0% error) but a tiny fluctuation with amplitude $\sim 1\text{E-}5\%$ can be seen in the global dry air mass (red thick oscillating line). Activating an additional iterative adjustment eliminates this oscillation (blue lines) and both tracer and dry mass remain constant.

To further validate this development, the following test was performed: an idealised passive tracer, with a background value which has CO₂-like spatial characteristics, was simulated in two different long-range forecasts of seven months at TCo399 resolution from the same initial conditions, each using a different version of the continuity equation. The tracer did not interact with the prognostic forecast fields and therefore did not modify the meteorology. At each time-step, the same amount of tracer mass was injected into the lowest model level, mimicking a strong volcanic emission. The emission points were distributed across nine different geographical locations, with each point emitting approximately 0.25 kg/m². The global changes in tracer mass and total mass of the model atmosphere, including water vapour and cloud fields, relative to their initial values are shown in the left panel of Fig. 7.3, while the changes in global air mass, both total wet and dry, are shown in the right panel. Although there is a small difference in the evolution of wet mass, the passive tracer evolves identically in the two forecasts, regardless of which continuity equation formulation is used. This demonstrates that passive tracer transport remains conservative independently of the underlying form of the continuity equation. Furthermore, as shown in the right panel, the default continuity formulation with the total pressure fixer keeps total atmospheric mass constant, whereas the NODRYFLX option with the dry mass fixer keeps dry atmospheric mass constant. As expected, in the default formulation the dry air mass is anti-correlated with the wet mass, whereas in the alternative formulation the total atmospheric mass change is correlated with the wet mass change, while the dry atmospheric mass remains constant. This is the physically consistent behaviour.

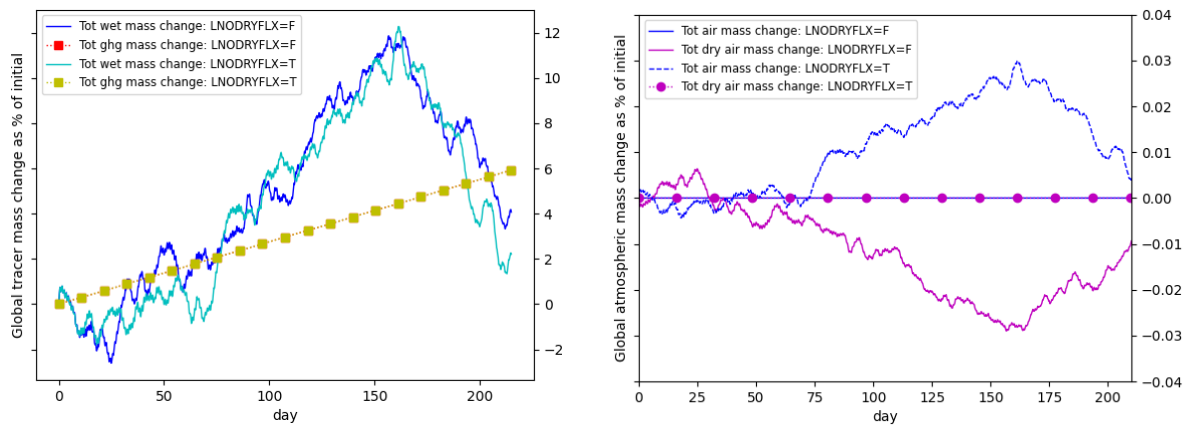


Figure 7.3. Global tracer mass change (left) and atmospheric mass change (right) for a single long (7-month) IFS forecast test case at TCo399 resolution. Two methods are compared: the operational continuity (LNODRYFLX=F) and the alternative form conserving dry mass of air (LNODRYFLX=T).

Changing the form of the continuity equation changes the main forecast fields and therefore it is essential to perform an evaluation on the meteorological impacts of the NODRYFLX continuity combined with the previously listed changes. Standard weather forecast tests at operational resolution (9 km grid spacing) show that there was no change in forecast skill with respect to the operational continuity equation configuration. This is illustrated in Fig. 7.4 where the Mean Sea Level forecast and 500 hPa geopotential headline scores of a forecast using the NODRYFLX continuity is compared against the operational forecast. The skill remains unchanged and in fact there is a slight improvement in the scores in the northern hemisphere. This is encouraging as maintaining a good weather forecast skill is essential for CAMS, CO2MVS inversions and for the unified nature of the IFS forecast system and confirms that this approach could be viable in the future.

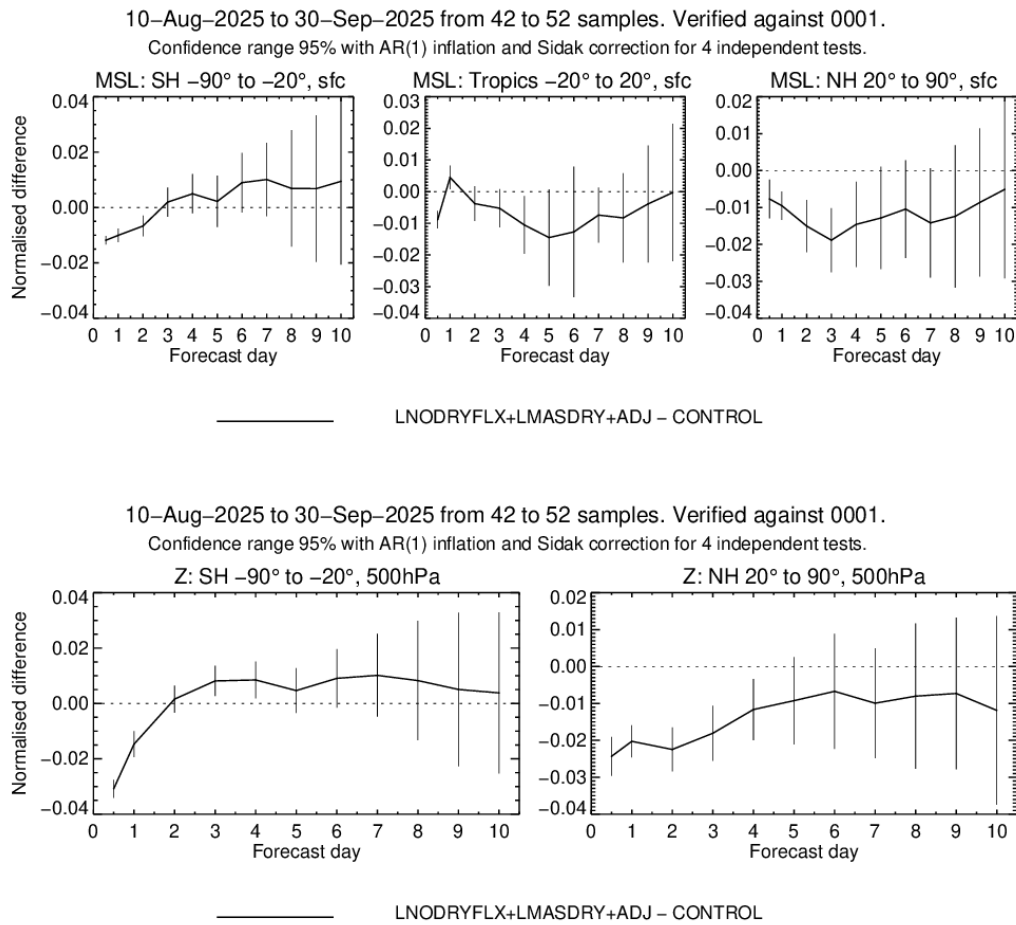


Figure 7.4. Relative change in RMSE with respect to the control forecast when the NODRYFLX continuity equation together with the tracer mass fixer changes described in this section and the dry pressure fixer are applied in IFS. Results are shown for two headline forecast scores: Mean Sea Level pressure (top) and 500 hPa geopotential (bottom). The LNODRYFLX option which conserves dry mass (black line) is compared against the default continuity option used in the operational IFS (including CAMS). The vertical lines at each forecast day indicate the range of statistically significant relative score changes for that forecast time-step. The testing period is 10-08-2025 until 30-09-2025.

This option was tested further by repeating a subset of the WP8 simulations for the 2022–2023 period. In particular, we repeated the experiment based on the current operational CAMS configuration, which uses the LQM3D limiter together with the tracer mass fixer, but replaced the operational continuity formulation with the NODRYFLX formulation and applied the modifications to the fixers described above. The model remained stable, and its meteorological performance was essentially unchanged. However, changes in the GHG bias were apparent both in the comparison with TCCON observations and in the global GHG mass budget. As shown in Fig. 7.5, the NODRYFLX continuity produces a similar magnitude negative rather than positive bias and increases the standard deviation.

One possible explanation for these larger differences in error metrics is an inconsistency introduced each time the meteorology is re-initialised. Every 24 hrs, each forecast is initialised from an ERA5 analysis generated using the operational continuity formulation, whereas the subsequent forecast uses NODRYFLX continuity. The resulting small inconsistency in the air mass evolution may affect the diagnosed GHG tracer mass and thus the mass fixer correction, effectively introducing a spurious tracer source or sink at each restart and thereby likely

contributing to the observed bias. This hypothesis is supported further by the fact that there is a gradual increase in the bias as we can see in Fig. 7.5 which suggests that this is systematic and builds up slowly i.e. each initialisation contributes by a small amount to it. Nevertheless, the results are not far from the observations during the first 6-7 months of the simulation which suggests that the method can deliver accurate results.

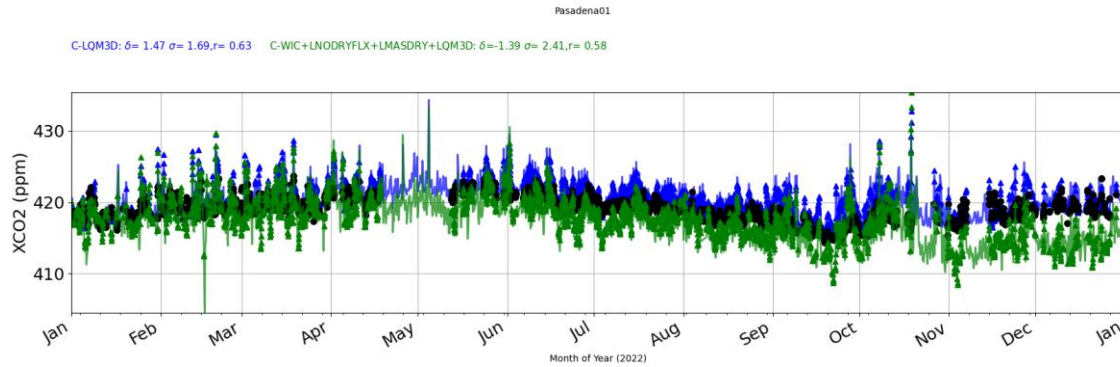


Figure 7.5. Time series (January 2022- January 2023) of daily average XCO₂ compared to TCCON observations for the Pasadena site. Two experiments are compared, one using the default continuity (blue curve) and one the NODRYFLX continuity (green curve). The bias, standard deviation of errors and correlation coefficient is shown at the top for each simulation.

Coupling the continuity equation with the change of water mass in the parametrizations also led to a thorough analysis of the moist equations used in the model and the consistency of the hypotheses made in the dynamical core, the physics parametrizations and the coupling between the dynamical core and the physics package. The IFS equations for momentum, enthalpy and specific ratios are written in advective form, i.e. the time evolution of the density is not anymore part of these equations. In order to obtain the advective form, the continuity equation is subtracted from the original flux form budget equation. Any change in the continuity equation will then result in a modification of all the equations in advective forms. So far, this modification has been included in the tracer equations only. A similar modification in the momentum and temperature equation is currently tested. In practice the impact from these changes is expected to be small. It has been already tested in the ARPEGE model in Météo-France which shares the same dyncore with the IFS but uses a different set of parametrizations and it was found that the scores for the meteorology are indeed neutral. Further tests will be performed in the IFS in order to confirm that the impact is also negligible for atmospheric composition applications.

Furthermore, a prototype implementation of the dry mass continuity approach proposed by Peng et al. (2020) has been developed. This approach differs from that of Malardel et al. (2019) in that it formulates the continuity equation in terms of dry pressure and uses dry mixing ratios instead of specific (moist) mixing ratios. However, the approach represents a more substantial and intrusive model change, with large implications for data assimilation that are beyond the scope of this project. The current development has progressed to the point where we can run this dry mass conserving version of the dynamical core together with physical parametrizations and perform weather forecast experiments. At TCo399 resolution (~28 km), it delivers skill comparable to the operational formulation, but higher-resolution testing has revealed errors linked to the moist pressure departure gradient term introduced into the momentum equation. As explained earlier, robust and accurate performance in weather

forecast cases must be ensured first, as maintaining the strong meteorological skill of the IFS is a prerequisite for reliable atmospheric composition forecasts.

This section has demonstrated that alternative forms of the continuity which conserve the dry mass of air have been developed and tested. These alternatives more accurately reflect atmospheric physics, since in nature only the wet atmospheric mass changes because of evaporation and precipitation. They can also support better use of satellite observations for GHG which are dry mixing ratios rather than the moist mixing ratios used by the IFS. Among these new dry mass conserving options, the NODRYFLX option is the most mature and least invasive option. Nevertheless, as such changes have impact in the remaining equations of the model and implications for the 4D-Var assimilation system and overall the ECMWF weather forecast system it is not straightforward to activate them in the near future, considering a time horizon of 2-3 years. The fact that meteorological scores remain neutral is encouraging. The hope is that there may be benefits for the prediction of intense precipitation systems which will make a stronger case to be adopted by the ECMWF model. Investigations so far have not demonstrated this point but before firm conclusions can be drawn further development and testing is required.

8 Recommendations for CO2MVS and CAMS

The results presented in this deliverable support the following recommendations for the configuration and future development of the IFS tracer advection scheme in CO2MVS and CAMS.

1. **COMAD with the LQM3DCONS limiter and the tracer mass fixer is a strong candidate for CO2MVS and for CAMS GHG forecasts.** This option is mature, already available in the IFS, and has consistently demonstrated good performance for GHG transport, particularly for CO₂. It substantially improves conservation compared with the current operational limiter while maintaining the accuracy, stability and computational efficiency required for long CAMS simulations and CO2MVS inversions.
2. **Continue testing of the ILMC limiter as a very promising option for tracer transport and consider activating it for applications that exhibit rapid local mass growth such as volcanic transport forecasts.** ILMC provides the largest reduction in mass-conservation error, in some idealised plume and point-source tests by up to two orders of magnitude, and performs very well in realistic CO₂ simulations, including experiments without the global mass fixer. Further optimisation is recommended to reduce its computational cost, and additional research is needed to better understand its impact on inversions.
3. **SWEEP interpolation is a strong candidate for the multi-tracer applications in CAMS, particularly for ozone and chemical tracers.** SWEEP reduces interpolation cost for simulations with many tracers and improves several error metrics in CAMS experiments, including standard deviation of errors, RMSE and correlation in some cases. Its combination with the current LQM3D limiter already performs competitively and appears suitable. However, before the recommended operational configuration is fixed, further tests will be needed combining SWEEP with the new limiters.
4. **Retain the tracer mass fixer in CO2MVS and CAMS configurations.** The mass fixer remains essential for preventing slow global tracer mass drift and for reducing sensitivity to the choice of interpolation scheme and limiter, particularly in long GHG simulations. For the current inversion configuration, based on the OSSE experiments, the preferred option is to keep the mass fixer active in the nonlinear trajectory but exclude it from the TL/AD minimisation unless future regularised formulations demonstrate clear benefit.
5. **Use the completed TL/AD developments for COMAD, LQM3DCONS and SWEEP in inversion.** Further work should focus on quantifying their impact on emission increments, posterior uncertainty and robustness across different observing networks and meteorological regimes.
6. **Continue developing dry-mass-conserving continuity formulations as research and development options rather than near-term operational options.** The NODRYFLX formulation and related dry-mass-conserving developments are physically attractive and technically more mature than before, but recent experiments indicate that further work is needed to ensure full consistency with the entire prognostic equation set, data assimilation and model restarts, before adoption in CO2MVS or CAMS.

Overall, the developments presented in this deliverable significantly improve the conservation, accuracy and flexibility of IFS tracer transport. Several components, including COMAD, LQM3DCONS, SWEEP and their TL/AD counterparts, are now sufficiently mature for operational consideration. ILMC is nearly mature, but it would benefit from further computational optimization, if this proves achievable, and requires testing with chemical tracers in CAMS and in CO2MVS inversions. Dry mass conserving continuity formulations represent promising directions for future research but cannot be activated in CAMS operations for at least the next two years. Together, these developments provide a solid foundation for

more accurate GHG forecasting and atmospheric inversion systems within CO2MVS and CAMS.

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