

The ECMWF contribution to the CEOP public domain dataset

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A model archive that would satisfy traditional atmospheric circulation studies, more detailed energy and water budgets, and remote sensing requirements is presented. Proper consideration has been given to data volume, numerics and conservation issues associated with the budgets, and the need to have a relatively simple archive, yet enabling a sound computation of the different budget terms. The energy and water budget part of the proposal is based on the vertically integrated water and energy budget components currently produced in ERA40, as defined in close collaboration with Kevin Trenberth. The vertical and horizontal resolutions and the time sampling are commensurable with the fine resolution of the ERA40.

1 Background and rationale

The Coordinated Enhanced Observing Period (CEOP) Initiative (Bosilovich and Lawford, 2002) is now in the process of firming up the contributions of the atmospheric modelling centres to the CEOP archive centre for model data. Requests to ECMWF for a data contribution were originally made in September 2001 on a letter from the World Climate Research Programme (WCRP), accompanied by a letter from Dr. Toshio Koike, CEOP Lead Scientist. More recently a Strawman Proposal is being drafted by the CEOP International Coordinator, with contributions from different researchers. Apart from more traditional atmospheric circulation variables, a large number of 3D model fields related to energy and water budget computations is included in the list of fields, which is mostly inspired by Dr. John Roads, Chair of the CEOP Water and Energy Cycle Simulation and Prediction activity.

This proposal addresses research needs in three different communities: (a) “Conventional” atmospheric circulation studies; (b) Water and energy detailed studies; (c) Remote sensing studies.

Most of this proposal is on the model fields for CEOP. Model Output Location Time Series (MOLTS), for vertical columns of the atmosphere over 41 predefined points (see http://www.joss.ucar.edu/ghp/ceopdm/ceop_world_molts.html), will be also provided by ECMWF. They will be based on the ECMWF capability so-called DDH (Diagnostiques sur Domaines Horizontaux) and we will try to provide as many model physical tendencies and fluxes as possible. Since these are single point fields, data volume is not an issue. Hourly time series for forecasts up to 36 hours will be provided.

2 Integrated water and energy budgets

A detailed vertical description of atmospheric water and energy budgets represents a large data volume and presumably is of use only to a small community of researchers. It can only

be done properly from the full resolution model level fields. A useful simplification, proposed here, is to have a complete set of 2-D fields describing vertically integrated energy, water and mass budget equations.

Apart from the data volume there are several reasons why having vertical detail can lead to incorrect use of the data (see review in Trenberth 1997). Let us consider first the possibility of making all model level data available. As Trenberth (1995) points out, model level data has to be handled at full spectral resolution; spectrally truncating model level data is an ill-defined operation and leads to problems in the vicinity of orography, because the vertical coordinate changes with the truncation. To make the fields available on a selected number of pressure levels would reduce data volume, but is an even less satisfactory alternative. Disadvantages include: (a) Insufficient detail to resolve model transport in the lower troposphere; (b) The equation of continuity can no longer be satisfied, with the result that all budgets based on pressure level data will see artificial sources and sinks of mass; (c) The lower boundary condition is more complex to formulate, a problem for vertical integrals; (d) Extrapolation below the earth's surface is arbitrary and pollutes the low level data.

For all the above reasons, the ERA40 project decided to produce a set of fields (http://www.ecmwf.int/research/era/_docs/ArchivePlan.ps) that are essentially what we are offering here for CEOP. We propose to provide vertically integrated fields that are the essential components in the computation of the different terms in the energy, mass and water budget equations for an atmospheric column. ECMWF will compute the vertical integrals at full resolution and fully compatible with the model horizontal and vertical discretisation. The final results will be interpolated and delivered on a regular lat-lon grid (see Section 3 below).

Using the fields provided, researchers can perform budgets for the following quantities on an entire atmospheric column (see Appendix A, Table A2, for a complete list of fields, and Appendix D for the integrated budget equations and a list of symbols): (a) Mass; (b) Water vapour; (c) Kinetic energy; (d) Enthalpy ($C_p T$); (d) Total dry energy ($C_p T + k$); (e) Total energy ($C_p T + k + Lq + \phi_s$).

For the surface, we will provide similar soil integrated dry and moist energy and total soil water, together with a number of fields that characterize the soil and near-surface state for remote sensing. These, together with the surface fluxes and runoff, allow the calculation of an integrated energy and water budget for the soil. Appendix A, Tables A3-A4, lists the complete set of 2-D fields, while the bottom part of Table A3 contains the soil integrated quantities.

3 Synopsis of remaining variables

3.1 Fluxes

The r.h.s of the energy and water budget equations are fluxes at the top and bottom of the atmosphere computed by the model physical parameterisations. The fluxes provided will be time accumulated during the forecast. See Appendix A, Table A4, for further details.

3.2 Atmospheric variables

More “traditional” atmospheric variables (e.g., wind components, geopotential, moisture, temperature) will be provided in pressure levels. See Appendix A, Table D, for further details.

3.3 Resolution, data representation, and time sampling

All fields will be provided on a 1.25x1.25 degree grid. Three-dimensional fields will be provided at 23 pressure levels, from 1000 hPa to 1 hPa. Fields will be sampled every 6 hours. This is an essential requirement to avoid spurious tidal signals in the mass, moisture and heat budgets (Trenberth 1997).

3.4 Analysis vs. forecast

Model prognostic variables, instantaneous diagnostic quantities and vertically integrated quantities associated to budgets will be based on analyses. Fluxes will be accumulated during the forecasts. Since some of the fluxes (especially precipitation) have considerable “spin-up”, they will be provided both for 4-times daily 6 hour forecasts and 12-24 forecasts starting at 00 and 12 UTC.

4 Operations vs. reanalysis

The vertically integrated budget components are not produced for the operational data assimilation and to introduce them in the production suite would take several months due to a number of practical considerations. Those fields are part of the ERA40 atmospheric reanalysis archiving suite, and that is the reason why *we propose to base all the data above on ERA40 and its continuation. 3 years of data, 1 October 2001-31 December 2004, covering the entire CEOP period, will be made available.*

ERA40 covers the period 1958-2001, and it will finish production in March 2003. Only the last 3 months of 2001 will cover the CEOP period. There are firm plans of reanalysing a recent period (possibly 1979-present, and continuing in near-real time) with a better assimilation system and better usage of data than ERA40. This will probably start next year by running through 2002, and it will continue in near-real time (3-12 months after the fact).

There is one additional reason why we consider reanalysis to be a better option than operations. It will be a strong motivation and it will give a real deadline for getting the radiosonde and surface data collected in CEOP in the shape that allows usage by the data assimilation groups. This will greatly improve the quality of the analysis in the Continental Scale Experiment areas.

Note that we intend to provide *MOLTS data for all locations from the operational high-resolution suite, as well as for the reanalysis suite.* The necessary model input preparation has been done and a number of technical steps are still needed, but we think that MOLTS data from the operational suite can be available from 1 December 2002. If there is a need for it, we can recreate MOLTS data from a high resolution integration before that date. Data will be provided in ASCII files, supported by a complete set of documentation.

References

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Appendix A: Complete list of fields and discretization

Table A1: 3-D fields on pressure levels. All data from Analysis, 4 times daily (00, 06, 12, 18 UTC).

| Level (hPa) | Parameters | Units |
|-------------|-----------------------------|--|
| 1 | Z, T, U, V, Q, R, omega, O3 | m^2s^{-2} , K, ms^{-1} , ms^{-1} , $kgkg^{-1}$, [0-1], Pas^{-1} , $kgkg^{-1}$ |
| 2 | Z, T, U, V, Q, R, omega, O3 | |
| 3 | Z, T, U, V, Q, R, omega, O3 | |
| 5 | Z, T, U, V, Q, R, omega, O3 | |
| 7 | Z, T, U, V, Q, R, omega, O3 | |
| 10 | Z, T, U, V, Q, R, omega, O3 | |
| 20 | Z, T, U, V, Q, R, omega, O3 | |
| 30 | Z, T, U, V, Q, R, omega, O3 | |
| 50 | Z, T, U, V, Q, R, omega, O3 | |
| 70 | Z, T, U, V, Q, R, omega, O3 | |
| 100 | Z, T, U, V, Q, R, omega, O3 | |
| 150 | Z, T, U, V, Q, R, omega, O3 | |
| 200 | Z, T, U, V, Q, R, omega, O3 | |
| 250 | Z, T, U, V, Q, R, omega, O3 | |
| 300 | Z, T, U, V, Q, R, omega, O3 | |
| 400 | Z, T, U, V, Q, R, omega, O3 | |
| 500 | Z, T, U, V, Q, R, omega, O3 | |
| 600 | Z, T, U, V, Q, R, omega, O3 | |
| 700 | Z, T, U, V, Q, R, omega, O3 | |
| 775 | Z, T, U, V, Q, R, omega, O3 | |
| 850 | Z, T, U, V, Q, R, omega, O3 | |
| 925 | Z, T, U, V, Q, R, omega, O3 | |
| 1000 | Z, T, U, V, Q, R, omega, O3 | |

Table A2: Vertically integrated budget component fields. All data from Analysis, 4 times daily (00, 06, 12, 18 UTC).

| Field | Definition | Units |
|------------------------------|---|--------------------------------|
| Surface geopotential | $\frac{1}{g} \int_0^1 \phi_s \frac{\partial p}{\partial \eta} d\eta$ | Jm^{-2} |
| Total mass | $\frac{p_s}{g}$ | kg m^{-2} |
| Mass u-flux | $\frac{1}{g} \int_0^1 u \frac{\partial p}{\partial \eta} d\eta$ | $\text{kgm}^{-1}\text{s}^{-1}$ |
| Mass v-flux | $\frac{1}{g} \int_0^1 v \frac{\partial p}{\partial \eta} d\eta$ | $\text{kgm}^{-1}\text{s}^{-1}$ |
| Mass flux divergence | $\nabla \cdot \frac{1}{g} \int_0^1 \mathbf{v} \frac{\partial p}{\partial \eta} d\eta$ | $\text{kgm}^{-2}\text{s}^{-1}$ |
| Geopotential | $\frac{1}{g} \int_0^1 \phi \frac{\partial p}{\partial \eta} d\eta$ | Jm^{-2} |
| Geopotential u-flux | $\frac{1}{g} \int_0^1 \phi u \frac{\partial p}{\partial \eta} d\eta$ | $\text{Jm}^{-1}\text{s}^{-1}$ |
| Geopotential v- flux | $\frac{1}{g} \int_0^1 \phi v \frac{\partial p}{\partial \eta} d\eta$ | $\text{Jm}^{-1}\text{s}^{-1}$ |
| Geopotential flux divergence | $\nabla \cdot \frac{1}{g} \int_0^1 \phi \mathbf{v} \frac{\partial p}{\partial \eta} d\eta$ | $\text{Jm}^{-2}\text{s}^{-1}$ |
| Enthalpy | $\frac{1}{g} \int_0^1 C_p T \frac{\partial p}{\partial \eta} d\eta$ | Jm^{-2} |
| Enthalpy u-flux | $\frac{1}{g} \int_0^1 C_p T u \frac{\partial p}{\partial \eta} d\eta$ | $\text{Jm}^{-1}\text{s}^{-1}$ |
| Enthalpy v- flux | $\frac{1}{g} \int_0^1 C_p T v \frac{\partial p}{\partial \eta} d\eta$ | $\text{Jm}^{-1}\text{s}^{-1}$ |
| Enthalpy flux divergence | $\nabla \cdot \frac{1}{g} \int_0^1 C_p T \mathbf{v} \frac{\partial p}{\partial \eta} d\eta$ | $\text{Jm}^{-2}\text{s}^{-1}$ |
| Water vapour | $\frac{1}{g} \int_0^1 q \frac{\partial p}{\partial \eta} d\eta$ | kgm^{-2} |
| Moisture u-flux | $\frac{1}{g} \int_0^1 q u \frac{\partial p}{\partial \eta} d\eta$ | $\text{kgm}^{-1}\text{s}^{-1}$ |
| Moisture v- flux | $\frac{1}{g} \int_0^1 q v \frac{\partial p}{\partial \eta} d\eta$ | $\text{kgm}^{-1}\text{s}^{-1}$ |
| Moisture flux divergence | $\nabla \cdot \frac{1}{g} \int_0^1 q \mathbf{v} \frac{\partial p}{\partial \eta} d\eta$ | $\text{kgm}^{-2}\text{s}^{-1}$ |

| | | |
|---|---|--------------------------------|
| Cloud liquid water | $\frac{1}{g} \int_0^1 q_l \frac{\partial p}{\partial \eta} d\eta$ | kgm^{-2} |
| Cloud ice | $\frac{1}{g} \int_0^1 q_i \frac{\partial p}{\partial \eta} d\eta$ | kgm^{-2} |
| Ozone | $\frac{1}{g} \int_0^1 O_3 \frac{\partial p}{\partial \eta} d\eta$ | kgm^{-2} |
| Ozone u-flux | $\frac{1}{g} \int_0^1 O_3 u \frac{\partial p}{\partial \eta} d\eta$ | $\text{kgm}^{-1}\text{s}^{-1}$ |
| Ozone v- flux | $\frac{1}{g} \int_0^1 O_3 v \frac{\partial p}{\partial \eta} d\eta$ | $\text{kgm}^{-1}\text{s}^{-1}$ |
| Ozone flux divergence | $\nabla \cdot \frac{1}{g} \int_0^1 O_3 \mathbf{v} \frac{\partial p}{\partial \eta} d\eta$ | $\text{kgm}^{-2}\text{s}^{-1}$ |
| Kinetic energy [$k = \frac{1}{2}(u^2 + v^2)$] | $\frac{1}{g} \int_0^1 k \frac{\partial p}{\partial \eta} d\eta$ | Jm^{-2} |
| Kinetic energy u-flux | $\frac{1}{g} \int_0^1 ku \frac{\partial p}{\partial \eta} d\eta$ | $\text{Jm}^{-1}\text{s}^{-1}$ |
| Kinetic energy v- flux | $\frac{1}{g} \int_0^1 kv \frac{\partial p}{\partial \eta} d\eta$ | $\text{Jm}^{-1}\text{s}^{-1}$ |
| Kinetic energy flux divergence | $\nabla \cdot \frac{1}{g} \int_0^1 k\mathbf{v} \frac{\partial p}{\partial \eta} d\eta$ | $\text{Jm}^{-2}\text{s}^{-1}$ |
| Dry static energy ($s = C_p T + gz$) | $\frac{1}{g} \int_0^1 s \frac{\partial p}{\partial \eta} d\eta$ | Jm^{-2} |
| Moist static energy ($h = s + Lq$) | $\frac{1}{g} \int_0^1 h \frac{\partial p}{\partial \eta} d\eta$ | Jm^{-2} |
| Total energy | $\frac{1}{g} \int_0^1 (C_p T + k + Lq + \phi_s) \frac{\partial p}{\partial \eta} d\eta$ | Jm^{-2} |
| Total energy u-flux | $\frac{1}{g} \int_0^1 (h + k)u \frac{\partial p}{\partial \eta} d\eta$ | $\text{Jm}^{-1}\text{s}^{-1}$ |
| Total energy v- flux | $\frac{1}{g} \int_0^1 (h + k)v \frac{\partial p}{\partial \eta} d\eta$ | $\text{Jm}^{-1}\text{s}^{-1}$ |
| Total energy flux divergence | $\nabla \cdot \frac{1}{g} \int_0^1 (h + k)\mathbf{v} \frac{\partial p}{\partial \eta} d\eta$ | $\text{Jm}^{-2}\text{s}^{-1}$ |
| Energy conversion | $\frac{1}{g} \int_0^1 \left(-\omega \frac{RT}{p} \right) \frac{\partial p}{\partial \eta} d\eta$ | $\text{Jm}^{-2}\text{s}^{-1}$ |

Table A3: 2-D analysis fields. All data from Analysis, 4 times daily (00, 06, 12, 18 UTC).

| Fields | Definition | Units |
|-----------------------------------|---|--------------------------------|
| Surface pressure | | Pa |
| Temperature at 2m level | | K |
| Dewpoint at 2m level | | K |
| U-component wind at 10 m level | | ms ⁻¹ |
| V-component wind at 10 m level | | ms ⁻¹ |
| Low cloud cover | | [0-1] |
| Medium cloud cover | | [0-1] |
| High cloud cover | | [0-1] |
| Total cloud cover | | [0-1] |
| Skin temperature | | K |
| Surface temperature layer 1 | [Top soil (0-7 cm depth) temperature over land, SST in the open ocean and top ice layer temperature over sea ice] | K |
| Soil temperature layer 2 | 7-28 cm depth | K |
| Soil temperature layer 3 | 28-100 cm depth | K |
| Soil temperature layer 4 | 100-289 cm depth | K |
| Ice temperature layer 1 | 0-7 cm depth | K |
| Ice temperature layer 2 | 7-28 cm depth | K |
| Ice temperature layer 3 | 28-100 cm depth | K |
| Ice temperature layer 4 | 100-150 cm depth | K |
| Sea surface temperature | Temperature of open sea and lakes | K |
| Sea ice fraction | | [0-1] |
| Snow mass (snow water equivalent) | | m |
| Volumetric soil water layer 1 | 0-7 cm depth | m ³ m ⁻³ |
| Volumetric soil water layer 2 | 7-28 cm depth | m ³ m ⁻³ |
| Volumetric soil water layer 3 | 28-100 cm depth | m ³ m ⁻³ |
| Volumetric soil water layer 4 | 100-189 cm depth | m ³ m ⁻³ |
| Snow temperature | | K |
| Snow density | | kgm ⁻³ |
| Albedo | Background (snow-free) albedo over land | [0-1] |
| Bare ground soil water index | Can be computed, see Annex E | [0-1] |
| Root zone soil water index | Can be computed, see Annex E | [0-1] |

| | | |
|---|---|------------------|
| Total soil water | $\sum_{i=1}^4 \theta_i d_i$, can be computed, see Annex E | m |
| Total soil sensible energy | $\sum_{i=1}^4 (\rho C)_i T_i d_i$, can be computed, see Annex E | Jm ⁻² |
| Total soil energy (sensible + latent) (Includes the thermal effect of phase changes in the soil, Viterbo et al 1999) | $\sum_{i=1}^4 \left[(\rho C)_i T_i - L \rho_w \theta_f \frac{\partial f}{\partial T} \right] d_i$, can be computed, see Annex E | Jm ⁻² |

Table A4: 2-D surface and top of the atmosphere fluxes fields. 6-hourly data from two forecast periods: (a) 6-hours forecasts from 00, 06, 12, 18 UTC; (b) 12-24 hour forecasts from 00 and 12 UTC. Note: Fields marked with * are time integrated since the beginning of forecast.

| Fields | | Units |
|--------------------------------------|-------------------------|--------------------------------|
| U-stress * | | Nm ⁻² s |
| V-stress * | | Nm ⁻² s |
| U- orographic stress * | | Nm ⁻² s |
| V- orographic stress * | | Nm ⁻² s |
| Surface net SW radiation * | | Wm ⁻² s |
| Surface net LW radiation * | | Wm ⁻² s |
| Surface SW radiation downward * | | Wm ⁻² s |
| Surface LW radiation downward * | | Wm ⁻² s |
| Clear-sky surface net SW radiation * | | Wm ⁻² s |
| Clear-sky surface net LW radiation * | | Wm ⁻² s |
| Top net SW radiation * | | Wm ⁻² s |
| Top LW radiation * | | Wm ⁻² s |
| Clear-sky top net SW radiation * | | Wm ⁻² s |
| Clear-sky top LW radiation * | | Wm ⁻² s |
| Surface SH flux * | | Wm ⁻² s |
| Surface LH flux * | | Wm ⁻² s |
| Surface evaporation * | | m |
| Snow evaporation * | | m |
| Snowmelt * | | m |
| Large-scale precipitation * | | m |
| Convective precipitation * | | m |
| Snowfall * | | m |
| Runoff * | | m |
| Boundary layer height | (6 hour forecasts only) | m |
| Forecast albedo | (6 hour forecasts only) | [0-1] |
| Two-metre temperature | (6 hour forecasts only) | K |
| Two-metre dewpoint | (6 hour forecasts only) | K |
| U-component wind at 10 metre level | (6 hour forecasts only) | ms ⁻¹ |
| V-component wind at 10 metre level | (6 hour forecasts only) | ms ⁻¹ |
| Soil temperature layer 1 | (6 hour forecasts only) | K |
| Volumetric soil water layer 1 | (6 hour forecasts only) | m ³ m ⁻³ |
| Volumetric soil water layer 2 | (6 hour forecasts only) | m ³ m ⁻³ |
| Volumetric soil water layer 3 | (6 hour forecasts only) | m ³ m ⁻³ |

Snow mass (snow water equivalent)

(6 hour forecasts only) m

Table A5: Selected boundary layer fields at model levels. All data from Analysis, 4 times daily (00, 06, 12, 18 UTC).

| Fields | Units |
|----------------------------|--------------------|
| U-wind component level 57 | ms^{-1} |
| V-wind component level 57 | ms^{-1} |
| Temperature level 57 | K |
| Specific humidity level 57 | kgkg^{-1} |
| U-wind component level 60 | |
| V-wind component level 60 | |
| Temperature level 60 | |
| Specific humidity level 60 | |

Table A6: Invariant fields.

| Fields | Units |
|--|--------------------------------|
| Land-sea mask | [0-1] |
| Background albedo (monthly) | [0-1] |
| Surface roughness for momentum | m |
| Logarithm of surface roughness for heat (in m) | - |
| High vegetation fraction | [0-1] |
| Low vegetation fraction | [0-1] |
| High vegetation type | - |
| Low vegetation type | - |
| Geopotential of model surface (orography height*g) | m ² s ⁻² |

Appendix B: Data volume

Let N_a , N_b , N_s , N_{f1} , N_{f2} , N_m be the number of fields per pressure level, the number of budget fields, the number of surface analysis fields, the number of surface forecast fields for 06 and 18, the number of surface forecast fields for 00 and 12 UTC, the number of model level fields, and P the number of pressure levels. The total number of field per day is $N_{day}=(4*N_a*P+4*N_b+4*N_s+2*N_{f1}+2*N_{f2}*3+4*N_m*2)$. The number of fields per year is $365*N_{day}$.

From the tables in Appendix A, $N_a=8$, $P=23$, $N_b=34$, $N_s=28$, $N_{f1}=34$, $N_{f2}=23$, $N_m=4$, gives the number of fields per day, $N_{day}=1222$.

Assuming the unit storage size of a field as $s=0.085$ Mb, this represents 104 Mb/day, 38 Gb/year and 114 Gb as the total volume for the total ECMWF CEOP archive.

Appendix C: MOLTS variables

To be written ...

Appendix D: Integrated budget equations. Vertical integrals for energy, mass, water and ozone budgets

Annex 1 on budget equations from the ERA40 archive plan (ECMWF 2000) is included here for convenience.

The continuous, adiabatic, frictionless form of the model's primitive equations may be manipulated to give the following equations, in standard notation:

Kinetic energy:

$$\begin{aligned} \frac{\partial}{\partial t} \left(E \frac{\partial p}{\partial \eta} \right) = & -\nabla \cdot \left(\underline{v} E \frac{\partial p}{\partial \eta} \right) - \nabla \cdot \left(\underline{v} (\phi - \phi_s) \frac{\partial p}{\partial \eta} \right) - \frac{\partial}{\partial \eta} \left(\dot{\eta} E \frac{\partial p}{\partial \eta} \right) \\ & + \frac{\partial}{\partial \eta} \left((\phi - \phi_s) \int_0^\eta \nabla \cdot (\underline{v} \frac{\partial p}{\partial \eta}) d\eta \right) - \frac{RT\omega}{p} \frac{\partial p}{\partial \eta} - \underline{v} \frac{\partial p}{\partial \eta} \cdot \nabla \phi_s \end{aligned} \quad (D.1)$$

$$E = \frac{1}{2} (\underline{v} \cdot \underline{v})$$

Potential+Internal energy:

$$\begin{aligned} \frac{\partial}{\partial t} \left((c_p T + \phi_s) \frac{\partial p}{\partial \eta} \right) = & -\nabla \cdot \left(\underline{v} (c_p T + \phi_s) \frac{\partial p}{\partial \eta} \right) - \frac{\partial}{\partial \eta} \left(\dot{\eta} (c_p T + \phi_s) \frac{\partial p}{\partial \eta} \right) \\ & + \frac{RT\omega}{p} \frac{\partial p}{\partial \eta} + \underline{v} \frac{\partial p}{\partial \eta} \cdot \nabla \phi_s \end{aligned} \quad (D.2)$$

Mass:

$$\frac{\partial}{\partial t} \left(\frac{\partial p}{\partial \eta} \right) = -\nabla \cdot \left(\underline{v} \frac{\partial p}{\partial \eta} \right) - \frac{\partial}{\partial \eta} \left(\dot{\eta} \frac{\partial p}{\partial \eta} \right) \quad (D.3)$$

Water vapour:

$$\frac{\partial}{\partial t} \left(q \frac{\partial p}{\partial \eta} \right) = -\nabla \cdot \left(\underline{v} q \frac{\partial p}{\partial \eta} \right) - \frac{\partial}{\partial \eta} \left(\dot{\eta} q \frac{\partial p}{\partial \eta} \right) \quad (D.4)$$

Ozone:

$$\frac{\partial}{\partial t} \left(O_3 \frac{\partial p}{\partial \eta} \right) = -\nabla \cdot \left(\underline{v} O_3 \frac{\partial p}{\partial \eta} \right) - \frac{\partial}{\partial \eta} \left(\dot{\eta} O_3 \frac{\partial p}{\partial \eta} \right) \quad (D.5)$$

The notation is as in Simmons and Burridge (1981, *Mon.Wea.Rev.*, **109**, 758-766). The gas constant, R , and specific heat at constant pressure, c_p , vary with specific humidity, q :

$$R = R_d \left(1 + \left(\frac{R_v}{R_d} - 1 \right) q \right) \quad (D.6)$$

$$c_p = c_{pd} \left(1 + \left(\frac{c_{pv}}{c_{pd}} - 1 \right) q \right) \quad (\text{D.7})$$

where subscripts d and v denote values for dry air and water vapour respectively.

It should be noted that $(c_p T + \phi_s) \frac{\partial p}{\partial \eta}$ should strictly be interpreted in terms of potential+internal energy only when vertically integrated:

$$\begin{aligned} \int_0^1 (c_v T + \phi) \frac{\partial p}{\partial \eta} d\eta &= \int_0^1 (c_p T + \phi - RT) \frac{\partial p}{\partial \eta} d\eta = \int_0^1 \left(c_p T \frac{\partial p}{\partial \eta} + \frac{\partial}{\partial \eta} (p\phi) \right) d\eta \\ &= \int_0^1 (c_p T + \phi_s) \frac{\partial p}{\partial \eta} d\eta \end{aligned} \quad (\text{D.8})$$

Integrating the energy, mass, water vapour and ozone equations in the vertical, they may be written symbolically as:

$$\frac{\partial}{\partial t} KE = -(\nabla \cdot \underline{F}_{KE}) - (\nabla \cdot \underline{F}_{\phi-\phi_s}) + C_1 + C_2 \quad (\text{D.9})$$

$$\frac{\partial}{\partial t} PIE = -(\nabla \cdot \underline{F}_{PIE}) - C_1 - C_2 \quad (\text{D.10})$$

$$\frac{\partial}{\partial t} Mass = -(\nabla \cdot \underline{F}_M) \quad (\text{D.11})$$

$$\frac{\partial}{\partial t} TCWV = -(\nabla \cdot \underline{F}_q) \quad (\text{D.12})$$

$$\frac{\partial}{\partial t} TCO = -(\nabla \cdot \underline{F}_{O_3}) \quad (\text{D.13})$$

The vertically integrated variables are:

$$KE = \frac{1}{g} \int_0^1 \frac{1}{2} (\underline{v} \cdot \underline{v}) \frac{\partial p}{\partial \eta} d\eta \quad (\text{D.14})$$

$$PIE = \frac{1}{g} \int_0^1 (c_p T + \phi_s) \frac{\partial p}{\partial \eta} d\eta = CPT + \phi_s Mass \quad (\text{D.15})$$

$$CPT = \frac{1}{g} \int_0^1 c_p T \frac{\partial p}{\partial \eta} d\eta \quad (\text{D.16})$$

$$Mass = \frac{1}{g} \int_0^1 \frac{\partial p}{\partial \eta} d\eta = \frac{p_s}{g} \quad (\text{D.17})$$

$$TCWV = \frac{1}{g} \int_0^1 q \frac{\partial p}{\partial \eta} d\eta \quad (\text{D.18})$$

$$TCO = \frac{1}{g} \int_0^1 O_3 \frac{\partial p}{\partial \eta} d\eta \quad (\text{D.19})$$

The fluxes are:

$$F_{KE} = \frac{1}{g} \int_0^1 \tilde{\nu} \frac{1}{2} (\tilde{\nu} \cdot \tilde{\nu}) \frac{\partial p}{\partial \eta} d\eta \quad (D.20)$$

$$F_{\tilde{\nu}-\phi_s} = \frac{1}{g} \int_0^1 \tilde{\nu} (\phi - \phi_s) \frac{\partial p}{\partial \eta} d\eta = F_{\tilde{\nu}\phi} - F_{\tilde{\nu}\phi_s} \quad (D.21)$$

$$F_{\tilde{\nu}\phi} = \frac{1}{g} \int_0^1 \tilde{\nu} \phi \frac{\partial p}{\partial \eta} d\eta \quad (D.22)$$

$$F_{\tilde{\nu}\phi_s} = \frac{1}{g} \int_0^1 \tilde{\nu} \phi_s \frac{\partial p}{\partial \eta} d\eta = \phi_s F_M \quad (D.23)$$

$$F_{PIE} = \frac{1}{g} \int_0^1 \tilde{\nu} (c_p T + \phi_s) \frac{\partial p}{\partial \eta} d\eta = F_{CPT} + \phi_s F_M \quad (D.24)$$

$$F_{CPT} = \frac{1}{g} \int_0^1 \tilde{\nu} c_p T \frac{\partial p}{\partial \eta} d\eta \quad (D.25)$$

$$F_M = \frac{1}{g} \int_0^1 \tilde{\nu} \frac{\partial p}{\partial \eta} d\eta \quad (D.26)$$

$$F_q = \frac{1}{g} \int_0^1 \tilde{\nu} q \frac{\partial p}{\partial \eta} d\eta \quad (D.27)$$

$$F_{O_3} = \frac{1}{g} \int_0^1 \tilde{\nu} O_3 \frac{\partial p}{\partial \eta} d\eta \quad (D.28)$$

and the energy conversions are:

$$C_1 = -\frac{1}{g} \int_0^1 \frac{RT\omega}{p} \frac{\partial p}{\partial \eta} d\eta \quad (D.29)$$

$$C_2 = -\frac{1}{g} \int_0^1 \left(\tilde{\nu} \frac{\partial p}{\partial \eta} \cdot \nabla \phi_s \right) d\eta = -F_M \cdot \nabla \phi_s \quad (D.30)$$

The two energy equations can also be written:

$$\frac{\partial}{\partial t} KE = -(\nabla \cdot F_{KE}) - (\nabla \cdot F_{\tilde{\nu}\phi}) + C_1 + C_3 \quad (D.31)$$

$$\frac{\partial}{\partial t} PIE = -(\nabla \cdot F_{CPT}) - C_1 - C_3 \quad (D.32)$$

where

$$C_3 = -\nabla \cdot F_{\tilde{\nu}\phi_s} \quad (D.33)$$

The standard post-processing already produces the net mass of water vapour (total column water vapour, $TCWV$ above) and ozone (total column ozone, TCO above) in kg/m^2 for each grid point. Also available is surface geopotential, ϕ_s , enabling the component $\phi_s Mass$ of PIE to be simply computed if $Mass$ is known. Note that ϕ_s is a fixed field, so the calculation of $\phi_s Mass$ can be done on monthly means if required.

In addition to these fields, analysis and selected forecast values of the following will be archived:

- *KE, CPT and Mass*
- $F_{KE}, F_{\phi}, F_{CPT}, F_M, F_q,$ and F_{O_3}
- C_1

These are most directly appropriate for use of the energy equation in the form given by equations (D.31) and (D.32). The flux F_{ϕ_s} can be simply calculated as $\phi_s F_M$, and the conversion term C_3 is given by the convergence of this flux. The vertical integral $\frac{1}{g} \int_0^1 e \frac{\partial p}{\partial \eta} d\eta$, of a quantity e that is defined by its analyzed or forecast values e_k at the 60 full

model levels is evaluated as $\frac{1}{g} \sum_{k=1}^{60} e_k \left(p_{k+\frac{1}{2}} - p_{k-\frac{1}{2}} \right)$.

If the alternative form of the energy equations given by (D.9) and (D.10) is preferred, the fluxes $F_{\phi-\phi_s}$ and F_{PIE} can be computed simply by subtracting $\phi_s F_M$ from F_{ϕ} and adding it to F_{CPT} . The conversion term C_2 is given by:

$$C_2 = -F_M \cdot \nabla \phi_s = -\nabla \cdot F_{\phi_s} + \phi_s \nabla \cdot F_M = C_3 + \phi_s \nabla \cdot F_M \quad (\text{D.34})$$

All RHS terms in the budget equations (D.9)-(D.13) (or (D.31), (D.32), (D.11), (D.12) and (D.13)) can thus be computed in terms of the supplied integrals, applying a divergence operator and simple multiplications where needed. The operations can be carried out either on the instantaneous values or their monthly means.

Appendix E: Surface energy and water budgets