

Appendix A

Stomatal conductance model

The derivation of the stomatal conductance model here is similar to that of Cowan (1977; see also Lloyd, 1991), but includes boundary layer conductances. Shown first is the transpiration rate in terms of the vapour pressure deficit of the air, accounting for heat loss through the boundary layer. The leaf flux equations for water vapour and heat are:

$$E = \frac{1}{r_{se} + r_{be}} (e_i - e_a) \quad (\text{A1})$$

$$H = \frac{c_p}{r_{bH}} (\theta_l - \theta_a) \quad (\text{A2})$$

If we assume that intercellular vapour concentration is the saturation value at leaf temperature, then using the approximation $e_{sat}(\theta_l) \approx e_{sat}(\theta_a) + s(\theta_l - \theta_a)$ (recall that s is the slope of saturation vapour concentration with temperature) we find:

$$E = \frac{1}{r_{se} + r_{be}} [D_a + s(\theta_l - \theta_a)]$$

which, combined with Equation (A2) leads to:

$$E = \frac{D_a + \frac{\varepsilon}{\lambda_E} r_{bH} H}{r_{se} + r_{be}}$$

where $\varepsilon = s\lambda_E/c_p$. The energy balance equation (Equation (2.19)) can then be used to find:

$$E = \frac{1}{r_{se} + r_{be}} \left[D_a + \frac{\frac{\varepsilon}{\lambda_E} r_{bH} R_{n,abs}^* - \varepsilon r_{bH} E}{1 + \frac{4\varepsilon_l \sigma \theta_a^3}{c_p} r_{bH}} \right]$$

which, on rearrangement, reveals:

$$E = \frac{D_0}{r_{se} + r_{be} + \varepsilon r_{bH}^*} \quad (\text{A3})$$

where $r_{bH}^* = \frac{1}{g_{bH} + 4\varepsilon_l \sigma \theta_a^3 / c_p}$ and $D_0 = D_a + \varepsilon r_{bH}^* R_{n,abs}^* / \lambda_E$.

That D_0 is the leaf to air vapour pressure difference when the stomata are fully closed can be seen by equating Equations (A1) and (A3), so that:

$$e_i - e_a = \frac{D_0}{1 + \frac{\varepsilon r_{bH}^*}{r_{se} + r_{be}}}$$

which shows that $e_i - e_a \rightarrow D_0$ when $r_{se} \rightarrow \infty$.

Next we obtain an expression for assimilation rate with conductance being the only variable. First we note that for changes in c_i due to changes in stomatal conductance, assimilation is linear in c_i (Lloyd, 1991):

$$A = k(c_i - \Gamma)$$

Combining this with the leaf flux equation for CO_2 ,

$$A = g_c(c_a - c_i)$$

where $g_c = \frac{1}{r_{sc} + r_{bc}} = \frac{g_{sc}}{1 + r_{bc} g_{sc}}$ is the total conductance to CO_2 from the intercellular spaces to the canopy air space, we eliminate c_i to obtain:

$$A = \frac{k g_c (c_a - \Gamma)}{k + g_c} \quad (\text{A4})$$

Now to relate stomatal conductance to the marginal water loss per unit carbon gain, we start with the premise that the stomatal opening varies in such a way as to maintain

a constant ratio between the incremental change in assimilation and transpiration rates due to an incremental change in conductance (Cowan and Farquhar, 1977):

$$\frac{\partial E}{\partial g_{sc}} \bigg/ \frac{\partial A}{\partial g_{sc}} = \lambda \quad (\text{A5})$$

The derivative of A with respect to g_c is found from Equation (A4) as:

$$\frac{\partial A}{\partial g_c} = \frac{k^2(c_a - \Gamma)}{(k + g_c)^2}$$

Substituting $k = \frac{A}{c_a - \Gamma - A/g_c}$ from Equation (A4) we find:

$$\frac{\partial A}{\partial g_c} = \frac{A^2}{g_c^2(c_a - \Gamma)}$$

and to relate this to stomatal conductance only, note that:

$$\frac{\partial g_c}{\partial g_{sc}} = \frac{1}{(1 + r_{bc}g_{sc})^2}$$

so that the expression is equally valid for g_{sc} :

$$\frac{\partial A}{\partial g_{sc}} = \frac{\partial A}{\partial g_c} \frac{\partial g_c}{\partial g_{sc}} = \frac{A^2}{g_{sc}^2(c_a - \Gamma)} \quad (\text{A6})$$

The derivative of transpiration with respect to g_{sc} is found from Equation (A3), noting that $r_{se} = \frac{1}{1.6g_{sc}}$, as:

$$\frac{\partial E}{\partial g_{sc}} = \frac{1.6D_0}{[1 + 1.6g_{sc}(r_{bc} + \varepsilon r_{bH}^*)]^2} \quad (\text{A7})$$

From Equation (A5), we can then solve for g_{sc} to obtain:

$$g_{sc} = \frac{A}{\sqrt{\frac{1.6D_0}{\lambda} (c_a - \Gamma) - \frac{1.6A}{g_{be}^*}}}$$

where $g_{be}^* = \frac{1}{r_{be} + \varepsilon r_{bH}^*}$, which is Equation (2.16) in the text.

Appendix B

Analytic assimilation solutions

Equation (2.4) expressed as the assimilation flux per unit leaf area can be written as:

$$A = \frac{1}{r_{sc} + r_{bc}} (c_a - c_i) \quad (\text{B1})$$

where assimilation A is defined positive. From the biochemical equations for assimilation, intercellular CO_2 concentration can be expressed in terms of assimilation rate and maximum photosynthetic capacity or electron transport. From Equation (2.10) for the Rubisco-limited case we obtain:

$$c_i = \frac{-(V_l \Gamma_* + K' A_V)}{A_V - V_l} \quad (\text{B2})$$

and from Equation (2.11) for the electron transport-limited case:

$$c_i = \frac{-(8A_J \Gamma_* + J \Gamma_*)}{4A_J - J} \quad (\text{B3})$$

Quadratic solutions for the net assimilation rate are obtained by combining Equation (B1) with the expression for stomatal conductance (Equation (2.16)) and that for c_i in either the Rubisco-limited or electron transport-limited case (Equation (B2) or (B3)), as:

$$A = \frac{-b - \sqrt{b^2 - 4ac}}{2a}$$

where for the Rubisco-limited case we have:

$$\begin{aligned}
 a \text{ (Rubisco-ltd)} &= r_{bc} - \frac{1.6}{g_{be}^*} \\
 b \text{ (Rubisco-ltd)} &= \sqrt{\frac{1.6D_0(c_a - \Gamma)}{\lambda}} - c_a - K' + (R_l - V_l) \left(r_{bc} - \frac{1.6}{g_{be}^*} \right) \\
 c \text{ (Rubisco-ltd)} &= (R_l - V_l) \left(\sqrt{\frac{1.6D_0(c_a - \Gamma)}{\lambda}} - c_a \right) - V_l \Gamma_* - K' R_l
 \end{aligned}$$

and for the electron transport-limited case:

$$\begin{aligned}
 a \text{ (light-ltd)} &= 4 \left(r_{bc} - \frac{1.6}{g_{be}^*} \right) \\
 b \text{ (light-ltd)} &= 4 \left(\sqrt{\frac{1.6D_0(c_a - \Gamma)}{\lambda}} - c_a - 2\Gamma_* \right) + (4R_l - J) \left(r_{bc} - \frac{1.6}{g_{be}^*} \right) \\
 c \text{ (light-ltd)} &= (4R_l - J) \left(\sqrt{\frac{1.6D_0(c_a - \Gamma)}{\lambda}} - c_a \right) - \Gamma_* (J + 8R_l)
 \end{aligned}$$

These equations represent the exact solutions to the Farquhar biochemical photosynthesis model coupled to the Cowan/Farquhar stomatal conductance optimisation model. Analytic solutions are desirable where possible in modelling applications in order to avoid compounded round-off errors during iterations and potential degeneration into chaotic behaviour (Baldocchi, 1994).

Appendix C

Canopy long wave radiation

The long wave radiation penetration in a canopy is derived here for isothermal leaves (ie. leaves at air temperature), with the effect of leaf temperature being taken into account in the leaf energy balance (Equation (2.19)). Equations for long wave radiation from the sky and ground are given separately in §2.1. Considering first the downward long wave radiation I_{LW} in the canopy, an incremental increase in leaf area decreases the radiation penetration by an amount proportional to the leaf area increase and the radiation intensity. It also contributes an additional amount according to the Stefan-Boltzmann law, also in proportion to the additional leaf area:

$$\frac{dI_{LW,canopy} \downarrow}{dL} = -I_{LW,canopy} \downarrow + \varepsilon_l \sigma \theta_a^4$$

Integrating, with the initial condition that $I_{LW,canopy} \downarrow = 0$ when $L = 0$, we obtain:

$$I_{LW,canopy} \downarrow = \varepsilon \sigma \theta_a^4 (1 - e^{-L})$$

This equation assumes that the radiation is in the downward direction only and that the leaves are all horizontally aligned. Since long wave radiation is emitted in all directions equally and we have assumed a spherical leaf angle distribution, the coefficient for diffuse radiation is inserted to account for the effect of leaf angle as for diffuse radiation:

$$I_{LW,canopy} \downarrow = \varepsilon \sigma \theta_a^4 (1 - e^{-k_d L})$$

Similarly, radiation in the upward direction is found as:

$$I_{LW,canopy} \uparrow = \varepsilon \sigma \theta_a^4 \left(1 - e^{-k_d(\Lambda-L)} \right)$$

Appendix D

Optimisation procedure

The source forms given by Equations (2.4) to (2.6), with fluxes obtained from Equation (2.8), are input into Equations (2.2) and (2.3) with parameters initialised to calculate the concentration profile. The parameters are then adjusted to improve the fit of the modelled to measured concentration until the best possible fit is obtained.

Equation (2.1) can be represented by the function $C(z_i; \mathbf{a})$, a function of the model parameters $\mathbf{a} = (a_1, a_2, \dots, a_n)$ evaluated at height z_i . The goodness of fit of the modelled concentration to the measured concentration is measured by the “chi-square” function, given by:

$$\chi^2 = \sum_{i=1}^N \left(\frac{\hat{C}_i - C(z_i; \mathbf{a})}{\sigma_i} \right)^2 \quad (\text{D1})$$

where the sum is taken over the N levels at which the concentration is either measured or interpolated; $C(z_i; \mathbf{a})$ is the modelled concentration at level z_i ; \hat{C}_i is the measured concentration at level z_i ; and σ_i is the standard deviation of the measured concentration.

The model seeks to minimise χ^2 with respect to the a_k parameters. To do this, the χ^2 function is expanded as a Taylor series to second order, so that:

$$\chi_n^2 = \chi_c^2 + (\mathbf{a}_n - \mathbf{a}_c) \nabla \chi_c^2 + \frac{1}{2} (\mathbf{a}_n - \mathbf{a}_c) \nabla^2 \chi_c^2 (\mathbf{a}_n - \mathbf{a}_c)$$

where χ_n^2 is chi-square calculated with the new set of parameters \mathbf{a}_n ; χ_c^2 is that calculated

with the current set \mathbf{a}_c ; and $\nabla\chi^2$ and $\nabla^2\chi^2$ are the first and second derivative matrices, respectively, of χ^2 with respect to \mathbf{a} . From this Taylor expansion it can be seen that the function is minimised (with zero derivative) when:

$$\nabla^2\chi_c^2(\mathbf{a}_n - \mathbf{a}_c) = -\nabla\chi_c^2$$

Hence if the Taylor approximation is a good one, the final model parameters can be obtained immediately from this equation. In reality, though, we must start with an initial estimate of \mathbf{a} that is likely to be far from the optimised set, so that the initial χ^2 will also be far from the final one. It is then useful to use iterations of the ‘‘steepest descent’’ method, where a step is taken along the gradient towards the minimum by:

$$(\mathbf{a}_n - \mathbf{a}_c) = -(\text{constant}) \nabla\chi_c^2$$

The gradient of χ^2 with respect to the parameters \mathbf{a} has components:

$$\frac{\partial\chi^2}{\partial a_j} = -2 \sum_{i=1}^N \frac{[\hat{C}_i - C(z_i; \mathbf{a})]}{\sigma_i^2} \frac{\partial C(z_i; \mathbf{a})}{\partial a_j} \quad j = 1, \dots, 4 \quad (\text{D2})$$

and the Hessian or second derivative matrix has components:

$$\frac{\partial^2\chi^2}{\partial a_j \partial a_k} = 2 \sum_{i=1}^N \frac{1}{\sigma_i^2} \left[\frac{\partial C(z_i; \mathbf{a})}{\partial a_j} \frac{\partial C(z_i; \mathbf{a})}{\partial a_k} - [C_i - C(z_i; \mathbf{a})] \frac{\partial^2 C(z_i; \mathbf{a})}{\partial a_j \partial a_k} \right] \quad (\text{D3})$$

The second derivative term in Equation (D3) can generally be ignored because the multiplying term, the difference between the measured and modelled concentrations, should be just the random error of measurement at each point. This can be of either sign and should be have no systematic relationship with the model, and so will tend to cancel out when summed over the concentration levels (Press et al., 1992).

The equation to be solved, then, is:

$$\sum_{k=1}^M \alpha_{jk} \delta a_k = \beta_j \quad (\text{D4})$$

or, for the steepest descent method:

$$\delta a_j = (\text{constant}) \beta_j \quad (\text{D5})$$

where α_{jk} and β_j are defined as:

$$\alpha_{jk} \equiv \frac{1}{2} \frac{\partial^2 \chi^2}{\partial a_j \partial a_k} \quad \beta_j \equiv -\frac{1}{2} \frac{\partial \chi^2}{\partial a_j}$$

The usual method for deciding which of the two equations above to attempt to solve is the Levenberg-Marquardt method, which gives varying weight to the two methods depending on the distance from the minimum. The constant in Equation (D5) is set to the reciprocal of the diagonal elements of the Hessian matrix α_{jk} , multiplied by a scaling factor λ_{LM} . A new matrix α' is defined by:

$$\alpha'_{jk} = \begin{cases} \alpha_{jk} (1 + \lambda_{LM}), & j = k \\ \alpha_{jk}, & j \neq k \end{cases} \quad (\text{D6})$$

and this is substituted for α_{jk} in Equation (D4) to produce a single equation to be solved:

$$\sum_{k=1}^M \alpha'_{jk} \delta a_k = \beta_j \quad (\text{D7})$$

The scaling factor λ_{LM} allows Equation (D7) to revert to Equation (D4) near the minimum as λ_{LM} approaches zero, or to Equation (D5) away from the minimum when λ_{LM} is large, causing the diagonal elements to dominate. The value of λ_{LM} chosen for a given iteration depends on the improvement or otherwise of the χ^2 merit function over the previous iteration.

From Equations (D2) and (D3), which are needed to solve Equation (D7) above, it can be seen that it is necessary to compute the derivative of the modelled concentration $C(z_i; \mathbf{a})$ with respect to the parameters \mathbf{a} . This is composed of near field and far field components:

$$\begin{aligned} \frac{\partial C}{\partial a_k} &= \frac{\partial C_n}{\partial a_k} + \frac{\partial C_f}{\partial a_k} \\ &= \int_0^\infty \frac{1}{\sigma_{w0}} \frac{\partial S(z_0)}{\partial a_k} \left[k_n \left(\frac{z-z_0}{\sigma_{w0} T_{L0}} \right) + k_n \left(\frac{z+z_0}{\sigma_{w0} T_{L0}} \right) \right] \\ &\quad + \frac{S(z_0)}{\sigma_{w0}} \frac{\partial T_{L0}}{\partial a_k} \left\{ \frac{\partial k_n[(z-z_0)/(\sigma_{w0} T_{L0})]}{\partial T_{L0}} + \frac{\partial k_n[(z+z_0)/(\sigma_{w0} T_{L0})]}{\partial T_{L0}} \right\} dz_0 \\ &\quad - \frac{\partial C_n(z_R)}{\partial a_k} + \int_z^{z_R} \frac{1}{\sigma_w^2(z) T_L(z)} \left[\frac{\partial F(z)}{\partial a_k} - \frac{F(z)}{T_L} \frac{\partial T_L}{\partial a_k} \right] dz \end{aligned}$$

Since calculating the analytical derivatives of the source and flux profiles with respect to the adjustable parameters becomes very complicated, these are calculated numerically according to:

$$\frac{\partial S(z, \mathbf{a})}{\partial a_k} \approx \frac{S(z; \mathbf{a} : a_k + \varepsilon_k) - S(z; \mathbf{a} : a_k - \varepsilon_k)}{2\varepsilon_k}$$

where ε_k is chosen as 0.001 times the magnitude of the parameter in question. The flux, near-field kernel and Lagrangian time scale derivatives were treated in the same way. The flux itself is calculated numerically from the source profile using the trapezoidal rule applied to Equation (2.8).

The inverse of the Hessian matrix is the covariance matrix C_{ij} of the standard errors in the adjustable parameters (Press *et al.*, 1992): $[C] \equiv [\alpha]^{-1}$. Hence the diagonals of $[C]$ give the standard errors in the parameters, as:

$$\sigma(a_i) = \sqrt{C_{ii}}$$

and the parameter correlation coefficients are given by:

$$r_{ij} = \frac{C_{ij}}{\sqrt{C_{ii} C_{jj}}}$$

If the measurement errors are normally distributed, then the confidence intervals in the parameters $\pm\delta a_i$ are related to the standard error in the usual way, with the 68% confidence interval being $\pm\sigma(a_i)$, the 95% interval $\pm 2\sigma(a_i)$, and so on.

Appendix E

Pressure-height relation

The hydrostatic equation states that:

$$\frac{dp}{dz} = -\rho g \quad (\text{E1})$$

where p is the atmospheric pressure; z is the height above the ground; ρ is the air density and g is the acceleration due to gravity ($\sim 10 \text{ ms}^{-2}$). If we assume that temperature decreases with height at the adiabatic lapse rate γ , then temperature T can be written:

$$T = T_0 - \gamma z \quad (\text{E2})$$

where T_0 is the temperature at the ground. Combining Equations (E1) and (E2) with the universal gas law, $p = \rho R_m T$ we obtain:

$$\frac{d \ln p}{dz} = -\frac{g}{R_m(T_0 - \gamma z)}$$

which can be integrated to show:

$$\frac{p}{p_0} = \left(1 - \frac{\gamma z}{T_0}\right)^{\frac{g}{R_m \gamma}} \quad (\text{E3})$$

Equation (E3) can be rearranged to obtain height z in terms of pressure p , given by Equation (3.10). It can also be combined again with the universal gas law to find the variation in density with height:

$$\frac{\rho}{\rho_0} = \left(1 - \frac{\gamma z}{T_0}\right)^{\frac{g}{R_m \gamma} - 1}$$

Appendix F

Temperature correction

The rate of change of temperature measured by an instrument with a delayed response (T_{meas}) is related to the temperature difference between the sensor and ambient air at temperature T_{real} as (eg. Middleton and Spilhaus, 1953):

$$\frac{dT_{meas}}{dt} = -k(T_{meas} - T_{real})$$

where the proportionality constant k is the inverse time constant of the instrument. This equation can easily be integrated if the ambient temperature T_{real} is constant. In the application to measurement of temperature in the atmospheric boundary layer, however, ambient temperature is changing with height. If we consider that temperature decreases approximately linearly with height according to the adiabatic lapse rate, and if the rate of ascent of the aircraft is approximately constant, then ambient temperature will decrease linearly with time in an ascending flight. The reverse is true for a descending flight. The measured temperature is then related to the ambient temperature by:

$$\frac{dT_{meas}}{dt} = -k[T_{meas} - (T_0 + \beta t)] \quad (\text{F1})$$

where β is the time rate of change of temperature and T_0 is the ground temperature. Equation (F1) can be integrated to obtain real temperature in terms of measured temperature by multiplying both sides by the factor e^{kt} :

$$e^{kt} \frac{dT_{meas}}{dt} + kT_{meas}e^{kt} = ke^{kt}(T_0 + \beta t) \quad (\text{F2})$$

The left hand side is just the time derivative of the factor $T_{meas}e^{kt}$. The first term on the right hand side is also easily integrated, while the second can be integrated by parts using the rule:

$$\int u dv = uv - \int v du$$

We make the substitution $u = x$ and $dv = k\beta e^{kt}$, so that $du = dx$ and $v = \beta e^{kt}$. The integration can then be carried out as:

$$\begin{aligned} \int k\beta t e^{kt} dt &= \int u dv \\ &= uv - \int v du \\ &= \beta t e^{kt} - \int \beta e^{kt} dt \\ &= \beta t e^{kt} - \frac{\beta}{k} e^{kt} + c \end{aligned}$$

Assuming the sensor to be in equilibrium with the ambient air at the start of the flight, the constant c is evaluated as $\frac{\beta}{k}$ using the initial condition $T_{meas} = T_0$ at time $t = 0$ and the above result is substituted into Equation (F2) to obtain:

$$T_{meas}e^{kt} = T_0e^{kt} + \beta t e^{kt} - \frac{\beta}{k}e^{kt} + \frac{\beta}{k}$$

Multiplying both sides by e^{-kt} we find:

$$T_{meas} = T_0 + \beta t - \frac{\beta}{k}(1 - e^{-kt})$$

With our initial assumption that $T_{real} = T_0 + \beta t$ we then have:

$$T_{meas} = T_{real} - \frac{\beta}{k}(1 - e^{-kt})$$

Rearranging to solve for T_{real} and neglecting the exponential term at long times, we obtain Equation (3.11):

$$T_{real} = T_{meas} + \frac{\beta}{k}$$

Appendix G

Canopy model source code

G.1 Driver code

G.1.1 Full optimisation

The following Fortran 90 code carries out the optimisation of canopy and turbulence parameters plus variable ground fluxes for the ten periods with isotope data on 25 and 27 May 2000, by minimising the difference between modelled and measured concentrations.

```
$debug
PROGRAM CANMOD
! PROGRAM FOR FINDING CANOPY SOURCE DENSITY PROFILE S FROM
! CONCENTRATION PROFILE C, ASSUMING STEADY, ONE-DIMENSIONAL TRANSFER.
! CONVENTIONS AND USING MULTILAYER CANOPY MODEL WITH UNKNOWN
! PARAMETERS. DEVELOPED FROM INVERSE LAGRANGIAN SOURCE CODE OF
! RAUPACH 1988-1998. DATA INPUT SECTION MODIFIED BY RAY LEUNING 1996.
! MANY REDUNDANT ARRAYS AND ROUTINES STILL PRESENT
!
! Subroutines used
! comskp      (sousub15.for) skip comments in data input file
! air         (sousub15.for) calculate latent ht vap, RHO, CP, VOLM
! turb2       (sousub15.for) calculate sigw and TL
! dispm2      (sousub15.for) calculate dispersion matrix
! integr      (sousub15.for) integrate a function
! shsor2      (sousub15.for) sort profiles into ascending order
! phi         (sousub15.for) calculate phi for stability correction
! interp      (sousub15.for) interpolate concentration profiles
! intval      (sousub15.for) calculate interpolated value
! calce       (sousub15.for) calculate flux profiles
! calcs       (sousub15.for) calculate source profiles
! assim       (sousub15.for) calculate leaf level fluxes
!
! numfiles=615 for half hour, 308 for hour averages
!
PARAMETER(MMAX=20,NMAX=40,numfiles=308,NUML=20,NUMP=9,IFMAX=1000, &
          ISMAX=1000, NUMK=36,NISO=16,NUMAK=54,IDMAX=400)

! NUML=NUMBER OF CONCENTRATION LEVELS TO BE USED FROM SPLINE INTERPOLATION
! NUMP=NUMBER OF SCALAR INPUT PROFILES
! SOURCE ARRAYS, DIMENSION 0:M WHERE M IS NUMBER OF SOURCE LEVELS,
! Z=HEIGHT OF TOP OF SOURCE LAYERS; ZS=HEIGHT OF MIDDLE OF SOURCE LAYERS;
! DZ=WIDTH OF SOURCE LAYERS
```

```

! SA,SH,SE,SC = OUTPUT SOURCES; FA,FH,FE,FC = OUTPUT FLUXES
! DIS,DISN,DISF = DISPERSION MATRICES
! T,Q,EV,CC,CA,CH,CE = PROFILES INPUT TO MODEL (AFTER INTERPOLATION)
! ZC NO LONGER USED

      REAL, DIMENSION(:),ALLOCATABLE :: Z,ZS,DZ,FA,SA, &
          FH,SH,FE,SE,FC,SC,HH,BBADD
      REAL, DIMENSION(:,:), ALLOCATABLE :: DIS,DISN,DISF
      REAL, DIMENSION(:), ALLOCATABLE :: T,Q,EV,CC,CA,CH,CE,BB
      REAL*8, DIMENSION(:), ALLOCATABLE :: AA,AAL
      integer, dimension(:), allocatable :: IP
      REAL, DIMENSION(:,:), ALLOCATABLE :: ZC
      REAL A1,AH,AO,CCH,CCO,ALFAA,ALFAB,ALFAC,HC,SWREF,USREF
      COMMON /T/ ITURB,A1,AH,AO,CCH,CCO,alfaa,alfab,ALFAC, &
          HC,SWREF,USREF,IST_COR

      character mon*3,day(numfiles)*2,timdat*32
      character*60 exptnam,filenam,path_IP,path_OP
      character*90 path_file_IP,outfila,outfils,outdmtx

!   arrays needed for profile and flux data for "numfiles" half-hrs
      character*8                                & !time & date
      Ttdate(numfiles),VPdate(numfiles),C2date(numfiles), &
      Fxdate(numfiles),SIGCDAT(NUMFILES),SIGHDAT(NUMFILES), &
      SIGTDAT(NUMFILES),D13DAT(NISO)

      integer Tthr(numfiles),Ttmin(numfiles),VPhr(numfiles), &
          VPmin(numfiles),C2hr(numfiles),C2min(numfiles), &
          Fxhr(numfiles),Fxmin(numfiles),SIGCHR(NUMFILES),SIGCMIN(NUMFILES), &
          SIGHHR(NUMFILES),SIGHMIN(NUMFILES),SIGTHR(NUMFILES),SIGTMIN(NUMFILES), &
          D13HR(NISO),D13MIN(NISO),NLI(NISO),nday(numfiles),ISN(10),ICN(10)
      common /timx/ Tthr,Ttmin,VPhr,VPmin,C2hr,C2min, Fxhr,Fxmin
      integer timm(numfiles,10)
      equivalence (timm,Tthr)

!   Ttz,VPz,C2z = ORIGINAL HEIGHTS OF INPUT PROFILES
!   ZZZ = INCORPORATES ORIGINAL HEIGHTS OF ALL SCALAR PROFILES INTO ONE MATRIX AFTER SORTING
!   NLEV1 = ORIGINAL NUMBER OF LEVELS FOR PROFILE DATA
!   X,Y = HEIGHTS AND PROFILES AFTER INTERPOLATION
!   XPROF=X
!   Tt,VP,C2 = ORIGINAL INPUT PROFILES
!   PROF = INCORPORATES ALL ORIGINAL PROFILES INTO ONE MATRIX AFTER SORTING
!   PRAF = DUMMY MATRIX FOR SORTING
!   SPROF = ALL PROFILES AFTER INTERPOLATION IN ONE MATRIX

      REAL, DIMENSION(:), ALLOCATABLE :: Ttz, VPz, C2z, za,B,C13Z,O18Z
      REAL, DIMENSION(:,:), ALLOCATABLE :: ZZZ,C13ZZ
      integer nlev1(11),nref(11) !number of levels for each scalar
      REAL ZREF,Y(NUML),X(NUML),XPROF(NUML),NEWZ,NEWPROF

      REAL, DIMENSION(:,:), ALLOCATABLE :: Tt, VP, C2, PRAF,SPROF,F,SIGC,SIGH,SIGT,dcdt,DHDT,DTDT,&
          D13C,D18O
      REAL, DIMENSION(:,:,:), ALLOCATABLE :: PROF
      REAL*8 RL, DTIME(NUMFILES)

      real H(numfiles),E(numfiles),FC2(numfiles),zMonU(numfiles),us(numfiles),swr(numfiles), &
          LE(numfiles),RN(numfiles),Uh(numfiles), APRESS(NUMFILES),PAR(NUMFILES), fd(numfiles), &
          SWDR(NUMFILES),LWDR(NUMFILES),LZMON(10),LMON(NUMFILES)
      common /flxx/ H,E,FC2,sgw,us,ur
      real flxx(numfiles,7)
      equivalence (flxx,H)

!   ARRAYS FOR ALTERNATIVE MODEL USING BETA FUNCTION TO CONSTRAIN SOURCE AND FLUX PROFILES
      REAL SK(6,0:ISMAX),FK(6,0:IFMAX),DSK(5,0:IDMAX+1,NUMAK),PARAM(5), &
          CD(NUML),SREF(6,10),THETL(0:ISMAX), ESATL(0:ISMAX),DUMMY(NUML),DEF(0:ISMAX), &
          DELTA(0:ISMAX),CICA(0:ISMAX),DEL18(0:ISMAX),RAIR(10), &

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        SWDREF(10), LWDREF(10), TLPROF(0: ISMAX), ZOBUKHOV(0: ISMAX)
REAL   AK(NUMAK), ake(NUMAK), AKO(NUMAK), GF(3,10), GFO(3,10), GFE(3,10), &
        TL1(10), TL10(10), TL1E(10), TL2(10), TL20(10), TL2E(10), STL1(10), STL2(10)
REAL   CK(6, NUML), CKO(6, NUML), CKK(6, NUML), CKKK(6, NUML), CKE(6, NUML), &
        SIGCO2(NUML), SIGH20(NUML), SIGTEMP(NUML), SIG13C(NUML), SIG180(NUML), &
        SIG(5, NUML), SIGO(5, NUML)
REAL   SPROFALL(NUML, 9, 10), APROFALL(NUML, 4, 10), DCKALL(5, NUML, NUMAK, 10), CKALL(6, NUML, 10), &
        DCKEALL(5, NUML, NUMAK, 10), DCKOALL(5, NUML, NUMAK, 10), CKEALL(6, NUML, 10), &
        CKOALL(6, NUML, 10), &
        CKKALL(6, NUML, 10), DCKD(5, NUML, NUMAK, 10), DFKTOP(3, 10, NUMAK), FKTOP(3, 10), &
        SPROFD(NUML), APROFC(NUML), APROFO(NUML), SPROFP(NUML), APROFCP(NUML), APROFOP(NUML)
REAL   DFK(5, 0: IDMAX+1, NUMAK), DCK(5, NUML, NUMAK), FKS(6, 0: ISMAX), esource(0: ISMAX), &
        ESOURCE2(0: ISMAX), &
        HSOURCE(0: ISMAX), HFLUX(0: IFMAX), HSOURCE2(0: ISMAX), eflux(0: IFMAX), CFLUX(0: IFMAX), &
        CFLUX1(NUMAK, 0: IFMAX), CFLUX2(NUMAK, 0: IFMAX), CSOURCE(0: ISMAX), CSOURCE2(0: ISMAX), &
        ZPR(0: IFMAX), EFLUX1(NUMAK, 0: IFMAX), EFLUX2(NUMAK, 0: IFMAX), &
        HFLUX1(NUMAK, 0: IFMAX), HFLUX2(NUMAK, 0: IFMAX), EFLUXD(0: IFMAX), CFLUXD(0: IFMAX), &
        HFLUXD(0: IFMAX), &
        THETLE(0: ISMAX), ZOUT(IFMAX), C13FLUX(0: IFMAX), C13FLUXD(0: IFMAX), C13SOURCE(0: ISMAX), &
        RLAI(0: ISMAX), RC(0: ISMAX), RH(0: ISMAX), RNN(0: ISMAX), C13FLUX1(NUMAK, 0: IFMAX), &
        C13FLUX2(NUMAK, 0: IFMAX), RSUM13(5), RSUM14(5), RSUM15(5), RSUM18(5), &
        C13SOURCE2(0: ISMAX), rsum4(5), rsum5(5), rsum6(5), rsum7(5), rsum8(5), RSUM12(5), &
        RSUM10(5), &
        DFKS(10, 0: ISMAX), RSUM9(5), KBF, KDF, DCKO(5, NUML, NUMAK), DCKE(5, NUML, NUMAK), &
        O18SOURCE(0: ISMAX), O18FLUX(0: IFMAX), O18FLUXD(0: IFMAX), O18SOURCE2(0: ISMAX), &
        O18FLUX2(NUMAK, 0: IFMAX), O18FLUX1(NUMAK, 0: IFMAX), &
        H18SOURCE(0: ISMAX), H18FLUX(0: IFMAX), H18FLUXD(0: IFMAX), DEL_E(0: ISMAX), ZSOU(0: ISMAX)
REAL*8 ALP(NUMK, NUMK), BET(NUMK), DAK(NUMK), AINV(NUMK, NUMK), DSUM
REAL   LSIGC(2), LSIGH(2), LSIGT(2), BINT(3), BINT2(3), IPN(NUMK), DCT(6, 2), DCFT(5, 2), &
        DISC(NUML, 0: ISMAX), DISCN(NUML, 0: ISMAX), DISCF(NUML, 0: ISMAX), &
        APROF(NUML, 2, NISO), AZZ(NUML)
REAL*8 BETA12(3), costfn(10, 3, 9), HESS(NUMK, NUMK), &
        check(2, 2), xxxx(numk)
EXTERNAL BETA, BETAI
DATA RSTD /0.011894/, R18STD /0.0020672/

! PRESET PARAMETERS:
      rmain = 0.02897      ! molecular weights (kg/mol) for air
      rmh2o = 0.018016    ! for H2O
      rmco2 = 0.044022    ! for CO2
      pmb   = 1000.       ! atmospheric pressure
      PI    = 3.14159
      IWRITE=1            ! WRITE DISPERSION MATRIX
      ICOST=1

! open and read control information from sourcfil.dat
      open(1, file='sourcfil_15d.dat')
2      call comskp(1)      !skip comments

      read(1, *, end=450) exptnam      !experiment name
      read(1, 105, end=450) path_IP    !Input path name
      read(1, 105, end=450) path_OP    !Output path name
105   format(a60)
      flen_IP=len_trim(path_IP)
      flen_OP=len_trim(path_OP)

      do 10000 iblk=1, 300            !read up to 300 days' file names

      READ(1, *, end=450) (nlevl(I), I=1, 3), (NREF(i), i=1, 3), HC, PMB
      READ(1, *, err=450, END=450) ITURB, MO, M, A1, AH, A0, CCH, CO0, alfaa, alfab, ALFAC, ist_cor
      read(1, *, err=450, end=450) nfil

      MN=MAXVAL(NLEVL)
      ALLOCATE(Z(0:M), ZS(0:M), DZ(0:M), FA(0:M), SA(0:M), FH(0:M), SH(0:M), &
              FE(0:M), SE(0:M), FC(0:M), SC(0:M))
      ALLOCATE(AA((M+1)**2), BB(M+1), IP(M+1), AAL((M+1)**2), BBADD(M+1))

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ALLOCATE(T(NUML),Q(NUML),EV(NUML),CC(NUML), CA(NUML),CH(NUML),CE(NUML))
ALLOCATE(ZC(NUMP,MN),HH((M+1)**2))
ALLOCATE(Tt(MN,NUMFILES),C2(MN,NUMFILES),&
      VP(MN,NUMFILES),PROF(MN,NUMP,NUMFILES),SPROF(NUML,NUMP), &
      SIGC(MN,NUMFILES),SIGH(MN,NUMFILES),SIGT(MN,NUMFILES), &
      dcdt(mn,numfiles),DHDT(MN,NUMFILES),DTDT(MN,NUMFILES))
ALLOCATE(PRAF(MN,NUMFILES),D13C(MN,NISO),D18O(MN,NISO))
ALLOCATE(Ttz(MN),C2z(MN),VPz(MN),ZA(MN),ZZZ(MN,NUMP),B(MN),F(4,MN),C13Z(MN),O18Z(MN))
ALLOCATE(DIS(NUML,0:M),DISN(NUML,0:M),DISF(NUML,0:M),C13ZZ(MN,NISO))

do ifa=1,nfil                                !read data for profiles and fluxes
  read(1,105) filenam
  path_file_IP=path_IP(1:flen_IP)//filenam

  open(10,file=path_file_IP,mode='read')

  select case(filenam(1:1))
    case('C','c')
      select case(filenam(2:2))
        case('O','o')                                !CO2
          read(10,*)
          read(10,200) (C2z(j),j=1,nlevl(1))          !read in CO2 heights
          do i=1,numfiles                             !read in CO2 data
            read(10,210,end=100,err=460) &
              C2date(i),C2hr(i),C2min(i),(C2(j,i),j=1,nlevl(1))
          end do
100      continue
          nC2=i-1                                     !# CO2 records

        end select

    case('T','t')
      read(10,*)                                     !skip one line
      read(10,200) (Ttz(j),j=1,nlevl(2))             !read in Temp heights
      do i=1,numfiles                                !read in Temp data
        read(10,210,end=120,err=480) &
          Ttdate(i),Tthr(i),Ttmin(i),(Tt(j,i),j=1,nlevl(2))
      end do
120      continue
          nTt=i-1                                     !# Temp records

    case('V','v')
      read(10,*)                                     !skip one line
      read(10,200) (VPz(j),j=1,nlevl(3))             !read in VP heights
      do i=1,numfiles                                !read in VP data
        read(10,210,end=130,err=490) &
          VPdate(i),VPhr(i),VPmin(i),(VP(j,i),j=1,nlevl(3))
      end do
130      continue
          nVP=i-1                                     !# VP records

    case('F','f')
      read(10,*,end=140,err=500)                     !skip 1 lines
      do i=1,numfiles
        read(10,220,end=140) fxdate(i),fxhr(i),fxmin(i), &
          H(i),LE(i),E(i),FC2(i),us(i),swr(i),zMonU(i),Uh(i),rn(i), &
          PAR(I),fd(i),SWDR(I),LWDR(I)
      end do
140      continue
          nfx=i-1                                     !# flux records

  CASE('A','a')
    READ(10,*)
    DO I=1,NUMFILES
      READ(10,270,END=141) DTIME(I), apress(i)

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      ENDDO
141      CONTINUE
!      apress=1000.

      CASE('S','s')
      SELECT CASE(FILENAM(7:7))
      CASE('C')
        READ(10,*)
        READ(10,*)
        DO I=1,NUMFILES
          READ(10,230, END=150,ERR=510) nday(i),SIGCDAT(I),SIGCHR(I), &
            SIGCMIN(I),(SIGC(J,I),J=1,NLEVL(1))
        ENDDO
150      CONTINUE
      CASE('H')
        READ(10,*)
        READ(10,*)
        DO I=1,NUMFILES
          READ(10,231, END=160,ERR=520) SIGHDAT(I),SIGHHR(I), &
            SIGHMIN(I),(SIGH(J,I),J=1,NLEVL(3))
        ENDDO
160      CONTINUE
      CASE('T')
        READ(10,*)
        READ(10,*)
        DO I=1,NUMFILES
          READ(10,231, END=170,ERR=530) SIGTDAT(I),SIGTHR(I), &
            SIGTMIN(I),(SIGT(J,I),J=1,NLEVL(2))
        ENDDO
170      CONTINUE
      CASE('A')
        READ(10,*)
        READ(10,*)
        READ(10,232) (SIGCO2(J),J=1,NUML)
        READ(10,232) (SIGH20(J),J=1,NUML)
        READ(10,232) (SIGTEMP(J),J=1,NUML)
        READ(10,232) (SIG13C(J),J=1,NUML)
        READ(10,232) (SIG180(J),J=1,NUML)
      END SELECT

      CASE('D','d')
      SELECT CASE(FILENAM(2:2))
      CASE('C','c')
        READ(10,*)
        READ(10,*)
        DO I=1,NUMFILES
          READ(10,240,END=180) (DCDT(J,I),J=1,NLEVL(1))
        ENDDO
180      CONTINUE
      CASE('H','h')
        READ(10,*)
        READ(10,*)
        DO I=1,NUMFILES
          READ(10,240,END=190) (DHDT(J,I),J=1,NLEVL(1))
        ENDDO
190      CONTINUE
      CASE('T','t')
        READ(10,*)
        READ(10,*)
        DO I=1,NUMFILES
          READ(10,240,END=195) (DTDT(J,I),J=1,NLEVL(1))
        ENDDO
195      CONTINUE
      CASE('I','i')
      SELECT CASE(FILENAM(4:4))
      CASE('C','c')

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```

        READ(10,*)
        READ(10,260,END=196) (C13z(j),j=1,6)          !read in C13 heights
        DO I=1,NISO
            READ(10,250) D13DAT(I),D13HR(I),D13MIN(I),(D13C(J,I),J=1,6)
        ENDDO
196     CONTINUE
        CASE('0','o')
        READ(10,*)
        READ(10,200,END=197) (O18Z(J),J=1,6)
        DO I=1,NISO
            READ(10,260) (D180(J,I),J=1,6)
        ENDDO
197     CONTINUE
        END SELECT
        END SELECT

        case default
            stop 'Incorrect profile or flux file type'

        end select

200     format(18x,10f8.2)
210     format(a8,i5,1x,i2,10f8.2)
220     format(a8,i5,1x,i2,6f8.2,f9.2,6f8.2)
230     format(I5,a8,i5,1x,i2,10f8.3)
231     format(a8,i5,1x,i2,10f8.3)
232     FORMAT(8X,20F8.2)
240     FORMAT(16X,10ES11.3)
250     FORMAT(A8,I5,1X,I2,6F9.3)
260     FORMAT(16X,6F9.3)
270     FORMAT(F11.3,F8.2)

        end do                                     !end reading block
!
        of files

        IX=1
        RMSIGC=MAXVAL(SIGC)
        RMSIGH=MAXVAL(SIGH)
        RMSIGT=MAXVAL(SIGT)
        LSIGC=MAXLOC(SIGC)
        LSIGH=MAXLOC(SIGH)
        LSIGT=MAXLOC(SIGT)
        WRITE(*,*) RMSIGC, RMSIGH, RMSIGT
        WRITE(*,*) LSIGC, LSIGH, LSIGT
!
        assume numfiles 1/2h records available each day
        nrec=numfiles
        PROF(:,1,:)=C2
        PROF(:,2,:)=TT
        PROF(:,3,:)=VP
        PROF(:,4,:)=SIGC
        PROF(:,5,:)=SIGT
        PROF(:,6,:)=SIGH
        PROF(:,7,:)=DCDT
        PROF(:,8,:)=DDT
        PROF(:,9,:)=DHDT
        SIG(1,:)=SIGC02; SIG(2,:)=SIGTEMP; SIG(3,:)=SIGH20; SIG(4,:)=SIG13C; SIG(5,:)=SIG180
        SIG(1,:)=0.5*SIG(1,:);SIG(2,:)=0.2*SIG(2,:);SIG(3,:)=0.2*SIG(3,:);
        SIG(4,:)=0.4*SIG(4,:);SIG(5,:)=0.6*SIG(5,:) !WEIGHT TO EACH SPECIES
        ZZZ(:,1)=C2z
        ZZZ(:,2)=Ttz
        ZZZ(:,3)=VPz
        ZZZ(:,4)=C2z
        ZZZ(:,5)=Ttz
        ZZZ(:,6)=VPz
        ZZZ(:,7)=C2z
        ZZZ(:,8)=Ttz

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      ZZZ(:,9)=VPz
      PROF(:,4,:)=0.3; PROF(:,5,:)=0.3      !CONSTANT SIGMA FOR EACH (10X ACTUAL)
!     PROF(7:9,6,:)=0.3
      prof(:,6,:)=0.05
      DO I=4,9
        NLEVL(I)=NLEVL(I-3)
      ENDDO

! INTERPOLATE D13C, D180 PROFILES
      TH=28.0
      DO I=1,NISO
        NLI(I)=6;C13ZZ(:,I)=C13Z
        DO J=1,6      !CHECK FOR BAD DATA
          IF(ABS(D13C(J,I)).GT.100.) THEN
            NLI(I)=NLI(I)-1
            DO K=J,5
              D13C(K,I)=D13C(K+1,I)
              D180(K,I)=D180(K+1,I)
              C13ZZ(K,I)=C13Z(K+1)
            ENDDO
          ENDIF
        ENDDO
      ENDIF
! INTERPOLATE ISOTOPE PROFILES
      CALL INTERP(NLI(I),C13ZZ(:,I),D13C(:,I),X,Y,TH,NUML,NV,B,F)
      APROF(:,1,I)=Y; AZZ=X
      CALL INTERP(NLI(I),C13ZZ(:,I),D180(:,I),X,Y,TH,NUML,NV,B,F)
      APROF(:,2,I)=Y
      ENDDO

!     sort profiles into ascending height order - assume order read in is sequential
!     but may be in descending order
!     utilise equivalence between zzz(nv,nf) & Ttz(nv),VPz(nv,nf)...
!     and between prof(nv,nf,nr) & Tt(nv,nr),VP(nv,nr)...
      do nf=1,NUMP                                     !profile files
        if(zzz(1,nf).gt.zzz(nlevl(nf),nf)) then        !need to reverse order
          do nv=1,nlevl(nf)                             !n levels
            za(nv)=zzz(nlevl(nf)-nv+1,nf)              !write to scratch array
            do nr=1,nrec                                 !nrec records common to
! all profile files
              praf(nv,nr)=prof(nlevl(nf)-nv+1,nf,nr)    !write to scratch array
            end do
          end do
        end do
      end do
!     now overwrite arrays in ascending order
      do nv=1,nlevl(nf)
        zzz(nv,nf)=za(nv)
        do nr=1,nrec
          prof(nv,nf,nr)=praf(nv,nr)
        end do
      end do
    end if
  end do

DO II=1,NUMP
  DO nv=1,MN
    zc(II,nv)=ZZZ(nv,II)
  ENDDO
ENDDO

!     end data input section

!     *****

!     construct output file names from date info
      mon=Ttdate(1)(6:8)
      day(1)=Ttdate(1)(3:4)
      if(day(1).eq.' ') day(1)='0'

```



```

end if

      call air(tc,pmb,rho,volm,capp,rlam,qsat,epsi)
      LMON(NR)=USREF**3*(TC+273.15)*RHO*CAPP/0.4/10./HREF      !MONIN-OBUKHOV LENGTH

3000  continue

!*****
  I=1
  NUMISO=0
  DO 4004 NR=1,NREC
  NIS=3
!   IF((DAY(NR).EQ.'25'.OR.DAY(NR).EQ.'27').AND.(TTHR(NR).GE.6.AND.TTHR(NR).LT.21)) THEN
      ISOTOPE: DO NI=1,NISO
      IF(D13DAT(NI)(3:4).EQ.DAY(NR).AND.(D13HR(NI)+1).EQ.TTHR(NR).AND. &
      TTHR(NR).LT.21.AND.TTHR(NR).GE.6) THEN
          ISN(I)=NI; ICN(I)=NR; NUMISO=NUMISO+1
          DO II=1,3
          CALL INTERP(NLEVL(II),ZZZ(:,II),PROF(:,II,ICN(I)),X,Y,TH,NUML,NV,B,F)
          SPROFALL(:,II,I)=Y
          CALL INTERP(NLEVL(II),ZZZ(:,II),PROF(:,II+6,ICN(I)),X,Y,TH,NUML,NV,B,F)
          SPROFALL(:,II+6,I)=Y      ! STORAGE
          ENDDO
          CALL INTERP(NLI(NI),C13ZZ(:,NI),D13C(:,NI),X,Y,TH,NUML,NV,B,F)
          APROFALL(:,1,I)=Y; AZZ=X
          CALL INTERP(NLI(NI),C13ZZ(:,NI),D180(:,NI),X,Y,TH,NUML,NV,B,F)
          APROFALL(:,2,I)=Y
          I=I+1
          ENDDIF
          ENDDO ISOTOPE
4004 CONTINUE
      ISOTOPES=2 ! USE ISOTOPES IN OPTIMISATION: 0=NO, 1=NO BUT CALCULATE ISOTOPE PROFILES,
      ! 2=YES FOR 13C, 3=YES FOR 13C AND 18O
202  IEDDY=0 ! USE EDDY FLUXES TO CONSTRAIN 1=YES, 0=NO
      IDIS=0 ! USE DISPM SUBROUTINE FOR DERIV AND CONC CALC 1=YES, 0=NO
      ICOSTFN=2 ! 1=calculate cost function (chisq) only, no optimisation,
      ! 2=output error covariance matrix
      IFLAGC=0 ! exit after one iteration, including deriv calc
      IOPT=1 ! 0=OPTIMISE ONLY GROUND FLUXES, 1=ALSO OTHER PARAMS
      IPM=1
      IN=1
      IF(ISOTOPES.GE.1) THEN
          DO IT=1,NUMISO
          IF(IT.EQ.5.OR.IT.EQ.10) THEN
              CALL INTERP(NLEVL(1),ZZZ(:,1),PROF(:,1,ICN(IT)+3),X,Y,TH,NUML,NV,B,F)
              SPROFD=Y
              CALL INTERP(NLI(ISN(IT)+1),C13ZZ(:,ISN(IT)+1),D13C(:,ISN(IT)+1),X,Y,TH,NUML,NV,B,F)
              APROFC=Y
              CALL INTERP(NLI(ISN(IT)+1),C13ZZ(:,ISN(IT)+1),D180(:,ISN(IT)+1),X,Y,TH,NUML,NV,B,F)
              APROFO=Y
              SPROFP=SPROFALL(:,1,IT-1)
              APROFCP=APROFALL(:,1,IT-1)
              APROFOP=APROFALL(:,2,IT-1)
              APROFALL(:,3,IT)=(APROFALL(:,1,IT)/1000.+1.)*RSTD*(SPROFD-SPROFP)/6./3600.+ &
              (APROFC-APROFCP)/1000./6./3600.*RSTD*SPROFALL(:,1,IT)
              APROFALL(:,4,IT)=(APROFALL(:,2,IT)/1000.+1.)*R18STD*(SPROFD-SPROFP)/6./3600.+ &
              (APROFO-APROFOP)/1000./6./3600.*RSTD*SPROFALL(:,1,IT)
          ELSEIF(IT.EQ.1.OR.IT.EQ.6) THEN
              SPROFD=SPROFALL(:,1,IT+1)
              APROFC=APROFALL(:,1,IT+1)
              APROFO=APROFALL(:,2,IT+1)
              CALL INTERP(NLEVL(1),ZZZ(:,1),PROF(:,1,ICN(IT)-3),X,Y,TH,NUML,NV,B,F)
              SPROFP=Y
              APROFALL(:,3,IT)=(APROFALL(:,1,IT)/1000.+1.)*RSTD*(SPROFD-SPROFP)/6./3600.+ &
              (APROFC-APROFALL(:,1,IT))/1000./3./3600.*RSTD*SPROFALL(:,1,IT)
              APROFALL(:,4,IT)=(APROFALL(:,2,IT)/1000.+1.)*R18STD*(SPROFD-SPROFALL(:,1,IT)) &

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/3./3600.+ (APROFO-APROFALL(:,2,IT))/1000./3./3600.*RSTD*SPROFALL(:,1,IT)
ELSE
  SPROFD=SPROFALL(:,1,IT+1); SPROFP=SPROFALL(:,1,IT-1)
  APROFC=APROFALL(:,1,IT+1); APROFCP=APROFALL(:,1,IT-1)
  APROFO=APROFALL(:,2,IT+1); APROFOP=APROFALL(:,2,IT-1)
  APROFALL(:,3,IT)=(APROFALL(:,1,IT)/1000.+1.)*RSTD*(SPROFD-SPROFP)/6./3600.+ &
    (APROFC-APROFCP)/1000./6./3600.*RSTD*SPROFALL(:,1,IT)
  APROFALL(:,4,IT)=(APROFALL(:,2,IT)/1000.+1.)*R18STD*(SPROFD-SPROFP)/6./3600.+ &
    (APROFO-APROFOP)/1000./6./3600.*RSTD*SPROFALL(:,1,IT)
ENDIF
ENDDO
ENDIF
NIS=NI
open(unit=10, file='cprof')
OPEN(UNIT=11, FILE='SPROFC')
OPEN(UNIT=16, FILE='EPROF')
OPEN(UNIT=13, FILE='HPROF')
OPEN(UNIT=17, FILE='SPROFE')
OPEN(UNIT=14, FILE='SPROFH')
open(unit=12, file='FLUXC')
OPEN(UNIT=15, FILE='FLUXH')
OPEN(UNIT=18, FILE='FLUXE')
OPEN(UNIT=19, FILE='FLUXLE')
OPEN(UNIT=20, FILE='MOREPROFS')
OPEN(UNIT=21, FILE='C13PROF')
OPEN(UNIT=22, FILE='SPROFC13')
OPEN(UNIT=23, FILE='GROUNDFLUX')
OPEN(UNIT=24, FILE='PROFC')
OPEN(UNIT=25, FILE='PROFE')
OPEN(UNIT=26, FILE='PROFH')
OPEN(UNIT=27, FILE='PROFC13')
OPEN(UNIT=28, FILE='O18PROF')
OPEN(UNIT=29, FILE='SPROFO18')
OPEN(UNIT=30, FILE='H18PROF')
OPEN(UNIT=31, FILE='CHISQ')
IWRITE=0
IFLAG=0
DO IT=1,NUMISO
! GTEMP(IT)=PROF(1,2,ICN(IT)); RNREF(IT)=RN(ICN(IT));
  SWDREF(IT)=SWDR(ICN(IT)); LWDREF(IT)=LWDR(ICN(IT))
ENDDO

NUMLEV=NUML          ! USE INTERPOLATED DATA
SPROF(:,1)=SPROF(:,1)+9.8  !CORRECT FOR OFFSET OF IRGA DATA FROM FLASK DATA

SPROFALL(:,1,:)=SPROFALL(:,1,:)+9.8
IS2=50      !NUMBER OF SEGMENTS FOR DC/DA INTEGRALS
IS3=100     !NUMBER OF POINTS WHERE SOURCE AND FLUX ARE EVALUATED
IS4=50     !NUMBER OF POINTS WHERE FLUX IS CALCULATED INITIALLY

FIS2=FLOAT(IS2)
FIS3=FLOAT(IS3)
FIS4=FLOAT(IS4)

HCS=23.     ! CANOPY HEIGHT
COUNT=0.
DO IK=1,NUMLEV      ! NUMBER OF HEIGHTS BELOW HC
  IF(XPROF(IK).LE.HCS) THEN
    COUNT=COUNT+1
  ENDIF
ENDDO

RL=0.001          ! INITIALISE RL (LEV-MARQ LAMBDA)

SLA1=5.; SLA2=4.  ! LEAF AREA PROFILE SHAPE
GHR=0.003        ! GH MULTIPLIER

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WIND=3.      ! WIND EXTINCTION COEFFICIENT
CICA=0.6     ! INITIAL CI/CA
D13RESP=18. ! RESP. DISCR.
D18RESP=15. ! RESP. DISCR.
SIGO=SIG     !RETAIN ORIGINAL SIGMAS FOR CONCENTRATIONS

VM=1.       ! VMAX PARAMETER
SVMi=10.    ! SIGMA OF VMAX PARAMETER
ALAM=250.   ! LAMBDA FOR GS
SALAMi=2500. ! SIGMA FOR LAMBDA
TLP1=20.    ! TL EXP COEFF
STLP1I=200. ! SIGMA FOR TL EXP COEFF
TLP2=0.30   ! TL U*/H AT TOP OF CANOPY
STLP2I=3.   ! SIGMA FOR TL U*/H
KDF=0.78    ! DIFFUSE RADIATION EXTINCTION COEFFICIENT
SKDFI=8.    ! SIGMA FOR KDF
KBF=0.50    ! DIRECT RADIATION EXTINCTION COEFFICIENT
SKBFI=5.    ! SIGMA FOR KBF

AK(1:3)=(/0.0458,-0.0268,0.00566/) ! CO2, HEAT AND H2O FLUX AT GROUND
DO I=1,NUMISO ! GROUND FLUXES FOR EACH OF THE TEN PROFILE SETS
  GF(1,I)=0.05; GF(2,I)=-0.05; GF(3,I)=0.01
ENDDO
AK(4)=VM     ! VMAX PARAMETER
AK(5)=ALAM  ! LAMBDA FOR GS
AK(6)=TLP1  ! TL EXP COEFF
AK(7)=TLP2  ! TL U*/H AT TOP OF CANOPY
AK(8)=KDF   ! DIRECT RADIATION EXTINCTION COEFFICIENT
AK(9)=KBF   ! DIFFUSE RADIATION EXTINCTION COEFFICIENT
TL1=TLP1
TL2=TLP2
STL1=STLP1I
STL2=STLP2I

PARAM(1:2)=(/SLA1,SLA2/) ! SHAPE OF LEAF AREA PROFILE
PARAM(3)=GHR ! GH MULTIPLIER
PARAM(4)=4.3 ! TOTAL LEAF AREA INDEX
PARAM(5)=WIND ! WIND EXTINCTION COEFFICIENT

TENLOOPS: DO I=1,NUMISO
DO NPR=1,3
SREF(NPR,I)=SPROFALL(NUMLEV,NPR,I)
  DO J=1,NUMLEV ! CHECK FOR BAD STD DEVIATION + BAD DC/DT
    IF(SPROF(J,NPR+3).LT.0.001) SPROF(J,NPR+3)=1.
    IF(ABS(SPROF(J,NPR+3)).GT.900.) SPROF(J,NPR+3)=1.
    IF(ABS(SPROF(J,NPR+6)).GT.900.) SPROF(J,NPR+6)=0.
  ENDDO
ENDDO
IF(ISOTOPES.GE.1) THEN
  SREF(4,I)=(APROFALL(NUMLEV,1,I)/1000.+1)*RSTD*SREF(1,I)
  RAIR(I)=SREF(4,I)/SREF(1,I)
  SREF(5,I)=(APROFALL(NUMLEV,2,I)/1000.+1)*R18STD*SREF(1,I)
ENDIF
ZREF=XPROF(NUMLEV)
SMOW=0.0020052; DEL_S=-18.; ESTAR=9.2
D18VAP=-26.
SREF(6,I)=(1.+D18VAP/1000.)*SMOW*SREF(3,I)

DO N=1,NUMLEV
  DO L=1,6
    CKOALL(L,N,I)=SREF(L,I)
  ENDDO
ENDDO
CKALL=CKOALL; CKKALL=CKOALL; AKO=AK; AKE=AK; IFLAGO=1; GFO=GF; GFE=GF
TL1O=TL1; TL2O=TL2; TL1E=TL1; TL2E=TL2
ENDDO TENLOOPS

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NC=0.;X2=0.
do i=0,is3-1
  ZAH=FLOAT(I)/FIS3*COUNT
  J=NINT(ZAH)
  IF(J.EQ.0)THEN; X1=0.;ELSE; X1=XPROF(J); ENDIF
  IF(X1.EQ.X2) THEN; NC=0.; ELSE; NC=NC+1; ENDIF
  IF(J.LT.20)THEN;IF(XPROF(J+1).GT.HCS) THEN; X2=HCS; ELSE; X2=XPROF(J+1); ENDIF;ENDIF
  IF(J.GT.0)THEN;IF(XPROF(J).GT.HCS) THEN; X1=HCS; ENDIF;ENDIF
  ZAH=NC/FIS3*COUNT
  ZAL=X1+(X2-X1)*ZAH
  ZAH=ZAL/HCS
  ZSOU(I)=ZAL
ENDDO
ZSOU(IS3)=HCS

1122  AK=AK0; GF=GFO; TL1=TL10; TL2=TL20
      IF(ICOSTFN.EQ.1) THEN
        IF(IPM.EQ.2) THEN
          AK(IN)=AK(IN)+0.1*AK(IN)
        ELSEIF(IPM.EQ.3) THEN
          AK(IN)=AK(IN)-0.1*AK(IN)
        ENDIF
      ENDIF

      ITER=200
3035  DO 3025 IA=1,ITER          ! ITERATE FOR AK PARAMETERS

      LIM=0
      CKOALL=CKALL
      DCKOALL=DCKALL
      IF(AK(4).LT.0.1) THEN; SVM=SVM/2.; LIM=1; ELSEIF(IFLAGO.EQ.1) THEN; SVM=SVMI; ENDIF
      IF(AK(5).LT.50.) THEN; SALAM=SALAM/2.; LIM=1
      ELSEIF(AK(5).GT.1500.) THEN; SALAM=SALAM/2.; LIM=1;
      ELSEIF(IFLAGO.EQ.1) THEN; SALAM=SALAMI; ENDIF
      IF(NUMK.EQ.54) THEN
        DO IT=1,10
          IF(TL1(IT).LT.8.)THEN; STL1(IT)=STL1(IT)/2.; LIM=1
          ELSEIF(TL1(IT).GT.200.) THEN; STL1(IT)=STL1(IT)/2.; LIM=1
          ELSEIF(IFLAGO.EQ.1) THEN; STL1(IT)=STLP1I; ENDIF
          IF(TL2(IT).LT.0.1)THEN; STL2(IT)=STL2(IT)/2.; LIM=1
          ELSEIF(TL2(IT).GT.0.6)THEN; STL2(IT)=STL2(IT)/2.; LIM=1
          ELSEIF(IFLAGO.EQ.1)THEN; STL2(IT)=STLP2I; ENDIF
        ENDDO
      ELSEIF(NUMK.NE.54) THEN
        IF(AK(6).LT.8.) THEN; STLP1=STLP1/2.; LIM=1
        ELSEIF(AK(6).GT.200.) THEN; STLP1=STLP1/2.; LIM=1;
        ELSEIF(IFLAGO.EQ.1)THEN; STLP1=STLP1I; ENDIF
        IF(AK(7).LT.0.1) THEN; STLP2=STLP2/2.; LIM=1
        ELSEIF(AK(7).GT.0.6) THEN; STLP2=STLP2/2.; LIM=1;
        ELSEIF(IFLAGO.EQ.1)THEN; STLP2=STLP2I; ENDIF
        IF(AK(7).LE.0.1.AND.AK(6).LE.0.2) THEN
          STLP2=STLP2/2.; STLP1=STLP1/2.; LIM=1
        ENDIF
      ENDIF
      IF(AK(8).LT.0.01) THEN; SKDF=SKDF/2.; LIM=1;
      ELSEIF(AK(8).GT.1.) THEN; SKDF=SKDF/2.; LIM=1; ELSEIF(IFLAGO.EQ.1)THEN; SKDF=SKDFI; ENDIF
      IF(AK(9).LT.0.01) THEN; SKBF=SKBF/2.; LIM=1
      ELSEIF(AK(9).GT.1.) THEN; SKBF=SKBF/2.; LIM=1; ELSEIF(IFLAGO.EQ.1)THEN; SKBF=SKBFI; ENDIF
      IF(LIM.EQ.1) THEN; AK=AKE; DCKALL=DCKEALL; CKALL=CKEALL; GF=GFE
        TL1=TL1E; TL2=TL2E; IFLAGO=0; GOTO 808; ENDIF

2121 CONTINUE

      TENLOOPS2: DO IT=1,NUMISO
!         check if stability correction required

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if(ist_cor.eq.1) then
  IF(TTHR(ICN(IT)).LT.5) ZMON=10.
  IF(TTHR(ICN(IT)).GE.5.AND.TTHR(ICN(IT)).LT.7) ZMON=50.
  IF(TTHR(ICN(IT)).GE.7.AND.TTHR(ICN(IT)).LT.8) ZMON=100.
  IF(TTHR(ICN(IT)).GE.8.AND.TTHR(ICN(IT)).LT.10) ZMON=500.
  IF(TTHR(ICN(IT)).GE.10.AND.TTHR(ICN(IT)).LT.17) ZMON=1000.
  IF(TTHR(ICN(IT)).GE.17.AND.TTHR(ICN(IT)).LT.18) ZMON=500.
  IF(TTHR(ICN(IT)).GE.18.AND.TTHR(ICN(IT)).LT.19) ZMON=100.
  IF(TTHR(ICN(IT)).GE.19.AND.TTHR(ICN(IT)).LT.22) ZMON=50.
  IF(TTHR(ICN(IT)).GE.22) ZMON=10.
else
  zMon=-1000.                !set to large -ve value
!                               -> neutral
end if

call air(SREF(2,IT),APRESS(ICN(IT)),rho,volm,capp,rlam,qsat,epsi)
UHREF=UH(ICN(IT))/1.3
USTARR=US(ICN(IT))
SIGWR=SWR(ICN(IT))
AK(1:3)=GF(:,IT)
IFLAGO=1
IF(IDIS.EQ.1) THEN
  call DISPM2(USTARR,SIGWR,AK(6),AK(7),timdat,NUMLEV,NUMLEV,NUMLEV,0,IS3, &
  ZSOU,XPROF,zMon,DISC,DISCN,DISCF,IWRITE)
ENDIF
DO KK=1,3
! CALCULATE SOURCE AND FLUX PROFILES
CALL CALCS(PARAM,FD(ICN(IT)),PAR(ICN(IT)),DEF,SWDREF(IT),LWDREF(IT), &
DTIME(ICN(IT)),APRESS(ICN(IT)),CKALL(:, :, IT), &
XPROF,SREF(1,IT),ESATL,thet1,RLAI,RC,RH,RNN,ak, &
hcs,cica,CSOURCE,esource,is3,HSOURCE,C13SOURCE,O18SOURCE,H18SOURCE, &
UHREF,DRESP,DELTA,DEL18,DEL_E,ZSOU)
SK(3,:)=ESOURCE ! THESE ARE THE SOURCE PROFILES FROM Z=0 TO Z=H
SK(2,:)=HSOURCE
SK(1,:)=CSOURCE
SK(4,:)=C13SOURCE
SK(5,:)=O18SOURCE
SK(6,:)=H18SOURCE

CALL INTVAL(28., 28., TEMP, CO2, H2O,NLEVL,ZZZ,PROF,28.,20,ICN(IT))
ESAT=6.1375*EXP(17.502*TEMP/(240.97+TEMP))
SL=17.502*240.97/(240.97+TEMP)**2*esat
s1=0.622*pmb/(pmb-0.378*esat)**2*s1
ep=rlam/cApp*s1
eqg=ep*rnn(0)*.9/(ep+1.)
! AK(3)=EQG*VOLM/RLAM/18.015/1.E-6
CALL CALCE(APROFALL(:,3:4,IT),SPROFALL(:,7:9,IT),PARAM,FD(ICN(IT)), &
PAR(ICN(IT)),SWDREF(IT),LWDREF(IT), &
DTIME(ICN(IT)),APRESS(ICN(IT)),CKALL(:, :, IT),XPROF,SREF(1,IT),ak,hcs, &
CFLUX,eflux,is4,0.,ZREF,HFLUX, C13FLUX,O18FLUX,H18FLUX,UHREF,ZPR,0)
!WRITE TO DUMMY VARIABLES, FLUX PROFILES FROM Z=0 TO Z=H
EFLUXD=EFLUX; HFLUXD=HFLUX; CFLUXD=CFLUX; C13FLUXD=C13FLUX; O18FLUXD=O18FLUX
H18FLUXD=H18FLUX

IF(IST_COR.EQ.1) THEN
  LZMON(IT)=USREF**3*(TC+273.15)*RHO*CAPP/0.4/10./HFLUX(IS4) !MONIN-OBUKHOV LENGTH
  ZMON=LZMON(IT)
ENDIF

CKNR=0.;CKNR2=0.;CKNR3=0.;CKNR4=0.; CKNR5=0.;CKNR6=0. !CALCULATE NEAR FIELD CONC AT ZREF
NC=0.;X2=0.
DO I=0,IS3-1
  ZAH=FLOAT(I)/FIS3*COUNT
  J=NINT(ZAH)
  IF(J.EQ.0)THEN; X1=0.;ELSE; X1=XPROF(J); ENDIF
  IF(X1.EQ.X2) THEN; NC=0.; ELSE; NC=NC+1; ENDIF

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IF(J.LT.20)THEN;IF(XPROF(J+1).GT.HCS) THEN; X2=HCS; ELSE; X2=XPROF(J+1); ENDIF;ENDIF
IF(J.GT.0)THEN;IF(XPROF(J).GT.HCS) THEN; X1=HCS; ENDIF;ENDIF
ZAH=NC/FIS3*COUNT
ZI=X1+(X2-X1)*ZAH
ZID=ZI+(X2-X1)*COUNT/FIS3
IF(NUMK.NE.54) THEN
  CALL TURB2(USTARR,SIGWR,AK(6),AK(7),ZI,zMon,SWO,TLO)
  CALL TURB2(USTARR,SIGWR,AK(6),AK(7),ZID,zMon,SWD,TLD)
ELSEIF(NUMK.EQ.54) THEN
  CALL TURB2(USTARR,SIGWR,TL1(IT),TL2(IT),ZI,zMon,SWO,TLO)
  CALL TURB2(USTARR,SIGWR,TL1(IT),TL2(IT),ZID,zMon,SWD,TLD)
ENDIF
RKN1=RKN((ZREF-ZI)/SWO/TLO)+RKN((ZREF+ZI)/SWO/TLO)
RKN2=RKN((ZREF-ZID)/SWD/TLD)+RKN((ZREF+ZID)/SWD/TLD)
CKNR=CKNR+((SK(1,I))/SWO*RKN1+ (SK(1,I+1))/SWD*RKN2)/2./FIS3*HCS
CKNR2=CKNR2+((SK(2,I))/SWO*RKN1+ (SK(2,I+1))/SWD*RKN2)/2./FIS3*HCS
CKNR3=CKNR3+((SK(3,I))/SWO*RKN1+ (SK(3,I+1))/SWD*RKN2)/2./FIS3*HCS
CKNR4=CKNR4+((SK(4,I))/SWO*RKN1+ (SK(4,I+1))/SWD*RKN2)/2./FIS3*HCS
CKNR5=CKNR5+((SK(5,I))/SWO*RKN1+ (SK(5,I+1))/SWD*RKN2)/2./FIS3*HCS
CKNR6=CKNR6+(SK(6,I)/SWO*RKN1+ SK(6,I+1)/SWD*RKN2)/2./FIS3*HCS
ENDDO
DO N=1,NUMLEV          ! CALCULATE NEAR FIELD CONC AT EACH Zi (MEASUREMENT HEIGHTS)
CKF1=0.;CKF2=0.;CKF3=0.;CKF4=0.; CKF5=0.; CKF6=0.
CKN=0.;CKN2=0.;CKN3=0.;CKN4=0.; CKN5=0.; CKN6=0.
DCKF1E=0.;DCKF2E=0.;DCKF3E=0.;DCKF4E=0.; DCKF5E=0.
DCKNE=0.;DCKN2E=0.;DCKN3E=0.;DCKN4E=0.; DCKN5E=0.
DCKF1B=0.;DCKF2B=0.;DCKF3B=0.;DCKF4B=0.; DCKF5B=0.
DCKNB=0.;DCKN2B=0.;DCKN3B=0.;DCKN4B=0.; DCKF5B=0.
ZL=XPROF(N)
NC=0.;X2=0.
DO I=0,IS3-1
  ZAH=FLOAT(I)/FIS3
  ZI=ZAH*HCS
  ZID=ZI+HCS/FIS3
  ZAH=FLOAT(I)/FIS3*COUNT
  J=NINT(ZAH)
  IF(J.EQ.0)THEN; X1=0.;ELSE; X1=XPROF(J); ENDIF
  IF(X1.EQ.X2) THEN; NC=0.; ELSE; NC=NC+1; ENDIF
  IF(J.LT.20)THEN;IF(XPROF(J+1).GT.HCS) THEN; X2=HCS; ELSE; X2=XPROF(J+1); ENDIF;ENDIF
  IF(J.GT.0)THEN;IF(XPROF(J).GT.HCS) THEN; X1=HCS; ENDIF;ENDIF
  ZAH=NC/FIS3*COUNT
  ZI=X1+(X2-X1)*ZAH
  ZID=ZI+(X2-X1)*COUNT/FIS3
  IF(NUMK.NE.54) THEN
    EPS=0.001*AK(6)
    EPS2=0.001*AK(7)
    CALL TURB2(USTARR,SIGWR,AK(6),AK(7),ZI,zMon,SWO,TLO)
    CALL TURB2(USTARR,SIGWR,AK(6),AK(7),ZID,ZMON,SWD,TLD)
    CALL TURB2(USTARR,SIGWR,AK(6)+EPS,AK(7),ZI,zMon,SWO,TLOE)
    CALL TURB2(USTARR,SIGWR,AK(6)+EPS,AK(7),ZID,ZMON,SWD,TLDE)
    CALL TURB2(USTARR,SIGWR,AK(6),AK(7)+EPS2,ZI,zMon,SWO,TLOB)
    CALL TURB2(USTARR,SIGWR,AK(6),AK(7)+EPS2,ZID,ZMON,SWD,TLDB)
  ELSEIF(NUMK.EQ.54) THEN
    EPS=0.001*TL1(IT)
    EPS2=0.001*TL2(IT)
    CALL TURB2(USTARR,SIGWR,TL1(IT),TL2(IT),ZI,zMon,SWO,TLO)
    CALL TURB2(USTARR,SIGWR,TL1(IT),TL2(IT),ZID,ZMON,SWD,TLD)
    CALL TURB2(USTARR,SIGWR,TL1(IT)+EPS,TL2(IT),ZI,zMon,SWO,TLOE)
    CALL TURB2(USTARR,SIGWR,TL1(IT)+EPS,TL2(IT),ZID,ZMON,SWD,TLDE)
    CALL TURB2(USTARR,SIGWR,TL1(IT),TL2(IT)+EPS2,ZI,zMon,SWO,TLOB)
    CALL TURB2(USTARR,SIGWR,TL1(IT),TL2(IT)+EPS2,ZID,ZMON,SWD,TLDB)
  ENDIF
  IF((ZL-ZI).NE.0.0.AND.(ZL-ZID).NE.0.0) THEN
    RKN1=RKN((ZL-ZI)/SWO/TLO)+RKN((ZL+ZI)/SWO/TLO)
    RKN2=RKN((ZL-ZID)/SWD/TLD)+RKN((ZL+ZID)/SWD/TLD)
    RKN1E=RKN((ZL-ZI)/SWO/TLOE)+RKN((ZL+ZI)/SWO/TLOE)

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RKN2E=RKN((ZL-ZID)/SWD/TLDE)+RKN((ZL+ZID)/SWD/TLDE)
RKN1B=RKN((ZL-ZI)/SWO/TLOB)+RKN((ZL+ZI)/SWO/TLOB)
RKN2B=RKN((ZL-ZID)/SWD/TLDB)+RKN((ZL+ZID)/SWD/TLDB)
ELSEIF((ZL-ZI).EQ.0.0) THEN
RKN1=RKN(HCS/FIS3/SWO/TLO)+RKN((ZL+ZI)/SWO/TLO)
RKN2=RKN((ZL-ZID)/SWD/TLDE)+RKN((ZL+ZID)/SWD/TLDE)
RKN1E=RKN(HCS/FIS3/SWO/TLOE)+RKN((ZL+ZI)/SWO/TLOE)
RKN2E=RKN((ZL-ZID)/SWD/TLDE)+RKN((ZL+ZID)/SWD/TLDE)
RKN1B=RKN(HCS/FIS3/SWO/TLOB)+RKN((ZL+ZI)/SWO/TLOB)
RKN2B=RKN((ZL-ZID)/SWD/TLDB)+RKN((ZL+ZID)/SWD/TLDB)
ELSEIF((ZL-ZID).EQ.0.0) THEN
RKN1=RKN((ZL-ZI)/SWO/TLO)+RKN((ZL+ZI)/SWO/TLO)
RKN2=RKN(HCS/FIS3/SWO/TLDE)+RKN((ZL+ZID)/SWD/TLDE)
RKN1E=RKN((ZL-ZI)/SWO/TLOE)+RKN((ZL+ZI)/SWO/TLOE)
RKN2E=RKN(HCS/FIS3/SWO/TLDE)+RKN((ZL+ZID)/SWD/TLDE)
RKN1B=RKN((ZL-ZI)/SWO/TLOB)+RKN((ZL+ZI)/SWO/TLOB)
RKN2B=RKN(HCS/FIS3/SWO/TLDB)+RKN((ZL+ZID)/SWD/TLDB)
ENDIF
DRKN1=(RKN1E-RKN1)/EPS
DRKN2=(RKN2E-RKN2)/EPS
DRKN1B=(RKN1B-RKN1)/EPS2
DRKN2B=(RKN2B-RKN2)/EPS2
CKN=CKN+((SK(1,I))/SWO*RKN1+ (SK(1,I+1))/SWD*RKN2)/2./FIS3*HCS
CKN2=CKN2+((SK(2,I))/SWO*RKN1+ (SK(2,I+1))/SWD*RKN2)/2./FIS3*HCS
CKN3=CKN3+((SK(3,I))/SWO*RKN1+ (SK(3,I+1))/SWD*RKN2)/2./FIS3*HCS
CKN4=CKN4+((SK(4,I))/SWO*RKN1+ (SK(4,I+1))/SWD*RKN2)/2./FIS3*HCS
CKN5=CKN5+((SK(5,I))/SWO*RKN1+ (SK(5,I+1))/SWD*RKN2)/2./FIS3*HCS
CKN6=CKN6+((SK(6,I))/SWO*RKN1+ (SK(6,I+1))/SWD*RKN2)/2./FIS3*HCS
DCKNE=DCKNE+((SK(1,I))/SWO*DRKN1+ (SK(1,I+1))/SWD*DRKN2)/2./FIS3*HCS
DCKN2E=DCKN2E+((SK(2,I))/SWO*DRKN1+ (SK(2,I+1))/SWD*DRKN2)/2./FIS3*HCS
DCKN3E=DCKN3E+((SK(3,I))/SWO*DRKN1+ (SK(3,I+1))/SWD*DRKN2)/2./FIS3*HCS
DCKN4E=DCKN4E+((SK(4,I))/SWO*DRKN1+ (SK(4,I+1))/SWD*DRKN2)/2./FIS3*HCS
DCKN5E=DCKN5E+((SK(5,I))/SWO*DRKN1+ (SK(5,I+1))/SWD*DRKN2)/2./FIS3*HCS
DCKNB=DCKNB+((SK(1,I))/SWO*DRKN1B+ (SK(1,I+1))/SWD*DRKN2B)/2./FIS3*HCS
DCKN2B=DCKN2B+((SK(2,I))/SWO*DRKN1B+ (SK(2,I+1))/SWD*DRKN2B)/2./FIS3*HCS
DCKN3B=DCKN3B+((SK(3,I))/SWO*DRKN1B+ (SK(3,I+1))/SWD*DRKN2B)/2./FIS3*HCS
DCKN4B=DCKN4B+((SK(4,I))/SWO*DRKN1B+ (SK(4,I+1))/SWD*DRKN2B)/2./FIS3*HCS
DCKN5B=DCKN5B+((SK(5,I))/SWO*DRKN1B+ (SK(5,I+1))/SWD*DRKN2B)/2./FIS3*HCS
ENDDO
DO I=0,IS3
ZN=ZL+FLOAT(I)*(ZREF-ZL)/FIS3
IF(NUMK.NE.54) THEN
EPS=0.001*AK(6)
EPS2=0.001*AK(7)
CALL TURB2(USTARR,SIGWR,AK(6),AK(7),ZN,zMon,SWZ,TLZ)
CALL TURB2(USTARR,SIGWR,AK(6)+EPS,AK(7),ZN,zMon,SWZ,TLZE)
CALL TURB2(USTARR,SIGWR,AK(6),AK(7)+EPS2,ZN,zMon,SWZ,TLZB)
ELSEIF(NUMK.EQ.54) THEN
EPS=0.001*TL1(IT)
EPS2=0.001*TL2(IT)
CALL TURB2(USTARR,SIGWR,TL1(IT),TL2(IT),ZN,zMon,SWZ,TLZ)
CALL TURB2(USTARR,SIGWR,TL1(IT)+EPS,TL2(IT),ZN,zMon,SWZ,TLZE)
CALL TURB2(USTARR,SIGWR,TL1(IT),TL2(IT)+EPS2,ZN,zMon,SWZ,TLZB)
ENDIF
! GET FLUX PROFILES FROM Z=Zi TO Z=ZREF FOR CONCENTRATION INTEGRAL, WHERE Zi IS HEIGHT
! OF CONCENTRATION MEASUREMENT, FOR EACH Zi
IF(ZN.EQ.ZPR(IS4)) THEN
FK(3,I)=EFLUX(IS4); FK(2,I)=HFLUX(IS4); FK(1,I)=CFLUX(IS4); FK(4,I)=C13FLUX(IS4)
FK(5,I)=O18FLUX(IS4); FK(6,I)=H18FLUX(IS4)
ELSEIF(ZN.GT.ZPR(IS4).OR.ZN.LT.ZPR(0)) THEN
STOP 'ZN NOT IN RANGE FLUX CALC'
ENDIF
DO J=0,IS4-1
IF(ZN.EQ.ZPR(J)) THEN !IF Zi COINCIDES WITH A HEIGHT AT WHICH WE ALREADY HAVE
! THE FLUX CALCULATION, TAKE THAT FLUX
FK(3,I)=EFLUXD(J); FK(2,I)=HFLUXD(J); FK(1,I)=CFLUXD(J); FK(4,I)=C13FLUXD(J)

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      FK(5,I)=O18FLUXD(J); FK(6,I)=H18FLUXD(J)
      ELSEIF(ZN.LT.ZPR(J+1).AND.ZN.GT.ZPR(J)) THEN      ! OTHERWISE CALCULATE ADDITIONAL
                ! FLUX FROM HEIGHT WE HAVE TO HEIGHT WE WANT
      EADD=EFLUXD(J); HADD=HFLUXD(J); CADD=CFLUXD(J); C13ADD=C13FLUXD(J)
      O18ADD=O18FLUXD(J); H18ADD=H18FLUXD(J)
      ZR=ZPR(J)+(ZN-ZPR(J))*FIS4
      CALL CALCE(APROFALL(:,3:4,IT),SPROFALL(:,7:9,IT),PARAM,FD(ICN(IT)), &
      PAR(ICN(IT)),SWDREF(IT),LWDREF(IT), DTIME(ICN(IT)),APRESS(ICN(IT)), &
      CKALL(:,IT),XPROF,SREF(1,IT),ak,hcs,CFLUX,eflux,is4,ZPR(J),ZR,HFLUX, &
      C13FLUX,O18FLUX,H18FLUX,UHREF,ZOUT,1)
      FK(3,I)=EFLUX(1)+EADD
      FK(2,I)=HFLUX(1)+HADD
      FK(1,I)=CFLUX(1)+CADD
      FK(4,I)=C13FLUX(1)+C13ADD
      FK(5,I)=O18FLUX(1)+O18ADD
      FK(6,I)=H18FLUX(1)+H18ADD
      ENDIF
    ENDDO
  FKS(3,I)=FK(3,I)/SWZ**2/TLZ      ! DIVIDE BY SIGW^2 AND TL FOR INTEGRATION
  FKS(2,I)=FK(2,I)/SWZ**2/TLZ
  FKS(1,I)=FK(1,I)/SWZ**2/TLZ
  FKS(4,I)=FK(4,I)/SWZ**2/TLZ
  FKS(5,I)=FK(5,I)/SWZ**2/TLZ
  FKS(6,I)=FK(6,I)/SWZ**2/TLZ
  DTL=(TLZE-TLZ)/EPS
  DTLB=(TLZB-TLZ)/EPS2
  DFKS(3,I)=-FK(3,I)/SWZ**2/TLZ**2*DTL
  DFKS(2,I)=-FK(2,I)/SWZ**2/TLZ**2*DTL
  DFKS(1,I)=-FK(1,I)/SWZ**2/TLZ**2*DTL
  DFKS(4,I)=-FK(4,I)/SWZ**2/TLZ**2*DTL
  DFKS(5,I)=-FK(5,I)/SWZ**2/TLZ**2*DTL
  DFKS(6,I)=-FK(1,I)/SWZ**2/TLZ**2*DTLB
  DFKS(7,I)=-FK(2,I)/SWZ**2/TLZ**2*DTLB
  DFKS(8,I)=-FK(3,I)/SWZ**2/TLZ**2*DTLB
  DFKS(9,I)=-FK(4,I)/SWZ**2/TLZ**2*DTLB
  DFKS(10,I)=-FK(5,I)/SWZ**2/TLZ**2*DTLB
ENDDO
DO I=0,IS3-1
  CKF1=CKF1+(FKS(1,I)+FKS(1,I+1))/2./FIS3*(ZREF-ZL)      ! INTEGRATE FROM Zi TO ZREF
  CKF2=CKF2+(FKS(2,I)+FKS(2,I+1))/2./FIS3*(ZREF-ZL)
  CKF3=CKF3+(FKS(3,I)+FKS(3,I+1))/2./FIS3*(ZREF-ZL)
  CKF4=CKF4+(FKS(4,I)+FKS(4,I+1))/2./FIS3*(ZREF-ZL)
  CKF5=CKF5+(FKS(5,I)+FKS(5,I+1))/2./FIS3*(ZREF-ZL)
  CKF6=CKF6+(FKS(6,I)+FKS(6,I+1))/2./FIS3*(ZREF-ZL)
  DCKF1E=DCKF1E+(DFKS(1,I)+DFKS(1,I+1))/2./FIS3*(ZREF-ZL)      ! INTEGRATE FROM Zi TO ZREF
  DCKF2E=DCKF2E+(DFKS(2,I)+DFKS(2,I+1))/2./FIS3*(ZREF-ZL)
  DCKF3E=DCKF3E+(DFKS(3,I)+DFKS(3,I+1))/2./FIS3*(ZREF-ZL)
  DCKF4E=DCKF4E+(DFKS(4,I)+DFKS(4,I+1))/2./FIS3*(ZREF-ZL)
  DCKF5E=DCKF5E+(DFKS(5,I)+DFKS(5,I+1))/2./FIS3*(ZREF-ZL)
  DCKF1B=DCKF1B+(DFKS(6,I)+DFKS(6,I+1))/2./FIS3*(ZREF-ZL)      ! INTEGRATE FROM Zi TO ZREF
  DCKF2B=DCKF2B+(DFKS(7,I)+DFKS(7,I+1))/2./FIS3*(ZREF-ZL)
  DCKF3B=DCKF3B+(DFKS(8,I)+DFKS(8,I+1))/2./FIS3*(ZREF-ZL)
  DCKF4B=DCKF4B+(DFKS(9,I)+DFKS(9,I+1))/2./FIS3*(ZREF-ZL)
  DCKF5B=DCKF5B+(DFKS(10,I)+DFKS(10,I+1))/2./FIS3*(ZREF-ZL)
ENDDO
CKALL(1,N,IT)=(CKN+CKF1-CKNR)+SREF(1,IT)      ! CONCENTRATION = NEAR-FIELD + FAR-FIELD -
CKALL(2,N,IT)=(CKN2+CKF2-CKNR2)+SREF(2,IT)      ! NEAR-FIELD (ZREF) + CONC (ZREF)
CKALL(3,N,IT)=(CKN3+CKF3-CKNR3)+SREF(3,IT)
CKALL(4,N,IT)=(CKN4+CKF4-CKNR4)+SREF(4,IT)
CKALL(5,N,IT)=(CKN5+CKF5-CKNR5)+SREF(5,IT)
CKALL(6,N,IT)=(CKN6+CKF6-CKNR6)+SREF(6,IT)
DO IK=1,6
  CKALL(IK,N,IT)=MIN(CKALL(IK,N,IT),1000.)
  CKALL(IK,N,IT)=MAX(CKALL(IK,N,IT),-1000.)
  IF(ABS(CKALL(IK,N,IT)).EQ.1000.) THEN
    CKALL(IK,N,IT)=SREF(IK,IT)
  
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        INAN=1
        GOTO 2122
    ENDF
ENDDO
DCKD(1,N,6,IT)=DCKNE+DCKF1E
DCKD(2,N,6,IT)=DCKN2E+DCKF2E
DCKD(3,N,6,IT)=DCKN3E+DCKF3E
DCKD(4,N,6,IT)=DCKN4E+DCKF4E
DCKD(5,N,6,IT)=DCKN5E+DCKF5E
DCKD(1,N,7,IT)=DCKNB+DCKF1B
DCKD(2,N,7,IT)=DCKN2B+DCKF2B
DCKD(3,N,7,IT)=DCKN3B+DCKF3B
DCKD(4,N,7,IT)=DCKN4B+DCKF4B
DCKD(5,N,7,IT)=DCKN5B+DCKF5B
FKTOP(1,IT)=CFLUXD(IS4)
FKTOP(2,IT)=HFLUXD(IS4)
FKTOP(3,IT)=EFLUXD(IS4)
IF(IDIS.EQ.1) THEN
DO NPR=1,5
ASUM=0.
    DO I=1,IS3
        ASUM=ASUM+DISC(N,I)*SK(NPR,I)*(ZSOU(I)-ZSOU(I-1))
    ENDDO
    ASUM=ASUM+DISC(N,0)*FK(NPR,0)*ZSOU(1)
CK(NPR,N)=ASUM+SREF(NPR,IT)
ENDDO
ENDF
ENDDO
ENDDO
ENDDO TENLOOPS2

2122 CSUM=0.
TENLOOPS3: DO IT=1,NUMISO
DO N=1,NUMLEV ! CALCULATE CHI-SQUARE = SUM (C_MODEL - C_MEAS)^2 / SIGMA^2
DO NPR=1,3
    CSUM=CSUM+(CKALL(NPR,N,IT)-SPROFALL(N,NPR,IT))**2/SIG(NPR,N)**2
ENDDO
ENDDO
DO N=1,NUMLEV
    ZAN=FLOAT(N)/FLOAT(NUMLEV)
    IF(ISOTOPES.GT.1) THEN
!       C13K=(APROF(N,1,NIS)/1000.+1.)*RSTD*SPROF(N,1)
       C13K=(CKALL(4,N,IT)/CKALL(1,N,IT)/RSTD-1.)*1000.
       CSUM = CSUM + (C13K-APROFALL(N,1,IT))**2/SIG(4,N)**2
    ENDF
    IF(ISOTOPES.GT.2) THEN
       O18K=(CKALL(5,N,IT)/CKALL(1,N,IT)/R18STD-1.)*1000.
       CSUM = CSUM + (O18K-APROFALL(N,2,IT))**2/SIG(5,N)**2
    ENDF
ENDDO
IF(IEDDY.EQ.1) THEN
    SIGFC=ABS(0.05*FC2(ICN(IT))*VOLM) ! SIGMA OF TOTAL C FLUX
    SIGFH=ABS(0.1*H(ICN(IT))/CAPP/RHO) ! SIGMA OF TOTAL H FLUX
    SIGFE=ABS(0.1*E(ICN(IT))*VOLM) ! SIGMA OF TOTAL E FLUX
    CSUM = CSUM + (FC2(ICN(IT))*VOLM-CFLUX(IS4))**2/SIGFC**2
    CSUM = CSUM + (H(ICN(IT))/CAPP/RHO-HFLUX(IS4))**2/SIGFH**2
    CSUM = CSUM + (E(ICN(IT))*VOLM-EFLUX(IS4))**2/SIGFE**2
ENDF
ENDDO TENLOOPS3
! CSUM = CSUM + (AK(4)-VM)**2/SVM**2
! CSUM = CSUM + (AK(5)-ALAM)**2/SALAM**2
! CSUM = CSUM + (AK(6)-TLP1)**2/STLP1**2
! CSUM = CSUM + (AK(7)-TLP2)**2/STLP2**2
! CSUM = CSUM + (AK(8)-KDF)**2/SKDF**2
! CSUM = CSUM + (AK(9)-KBF)**2/SKBF**2

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CHISQN=CSUM

IF(ABS(CHISQN-CHISQ).LT.0.1) GOTO 3045 !EXIT LOOP IF NO IMPROVEMENT IN CHISQ
CHISQNN=0.
IF(IA.EQ.1.OR.IAC.EQ.1) THEN ! 1ST ITERATION
CHISQ=CHISQN
IAC=0
CKEALL=CKALL
ELSEIF(IA.EQ.ITER-1.AND.CHISQN.LE.CHISQ) THEN ! 2ND LAST ITERATION, EXIT IF CHISQ
AKO=DBLE(AK) ! BETTER THAN PREVIOUS
GOTO 3045
ELSEIF(RL.GT.1.E+2) THEN ! EXIT IF LAMBDA LARGE
CKALL=CKOALL; AK=SNGL(AKO); GF=GFO; TL1=TL10; TL2=TL20
GOTO 3045
ELSEIF(INAN.EQ.1) THEN
WRITE(*,*) 'CONC NAN, AK=',(AK(K),K=4,9)
AK=SNGL(AKO)
GF=GFO
TL1=TL10; TL2=TL20
CKALL=CKOALL
DCKALL=DCKOALL
RL=MAX(RL*100.,0.1)
INAN=0
GOTO 808
ELSE IF (CHISQN.GE.CHISQ) THEN ! INCREASE LAMBDA IF CHISQ WORSE AND USE PREVIOUS PARAMS
AK=SNGL(AKO)
GF=GFO
TL1=TL10; TL2=TL20
CKALL=CKOALL
DCKALL=DCKOALL
RL=MAX(RL*100.,0.1)
GOTO 808
ELSE IF (CHISQN.LT.CHISQ) THEN ! DECREASE LAMBDA IF CHISQ BETTER, AND CONTINUE
RL=RL/10.
CHISQ=CHISQN
AKE=AK; DCKEALL=DCKALL; CKEALL=CKALL; GFE=GF; TL1E=TL1; TL2E=TL2
ELSE
STOP 'PROBLEM SOMEWHERE, MAYBE PARAMS OUT OF RANGE'
AK=SNGL(AKO)
GF=GFO
TL1=TL10; TL2=TL20
CKALL=CKOALL
DCKALL=DCKOALL
RL=MAX(RL*100.,0.1)
GOTO 808
ENDIF
write(*,*) 'Chisq = ',chisq, 'Iterations:',ia, ' RL =',RL
WRITE(*,2233) 'AK =', (AK(K), K=4,9)
IF(NUMK.EQ.54) THEN
WRITE(*,2234) 'TL1 =', (TL1(K), K=1,10)
WRITE(*,2234) 'TL2 =', (TL2(K), K=1,10)
ENDIF
2233 FORMAT(A8,6F8.3)
2234 FORMAT(A8,10F7.2)
2235 FORMAT(A8,10F7.3)

1133 IF(ICOSTFN.EQ.1) THEN
COSTFN(ICOST,IPM,IN)=CHISQ
IF(IPM.EQ.1.OR.IPMEQ.2) THEN
IPM=IPM+1
GOTO 1122
ELSEIF(IPM.EQ.3.AND.IN.LT.9) THEN
IN=IN+1
IPM=2
GOTO 1122
ELSE

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        ICOST=ICOST+1
        GOTO 3045
    ENDIF
ENDIF

! CALCULATE DERIVATIVE OF SOURCE PROFILES WRT PARAMETERS
2022      ZL=0.

SVM=SVMI;SALAM=SALAMI;STLP1=STLP1I;STLP2=STLP2I;SKDF=SKDFI;SKBF=SKBFI
STL1=STLP1I;STL2=STLP2I
TENLOOPS4: DO IT=1,NUMISO
!      check if stability correction required
      if(ist_cor.eq.1) then
        IF(TTHR(ICN(IT)).LT.5) ZMON=10.
        IF(TTHR(ICN(IT)).GE.5.AND.TTHR(ICN(IT)).LT.7) ZMON=50.
        IF(TTHR(ICN(IT)).GE.7.AND.TTHR(ICN(IT)).LT.8) ZMON=100.
        IF(TTHR(ICN(IT)).GE.8.AND.TTHR(ICN(IT)).LT.10) ZMON=500.
        IF(TTHR(ICN(IT)).GE.10.AND.TTHR(ICN(IT)).LT.17) ZMON=1000.
        IF(TTHR(ICN(IT)).GE.17.AND.TTHR(ICN(IT)).LT.18) ZMON=500.
        IF(TTHR(ICN(IT)).GE.18.AND.TTHR(ICN(IT)).LT.19) ZMON=100.
        IF(TTHR(ICN(IT)).GE.19.AND.TTHR(ICN(IT)).LT.22) ZMON=50.
        IF(TTHR(ICN(IT)).GE.22) ZMON=10.
        ZMON=LZMON(IT)
      else
        zMon=-1000.                !set to large -ve value
!                                  -> neutral
      end if

call air(SREF(2,IT),APRESS(ICN(IT)),rho,volm,capp,rlam,qsat,epsi)
UHREF=UH(ICN(IT))/1.3
USTARR=US(ICN(IT))
SIGWR=SWR(ICN(IT))
AK(1:3)=GF(:,IT)
OPTIMIZE: IF(IOPT.EQ.1) THEN
  DO L=4,7
    K=L
    IF(L.EQ.6) K=8
    IF(L.EQ.7) K=9
    EPS=0.001*ABS(AK(K))          !DERIV SOURCE WRT AK(K)
    AKE=AK
    AKE(k)=AKE(k)+EPS
    CALL CALCS(PARAM,FD(ICN(IT)),PAR(ICN(IT)),DEF,SWDREF(IT),LWDREF(IT), &
      DTIME(ICN(IT)),APRESS(ICN(IT)), &
      CKALL(:, :, IT),XPROF,SREF(1,IT),ESATL,thet1e,RLAI,RC,RH,RNN,akE, &
      hcs,cica,CSOURCE,esource,is2,HSOURCE,C13SOURCE,O18SOURCE,H18SOURCE, &
      UHREF,DRESP,DELTA,DEL18,DEL_E,ZSOU)
    ESOURCE2=ESOURCE
    CSOURCE2=CSOURCE
    HSOURCE2=HSOURCE
    C13SOURCE2=C13SOURCE
    O18SOURCE2=O18SOURCE
    AKE=AK
    AKE(k)=AKE(k)-EPS
    CALL CALCS(PARAM,FD(ICN(IT)),PAR(ICN(IT)),DEF,SWDREF(IT),LWDREF(IT), &
      DTIME(ICN(IT)),APRESS(ICN(IT)), &
      CKALL(:, :, IT),XPROF,SREF(1,IT),ESATL,thet1e,RLAI,RC,RH,RNN,akE, &
      hcs,cica,CSOURCE,esource,is2,HSOURCE,C13SOURCE,O18SOURCE,H18SOURCE, &
      UHREF,DRESP,DELTA,DEL18,DEL_E,ZSOU)
    DO NK=0,is2
      EDIFF=(ESOURCE2(NK)-esource(NK))/2./EPS
      CDIFF=(CSOURCE2(NK)-CSOURCE(NK))/2./EPS
      HDIFF=(HSOURCE2(NK)-HSOURCE(NK))/2./EPS
      C13DIFF=(C13SOURCE2(NK)-C13SOURCE(NK))/2./EPS
      O18DIFF=(O18SOURCE2(NK)-O18SOURCE(NK))/2./EPS
      DSK(3,NK,K)=EDIFF
      DSK(1,NK,K)=CDIFF
    
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        DSK(2,NK,K)=HDIFF
        DSK(4,NK,K)=C13DIFF
        DSK(5,NK,K)=O18DIFF
    ENDDO
ENDDO

DO NPR=1,5      ! INTEGRATE SOURCE DERIVATIVES FROM Z=0 TO Z=H FOR DCN(ZREF)/DAK
RSUM1=0.; RSUM2=0.; RSUM3=0.
RSUM4(npr)=0.; RSUM5(npr)=0.; RSUM6(npr)=0.
RSUM7(npr)=0.; RSUM8(NPR)=0.; RSUM9(NPR)=0.
NC=0.; X2=0.
IF (IDIS.EQ.0) THEN
DO NK=0, IS2-1
    ZI=FLOAT(NK)/FIS2*HCS
    ZID=ZI+HCS/FIS2
    ZAH=FLOAT(NK)/FIS2*COUNT
    J=NINT(ZAH)
    IF (J.EQ.0) THEN; X1=0.; ELSE; X1=XPROF(J); ENDIF
    IF (X1.EQ.X2) THEN; NC=0.; ELSE; NC=NC+1; ENDIF
    IF (J.LT.20) THEN; IF (XPROF(J+1).GT.HCS) THEN; X2=HCS; ELSE; X2=XPROF(J+1); ENDIF; ENDIF
    IF (J.GT.0) THEN; IF (XPROF(J).GT.HCS) THEN; X1=HCS; ENDIF; ENDIF
    ZAH=NC/FIS2*COUNT
    ZI=X1+(X2-X1)*ZAH
    ZID=ZI+(X2-X1)*COUNT/FIS2
    IF (NUMK.NE.54) THEN
        CALL TURB2(USTARR, SIGWR, AK(6), AK(7), ZI, zMon, SW, TL)
        CALL TURB2(USTARR, SIGWR, AK(6), AK(7), ZID, zMon, SWD, TLD)
    ELSEIF (NUMK.EQ.54) THEN
        CALL TURB2(USTARR, SIGWR, TL1(IT), TL2(IT), ZI, zMon, SW, TL)
        CALL TURB2(USTARR, SIGWR, TL1(IT), TL2(IT), ZID, zMon, SWD, TLD)
    ENDIF
    RKNR=RKN((ZREF-ZI)/SWD/TLD)+RKN((ZREF+ZI)/SWD/TLD)
    RKNRD=RKN((ZREF-ZID)/SWD/TLD)+RKN((ZREF+ZID)/SWD/TLD)
    RSUM4(npr)=RSUM4(npr)+(DSK(NPR,NK,4)/SW*RKNR+ &
        DSK(NPR,NK+1,4)/SWD*RKNRD)/2./FIS2*HCS
    RSUM5(npr)=RSUM5(npr)+(DSK(NPR,NK,5)/SW*RKNR+ &
        DSK(NPR,NK+1,5)/SWD*RKNRD)/2./FIS2*HCS
    RSUM8(npr)=RSUM8(npr)+(DSK(NPR,NK,8)/SW*RKNR+ &
        DSK(NPR,NK+1,8)/SWD*RKNRD)/2./FIS2*HCS
    RSUM9(npr)=RSUM9(npr)+(DSK(NPR,NK,9)/SW*RKNR+ &
        DSK(NPR,NK+1,9)/SWD*RKNRD)/2./FIS2*HCS
ENDDO
ENDIF
IF (NPR.EQ.1) THEN      ! CALCULATE FLUX DERIVATIVES WRT PARAMETERS,
    ZL=0.                ! FIRST FROM Z=0 TO Z=ZREF
    DO L=4,7
        K=L
        IF (L.EQ.6) K=8
        IF (L.EQ.7) K=9
        EPS=0.001*ABS(AK(K))
        AKE=AK
        AKE(k)=AKE(k)+EPS    ! FIND FLUX WITH AK(K)+EPSILON, K=4,10
        CALL CALCE( APROFALL(:,3:4,IT), SPROFALL(:,7:9,IT), PARAM, FD(ICN(IT)), &
            PAR(ICN(IT)), SWDREF(IT), LWDREF(IT), &
            DTIME(ICN(IT)), APRESS(ICN(IT)), CKALL(:, :, IT), XPROF, SREF(1,IT), ake, hcs, &
            CFLUX, eflux, is4, ZL, ZREF, HFLUX, &
            C13FLUX, O18FLUX, H18FLUX, UHREF, ZPR, 0)
        EFLUX1(K,:)=EFLUX
        CFLUX1(K,:)=CFLUX
        HFLUX1(K,:)=HFLUX
        C13FLUX1(K,:)=C13FLUX
        O18FLUX1(K,:)=O18FLUX
        AKE=AK
        AKE(k)=AKE(k)-EPS    ! FIND FLUX WITH AK(K)-EPSILON, K=4,10
        CALL CALCE( APROFALL(:,3:4,IT), SPROFALL(:,7:9,IT), PARAM, FD(ICN(IT)), &
            PAR(ICN(IT)), SWDREF(IT), LWDREF(IT), &

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DTIME(ICN(IT)), APRESS(ICN(IT)), CKALL(:, :, IT), XPROF, SREF(1, IT), ake, hcs, &
CFLUX, eflux, is4, ZL, ZREF, HFLUX, &
C13FLUX, O18FLUX, H18FLUX, UHREF, ZPR, 0)
EFLUX2(K, :) = EFLUX
CFLUX2(K, :) = CFLUX
HFLUX2(K, :) = HFLUX
C13FLUX2(K, :) = C13FLUX
O18FLUX2(K, :) = O18FLUX
ENDDO
ENDIF
enddo
ENDIF OPTIMISE
DO N=1, NUMLEV
do npr=1, 5
ZL=XPROF(N)
SSUM1=0.; SSUM2=0.; SSUM3=0.
SSUM4=0.; SSUM5=0.; SSUM6=0.
SSUM7=0.; SSUM8=0.; SSUM9=0.
NC=0.; X2=0.
OPTIMISE2: IF(IOPT.EQ.1) THEN
IF(IDIS.EQ.0) THEN
DO NK=0, IS2-1
ZI=FLOAT(NK)/FIS2*HCS
ZID=ZI+HCS/FIS2
ZAH=FLOAT(NK)/FIS2*COUNT
J=NINT(ZAH)
IF(J.EQ.0) THEN; X1=0.; ELSE; X1=XPROF(J); ENDIF
IF(X1.EQ.X2) THEN; NC=0.; ELSE; NC=NC+1; ENDIF
IF(J.LT.20) THEN; IF(XPROF(J+1).GT.HCS) THEN; X2=HCS; ELSE; X2=XPROF(J+1); ENDIF; ENDIF
IF(J.GT.0) THEN; IF(XPROF(J).GT.HCS) THEN; X1=HCS; ENDIF; ENDIF
ZAH=NC/FIS2*COUNT
ZI=X1+(X2-X1)*ZAH
ZID=ZI+(X2-X1)*COUNT/FIS2
IF(NUMK.NE.54) THEN
CALL TURB2(USTARR, SIGWR, AK(6), AK(7), ZI, zMon, SW, TL)
CALL TURB2(USTARR, SIGWR, AK(6), AK(7), ZID, zMon, SWD, TLD)
ELSEIF(NUMK.EQ.54) THEN
CALL TURB2(USTARR, SIGWR, TL1(IT), TL2(IT), ZI, zMon, SW, TL)
CALL TURB2(USTARR, SIGWR, TL1(IT), TL2(IT), ZID, zMon, SWD, TLD)
ENDIF
IF((ZL-ZI).NE.0.0.AND.(ZL-ZID).NE.0.0) THEN !INTEGRATE OVER SOURCES
RKN0=RKN((ZL-ZI)/SW/TL)+RKN((ZL+ZI)/SW/TL)
RKN0=RKN((ZL-ZID)/SWD/TLD)+RKN((ZL+ZID)/SWD/TLD)
ELSEIF((ZL-ZI).EQ.0.0) THEN
RKN0=RKN(HCS/FIS2/SW/TL)+RKN((ZL+ZI)/SW/TL)
RKN0=RKN((ZL-ZID)/SWD/TLD)+RKN((ZL+ZID)/SWD/TLD)
ELSEIF((ZL-ZID).EQ.0.0) THEN
RKN0=RKN((ZL-ZI)/SW/TL)+RKN((ZL+ZI)/SW/TL)
RKN0=RKN(HCS/FIS2/SW/TL)+RKN((ZL+ZID)/SWD/TLD)
ENDIF
SSUM4=SSUM4+(DSK(NPR, NK, 4)/SW*RKN0+ &
DSK(NPR, NK+1, 4)/SWD*RKN0)/2./FIS2*HCS
SSUM5=SSUM5+(DSK(NPR, NK, 5)/SW*RKN0+ &
DSK(NPR, NK+1, 5)/SWD*RKN0)/2./FIS2*HCS
SSUM8=SSUM8+(DSK(NPR, NK, 8)/SW*RKN0+ &
DSK(NPR, NK+1, 8)/SWD*RKN0)/2./FIS2*HCS
SSUM9=SSUM9+(DSK(NPR, NK, 9)/SW*RKN0+ &
DSK(NPR, NK+1, 9)/SWD*RKN0)/2./FIS2*HCS
ENDDO
ENDIF
ENDIF OPTIMISE2
SUM1=0.; SUM2=0; SUM3=0.; SUM4=0.; SUM1A=0.; SUM5=0.; SUM8=0.; SUM9=0.; SUM1B=0.
OPTIMISE3: IF(IOPT.EQ.1) THEN
IF(NPR.EQ.1) THEN
DO NK=0, IS2
ZN=ZL+FLOAT(NK)*(ZREF-ZL)/FIS2

```

```

IF(ZN.EQ.ZPR(IS4)) THEN ! TOP HEIGHT
  DO L=4,7
    K=L
    IF(L.EQ.6) K=8
    IF(L.EQ.7) K=9
    EPS=0.001*ABS(AK(K))
    DFK(3,NK,K)=(EFLUX1(K,IS4)-eflux2(K,IS4))/2./EPS
    DFK(2,NK,K)=(HFLUX1(K,IS4)-Hflux2(K,IS4))/2./EPS
    DFK(1,NK,K)=(CFLUX1(K,IS4)-Cflux2(K,IS4))/2./EPS
    DFK(4,NK,K)=(C13FLUX1(K,IS4)-C13flux2(K,IS4))/2./EPS
    DFK(5,NK,K)=(O18FLUX1(K,IS4)-O18flux2(K,IS4))/2./EPS
  ENDDO
ELSEIF(ZN.GT.ZPR(IS4).OR.ZN.LT.ZPR(0)) THEN ! ZN OUTSIDE RANGE OF FLUX CALCULATIONS
  STOP 'ZN NOT IN RANGE DERIV CALC'
ENDIF
DO J=0,IS4-1 ! FIND FLUX DERIVS FROM Z=Zi TO Z=ZREF
  IF(ZN.EQ.ZPR(J)) THEN ! IF FLUX ALREADY CALCULATED FOR Zi, EASY
    DO L=4,7
      K=L
      IF(L.EQ.6) K=8
      IF(L.EQ.7) K=9
      EPS=0.001*ABS(AK(K)) ! FLUX DERIV WRT AK(K), K=4,10
      DFK(3,NK,K)=(EFLUX1(K,J)-eflux2(K,J))/2./EPS
      DFK(2,NK,K)=(HFLUX1(K,J)-Hflux2(K,J))/2./EPS
      DFK(1,NK,K)=(CFLUX1(K,J)-Cflux2(K,J))/2./EPS
      DFK(4,NK,K)=(C13FLUX1(K,J)-C13flux2(K,J))/2./EPS
      DFK(5,NK,K)=(O18FLUX1(K,J)-O18flux2(K,J))/2./EPS
    ENDDO
  ELSEIF(ZN.LT.ZPR(J+1).AND.ZN.GT.ZPR(J)) THEN ! OTHERWISE CALCULATE EXTRA FLUX FROM
    ZR=ZPR(J)+(ZN-ZPR(J))*FIS4 ! HEIGHT WE HAVE TO HEIGHT WE WANT
    DO L=4,7
      K=L
      IF(L.EQ.6) K=8
      IF(L.EQ.7) K=9
      EPS=0.001*ABS(AK(K))
      AKE=AK
      AKE(k)=AKE(k)+EPS
      CALL CALCE(APROFALL(:,3:4,IT),SPROFALL(:,7:9,IT),PARAM, &
        FD(ICN(IT)),PAR(ICN(IT)),SWDREF(IT),LWDREF(IT), &
        DTIME(ICN(IT)),APRESS(ICN(IT)),CKALL(:, :, IT),XPROF, &
        SREF(1,IT),ake,hcs,CFLUX,eflux,is4,ZPR(J),ZR,HFLUX, &
        C13FLUX,O18FLUX,H18FLUX,UHREF,ZOUT,1)
      EFL1=EFLUX(1)+EFLUX1(K,J); CFL1=CFLUX(1)+CFLUX1(K,J); HFL1=HFLUX(1)+HFLUX1(K,J)
      C13FL1=C13FLUX(1)+C13FLUX1(K,J); O18FL1=O18FLUX(1)+O18FLUX1(K,J)
      AKE=AK
      AKE(k)=AKE(k)-EPS
      CALL CALCE(APROFALL(:,3:4,IT),SPROFALL(:,7:9,IT),PARAM, &
        FD(ICN(IT)),PAR(ICN(IT)),SWDREF(IT),LWDREF(IT), &
        DTIME(ICN(IT)),APRESS(ICN(IT)),CKALL(:, :, IT),XPROF, &
        SREF(1,IT),ake,hcs,CFLUX,eflux,is4,ZPR(J),ZR,HFLUX, &
        C13FLUX,O18FLUX,H18FLUX,UHREF,ZOUT,1)
      EFL2=EFLUX(1)+EFLUX2(K,J); CFL2=CFLUX(1)+CFLUX2(K,J); HFL2=HFLUX(1)+HFLUX2(K,J)
      C13FL2=C13FLUX(1)+C13FLUX2(K,J); O18FL2=O18FLUX(1)+O18FLUX2(K,J)
      DFK(3,NK,K)=(EFL1-efl2)/2./EPS
      DFK(2,NK,K)=(HFL1-Hf12)/2./EPS
      DFK(1,NK,K)=(CFL1-Cf12)/2./EPS
      DFK(4,NK,K)=(C13FL1-C13f12)/2./EPS
      DFK(5,NK,K)=(O18FL1-O18f12)/2./EPS
      AKE=AK
    ENDDO
  ENDDO
ENDIF
ENDIF OPTIMISE3
IF(IDIS.EQ.0) THEN

```

```

DO NK=0, IS2-1
  ZN=ZL+FLOAT(NK)*(ZREF-ZL)/FIS2
  ZND=ZN+(ZREF-ZL)/FIS2
  IF (NUMK.NE.54) THEN
    CALL TURB2(USTARR, SIGWR, AK(6), AK(7), ZN, ZMON, SWZ, TLZ)
    CALL TURB2(USTARR, SIGWR, AK(6), AK(7), ZND, ZMON, SWZD, TLZD)
  ELSEIF (NUMK.EQ.54) THEN
    CALL TURB2(USTARR, SIGWR, TL1(IT), TL2(IT), ZN, ZMON, SWZ, TLZ)
    CALL TURB2(USTARR, SIGWR, TL1(IT), TL2(IT), ZND, ZMON, SWZD, TLZD)
  ENDIF
  IF (NK.LT.IS2) THEN      ! INTEGRATE FLUX DERIVS FROM Z=Zi TO Z=ZREF
    SUM1=SUM1+(1./SWZ**2/TLZ+1./SWZD**2/TLZD)/2./FIS2*(ZREF-ZL)
    SUM1A=SUM1A+(D13RESP/1000./SWZ**2/TLZ+D13RESP/1000./SWZD**2/TLZD)/2./FIS2*(ZREF-ZL)
    SUM1B=SUM1B+(D18RESP/1000./SWZ**2/TLZ+D18RESP/1000./SWZD**2/TLZD)/2./FIS2*(ZREF-ZL)
    SUM2=SUM2+(1./SWZ**2/TLZ+1./SWZD**2/TLZD)/2./FIS2*(ZREF-ZL)
    SUM3=SUM3+(1./SWZ**2/TLZ+1./SWZD**2/TLZD)/2./FIS2*(ZREF-ZL)
    SUM4=SUM4+(DFK(NPR, NK, 4)/SWZ**2/TLZ+DFK(NPR, NK+1, 4)/SWZD**2/TLZD)/2./FIS2*(ZREF-ZL)
    SUM5=SUM5+(DFK(NPR, NK, 5)/SWZ**2/TLZ+DFK(NPR, NK+1, 5)/SWZD**2/TLZD)/2./FIS2*(ZREF-ZL)
    SUM8=SUM8+(DFK(NPR, NK, 8)/SWZ**2/TLZ+DFK(NPR, NK+1, 8)/SWZD**2/TLZD)/2./FIS2*(ZREF-ZL)
    SUM9=SUM9+(DFK(NPR, NK, 9)/SWZ**2/TLZ+DFK(NPR, NK+1, 9)/SWZD**2/TLZD)/2./FIS2*(ZREF-ZL)
  ENDIF
ENDDO
ENDIF

DCKALL(1, N, 1, IT)=SUM1      ! CONC DERIVS = INT(SOURCE DERIV) + INT(FLUX DERIV) - dC(ZREF)/da
DCKALL(2, N, 2, IT)=SUM2
DCKALL(3, N, 3, IT)=SUM3
DCKALL(4, N, 1, IT)=SUM1A
DCKALL(5, N, 1, IT)=SUM1B
DCKALL(NPR, N, 4, IT)=SSUM4+SUM4-RSUM4(npr)
DCKALL(NPR, N, 5, IT)=SSUM5+SUM5-RSUM5(npr)
DCKALL(NPR, N, 8, IT)=SSUM8+SUM8-RSUM8(npr)
DCKALL(NPR, N, 9, IT)=SSUM9+SUM9-RSUM9(npr)
DFKTOP(1:3, IT, 1:2)=DFK(1:3, NK, 4:5)
DFKTOP(1:3, IT, 5:6)=DFK(1:3, NK, 8:9)
ENDDO
ENDDO

DO NPR=1, 3
  DFK(NPR, :, NPR)=1.
ENDDO
DFK(4, :, 1)=D13RESP/1000.
DFK(5, :, 1)=D18RESP/1000.

IF (IDIS.EQ.1) THEN
DO N=1, NUMLEV
DO NPR=1, 5
  DO L=1, 7
    K=L
    IF (L.EQ.6) K=8
    IF (L.EQ.7) K=9
    ASUM=0.
    DO I=1, IS3
      ASUM=ASUM+DISC(N, I)*DSK(NPR, I, K)*(ZSOU(I)-ZSOU(I-1))
    ENDDO
    ASUM=ASUM+DISC(N, 0)*DFK(NPR, 0, K)*ZSOU(1)
    DCKALL(NPR, N, K, IT)=ASUM
  ENDDO
ENDDO
ENDDO
ENDIF

IF (ISOTOPES.GT.1) THEN
DO K=1, NUMAK
  DCKALL(4, :, K, IT)=DCKALL(4, :, K, IT)/CKALL(1, :, IT)/RSTD*1000. - &
  CKALL(4, :, IT)/CKALL(1, :, IT)**2/RSTD*1000.*DCKALL(1, :, K, IT)

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      DCKALL(5, :, K, IT) = DCKALL(5, :, K, IT) / CKALL(1, :, IT) / R18STD * 1000. - &
      CKALL(5, :, IT) / CKALL(1, :, IT) ** 2 / R18STD * 1000. * DCKALL(1, :, K, IT)
      ENDDO
      ENDIF

      ENDDO TENLOOPS4

      CALL TURB2(USTARR, SIGWR, AK(6), AK(7), ZREF, ZMON, SWTOP, TLTOP)
      DCKD(:, :, 1:3, :) = DCKALL(:, :, 1:3, :)
      DCKALL(:, :, 1:6, :) = DCKALL(:, :, 4:9, :)
      DCKALL(:, :, 7:9, :) = 0.
      DCKALL(:, :, 3:4, :) = DCKD(:, :, 6:7, :)
      DO IT=0, NUMISO-1
        DCKALL(:, :, 7+IT*3:9+IT*3, IT+1) = DCKD(:, :, 1:3, IT+1)
        DFKTOP(:, IT+1, 7+IT*3:9+IT*3) = 1.
      ENDDO
      IF (IOPT.EQ.0) THEN
        DCKALL(:, :, 1:30, :) = DCKALL(:, :, 7:36, :)
      ENDIF
      IF (NUMK.EQ.35) THEN ! NO TL1
        DCKALL(:, :, 3:35, :) = DCKALL(:, :, 4:36, :)
        DFKTOP(:, :, 3:35) = DFKTOP(:, :, 4:36)
      ELSEIF (NUMK.EQ.33) THEN
        DCKALL(:, :, 1, :) = DCKALL(:, :, 2, :); DCKALL(:, :, 2:3, :) = DCKALL(:, :, 4:5, :)
        DCKALL(:, :, 4:33, :) = DCKALL(:, :, 7:36, :)
      ELSEIF (NUMK.EQ.34) THEN ! NO TL1, NO VM
        DCKALL(:, :, 3:35, :) = DCKALL(:, :, 4:36, :)
        DCKALL(:, :, 1:34, :) = DCKALL(:, :, 2:35, :)
        DFKTOP(:, :, 3:35) = DFKTOP(:, :, 4:36)
        DFKTOP(:, :, 1:34) = DFKTOP(:, :, 2:35)
      ELSEIF (NUMK.EQ.54) THEN ! OPTIMISE TL1 AND TL2 FOR EACH PROFILE SET SEPARATELY
        DCKALL(:, :, 3:4, :) = DCKALL(:, :, 5:6, :)
        DCKALL(:, :, 25:54, :) = DCKALL(:, :, 7:36, :)
        DCKALL(:, :, 5:24, :) = 0.
        DO IT=1, 10
          DCKALL(:, :, 3+IT*2:4+IT*2, IT) = DCKD(:, :, 6:7, IT)
        ENDDO
      ENDIF

      IF (IA.EQ.1) DCKEALL = DCKALL

808 DO J=1, NUMK
      DO K=1, NUMK
        DSUM=0.
        TENLOOPS5: DO IT=1, NUMISO
          DO N=1, NUMLEV
            DO NPR=1, 3
              DSUM = DSUM + DCKALL(NPR, N, J, IT) * DCKALL(NPR, N, K, IT) / SIG(NPR, N) ** 2
            ENDDO
            IF (ISOTOPE.S.GT.1) THEN
              DSUM = DSUM + DCKALL(4, N, J, IT) * DCKALL(4, N, K, IT) / SIG(4, N) ** 2
            ENDIF
            IF (ISOTOPE.S.GT.2) THEN
              DSUM = DSUM + DCKALL(5, N, J, IT) * DCKALL(5, N, K, IT) / SIG(5, N) ** 2
            ENDIF
          ENDDO
        ENDDO TENLOOPS5
        HESS(J, K) = DSUM ! RETAIN HESSIAN MATRIX
        DO N=1, NUMLEV
          IF (IOPT.EQ.1) THEN
            IF (NUMK.NE.54) THEN
              IF (J.EQ.1.AND.K.EQ.1) THEN
                DSUM = DSUM + 1. / SVM ** 2
              ELSEIF (J.EQ.2.AND.K.EQ.2) THEN
                DSUM = DSUM + 1. / SALAM ** 2
              ENDIF
            ENDIF
          ENDIF
        ENDDO
      ENDDO
    ENDDO
  ENDDO

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ELSEIF(J.EQ.3.AND.K.EQ.3) THEN
  DSUM=DSUM+1./STLP1**2
ELSEIF(J.EQ.4.AND.K.EQ.4) THEN
  DSUM=DSUM+1./STLP2**2
ELSEIF(J.EQ.5.AND.K.EQ.5) THEN
  DSUM=DSUM+1./SKDF**2
ELSEIF(J.EQ.6.AND.K.EQ.6) THEN
  DSUM=DSUM+1./SKBF**2
ENDIF
ELSEIF(NUMK.EQ.54) THEN
IF(J.EQ.1.AND.K.EQ.1) THEN
  DSUM=DSUM+1./SVM**2
ELSEIF(J.EQ.2.AND.K.EQ.2) THEN
  DSUM=DSUM+1./SALAM**2
ELSEIF(J.EQ.3.AND.K.EQ.3) THEN
  DSUM=DSUM+1./SKDF**2
ELSEIF(J.EQ.4.AND.K.EQ.4) THEN
  DSUM=DSUM+1./SKBF**2
ELSEIF(J.EQ.5.AND.K.EQ.5) THEN
  DSUM=DSUM+1./STL1(1)**2
ELSEIF(J.EQ.6.AND.K.EQ.6) THEN
  DSUM=DSUM+1./STL2(1)**2
ELSEIF(J.EQ.7.AND.K.EQ.7) THEN
  DSUM=DSUM+1./STL1(2)**2
ELSEIF(J.EQ.8.AND.K.EQ.8) THEN
  DSUM=DSUM+1./STL2(2)**2
ELSEIF(J.EQ.9.AND.K.EQ.9) THEN
  DSUM=DSUM+1./STL1(3)**2
ELSEIF(J.EQ.10.AND.K.EQ.10) THEN
  DSUM=DSUM+1./STL2(3)**2
ELSEIF(J.EQ.11.AND.K.EQ.11) THEN
  DSUM=DSUM+1./STL1(4)**2
ELSEIF(J.EQ.12.AND.K.EQ.12) THEN
  DSUM=DSUM+1./STL2(4)**2
ELSEIF(J.EQ.13.AND.K.EQ.13) THEN
  DSUM=DSUM+1./STL1(5)**2
ELSEIF(J.EQ.14.AND.K.EQ.14) THEN
  DSUM=DSUM+1./STL2(5)**2
ELSEIF(J.EQ.15.AND.K.EQ.15) THEN
  DSUM=DSUM+1./STL1(6)**2
ELSEIF(J.EQ.16.AND.K.EQ.16) THEN
  DSUM=DSUM+1./STL2(6)**2
ELSEIF(J.EQ.17.AND.K.EQ.17) THEN
  DSUM=DSUM+1./STL1(7)**2
ELSEIF(J.EQ.18.AND.K.EQ.18) THEN
  DSUM=DSUM+1./STL2(7)**2
ELSEIF(J.EQ.19.AND.K.EQ.19) THEN
  DSUM=DSUM+1./STL1(8)**2
ELSEIF(J.EQ.20.AND.K.EQ.20) THEN
  DSUM=DSUM+1./STL2(8)**2
ELSEIF(J.EQ.21.AND.K.EQ.21) THEN
  DSUM=DSUM+1./STL1(9)**2
ELSEIF(J.EQ.22.AND.K.EQ.22) THEN
  DSUM=DSUM+1./STL2(9)**2
ELSEIF(J.EQ.23.AND.K.EQ.23) THEN
  DSUM=DSUM+1./STL1(10)**2
ELSEIF(J.EQ.24.AND.K.EQ.24) THEN
  DSUM=DSUM+1./STL2(10)**2
ENDIF
ENDIF
ENDIF
ENDDO
IF(IEDDY.EQ.1) THEN
  TENLOOPS6: DO IT=1,NUMISO
    SIGFC=ABS(0.05*FC2(ICN(IT))*VOLM) ! SIGMA OF TOTAL C FLUX
    SIGFH=ABS(0.1*H(ICN(IT))/CAPP/RHO) ! SIGMA OF TOTAL H FLUX
  
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      SIGFE=ABS(0.1*E(ICN(IT))*VOLM) ! SIGMA OF TOTAL E FLUX
      DSUM = DSUM + DFKTOP(1,IT,J)*DFKTOP(1,IT,K)/SIGFC**2
      DSUM = DSUM + DFKTOP(2,IT,J)*DFKTOP(2,IT,K)/SIGFH**2
      DSUM = DSUM + DFKTOP(3,IT,J)*DFKTOP(3,IT,K)/SIGFE**2
      ENDDO TENLOOPS6
    ENDIF
    IF(J.EQ.K) THEN
      ! ALPHA(J,K) = SUM( dC/dAj * dC/dAk)/SIGMA^2
      ALP(J,K)=DSUM*(1.+RL) ! *(1 + LAMBDA) ON DIAGONALS
    ELSE
      ALP(J,K)=DSUM
    ENDIF
  ENDDO
  DSUM=0.
  TENLOOPS7: DO IT=1,NUMISO
  DO NPR=1,3
    DO N=1,NUMLEV
      IF(DCKALL(NPR,N,J,IT).NE.0.) THEN
        DSUM=DSUM+(-CKALL(NPR,N,IT)+SPROFALL(N,NPR,IT))*DCKALL(NPR,N,J,IT)/SIG(NPR,N)**2
      ENDIF
    ENDDO
  ENDDO
  ENDDO TENLOOPS7
  DO N=1,NUMLEV
    ZAH=FLOAT(N)/FLOAT(NUMLEV)
    TENLOOPS8: DO IT=1,NUMISO
    IF(ISOTOPE.S.GT.1) THEN
      C13K=(CKALL(4,N,IT)/CKALL(1,N,IT)/RSTD-1.)*1000.
      DSUM=DSUM+(-C13K+APROFALL(N,1,IT))*DCKALL(4,N,J,IT)/SIG(4,N)**2
    ENDIF
    IF(ISOTOPE.S.GT.2) THEN
      O18K=(CKALL(5,N,IT)/CKALL(1,N,IT)/R18STD-1.)*1000.
      DSUM=DSUM+(-O18K+APROFALL(N,2,IT))*DCKALL(5,N,J,IT)/SIG(5,N)**2
    ENDIF
  ENDDO TENLOOPS8
  IF(IOPT.EQ.1) THEN
    IF(NUMK.NE.54) THEN
      IF(J.EQ.1) THEN
        DSUM=DSUM+(-AK(4)+VM)/SVM**2
      ELSEIF(J.EQ.2) THEN
        DSUM=DSUM+(-AK(5)+ALAM)/SALAM**2
      ELSEIF(J.EQ.3) THEN
        DSUM=DSUM+(-AK(6)+TLP1)/STLP1**2
      ELSEIF(J.EQ.4) THEN
        DSUM=DSUM+(-AK(7)+TLP2)/STLP2**2
      ELSEIF(J.EQ.5) THEN
        DSUM=DSUM+(-AK(8)+KDF)/SKDF**2
      ELSEIF(J.EQ.6) THEN
        DSUM=DSUM+(-AK(9)+KBF)/SKBF**2
      ENDIF
    ELSEIF(NUMK.EQ.54) THEN
      IF(J.EQ.1) THEN
        DSUM=DSUM+(-AK(4)+VM)/SVM**2
      ELSEIF(J.EQ.2) THEN
        DSUM=DSUM+(-AK(5)+ALAM)/SALAM**2
      ELSEIF(J.EQ.3) THEN
        DSUM=DSUM+(-AK(8)+KDF)/SKDF**2
      ELSEIF(J.EQ.4) THEN
        DSUM=DSUM+(-AK(9)+KBF)/SKBF**2
      ELSEIF(J.EQ.5) THEN
        DSUM=DSUM+(-TL1(1)+TLP1)/STL1(1)**2
      ELSEIF(J.EQ.6) THEN
        DSUM=DSUM+(-TL2(1)+TLP2)/STL2(1)**2
      ELSEIF(J.EQ.7) THEN
        DSUM=DSUM+(-TL1(2)+TLP1)/STL1(2)**2
      ELSEIF(J.EQ.8) THEN
        DSUM=DSUM+(-TL2(2)+TLP2)/STL2(2)**2
    ENDIF
  ENDIF

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ELSEIF(J.EQ.9) THEN
  DSUM=DSUM+(-TL1(3)+TLP1)/STL1(3)**2
ELSEIF(J.EQ.10) THEN
  DSUM=DSUM+(-TL2(3)+TLP2)/STL2(3)**2
ELSEIF(J.EQ.11) THEN
  DSUM=DSUM+(-TL1(4)+TLP1)/STL1(4)**2
ELSEIF(J.EQ.12) THEN
  DSUM=DSUM+(-TL2(4)+TLP2)/STL2(4)**2
ELSEIF(J.EQ.13) THEN
  DSUM=DSUM+(-TL1(5)+TLP1)/STL1(5)**2
ELSEIF(J.EQ.14) THEN
  DSUM=DSUM+(-TL2(5)+TLP2)/STL2(5)**2
ELSEIF(J.EQ.15) THEN
  DSUM=DSUM+(-TL1(6)+TLP1)/STL1(6)**2
ELSEIF(J.EQ.16) THEN
  DSUM=DSUM+(-TL2(6)+TLP2)/STL2(6)**2
ELSEIF(J.EQ.17) THEN
  DSUM=DSUM+(-TL1(7)+TLP1)/STL1(7)**2
ELSEIF(J.EQ.18) THEN
  DSUM=DSUM+(-TL2(7)+TLP2)/STL2(7)**2
ELSEIF(J.EQ.19) THEN
  DSUM=DSUM+(-TL1(8)+TLP1)/STL1(8)**2
ELSEIF(J.EQ.20) THEN
  DSUM=DSUM+(-TL2(8)+TLP2)/STL2(8)**2
ELSEIF(J.EQ.21) THEN
  DSUM=DSUM+(-TL1(9)+TLP1)/STL1(9)**2
ELSEIF(J.EQ.22) THEN
  DSUM=DSUM+(-TL2(9)+TLP2)/STL2(9)**2
ELSEIF(J.EQ.23) THEN
  DSUM=DSUM+(-TL1(10)+TLP1)/STL1(10)**2
ELSEIF(J.EQ.24) THEN
  DSUM=DSUM+(-TL2(10)+TLP2)/STL2(10)**2
ENDIF
ENDIF
ENDIF
ENDDO
IF(IEDDY.EQ.1) THEN
  TENLOOPS8A: DO IT=1,NUMISO
    SIGFC=ABS(0.05*FC2(ICN(IT))*VOLM) ! SIGMA OF TOTAL C FLUX
    SIGFH=ABS(0.1*H(ICN(IT))/CAPP/RHO) ! SIGMA OF TOTAL H FLUX
    SIGFE=ABS(0.1*E(ICN(IT))*VOLM) ! SIGMA OF TOTAL E FLUX
    DSUM = DSUM + (-FKTOP(1,IT)+FC2(ICN(IT))*VOLM)*DFKTOP(1,IT,J)/SIGFC**2
    DSUM = DSUM + (-FKTOP(2,IT)+H(ICN(IT))/CAPP/RHO)*DFKTOP(2,IT,J)/SIGFH**2
    DSUM = DSUM + (-FKTOP(3,IT)+E(ICN(IT))*VOLM)*DFKTOP(3,IT,J)/SIGFE**2
  ENDDO TENLOOPS8A
ENDIF
BET(J)=DSUM ! BETA(J) = SUM (C_MOD - C_MEAS) * dC/dAj / SIGMA^2
ENDDO

! SOLVE ALP*DAK=BET
IF(IOPT.EQ.0) THEN
  DO J=1,NUMK
    DAK(J)=1./ALP(J,J)*BET(J)
  ENDDO
ELSE
  CALL DLSGRR(NUMK,NUMK,ALP,NUMK,1.E-12,IRANK,AINV,NUMK)
  ! INVERSE OF ALP BY SINGULAR VALUE DECOMPOSITION
  DO K=1,NUMK
    DSUM=0.
    DO J=1,NUMK
      DSUM=DSUM+AINV(K,J)*BET(J)
    ENDDO
    DAK(K)=DSUM
  ENDDO
ENDIF

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ENDIF
AKO=DBLE(AK)      ! KEEP OLD PARAMETERS, ADJUST NEW PARAMS
GFO=GF
TL10=TL1; TL20=TL2
IF(IOPT.EQ.0) THEN
  DO I=1,NUMISO
    GF(:,I)=GF(:,I)+SNGL(DAK(I*3-2:I*3))
  ENDDO
ELSE
  DO I=1,NUMISO
    IF(NUMK.EQ.33) THEN
      GF(:,I)=GF(:,I)+SNGL(DAK(1+I*3:3+I*3))
    ELSEIF(NUMK.EQ.34) THEN
      GF(:,I)=GF(:,I)+SNGL(DAK(2+I*3:4+I*3))
    ELSEIF(NUMK.EQ.35) THEN
      GF(:,I)=GF(:,I)+SNGL(DAK(3+I*3:5+I*3))
    ELSEIF(NUMK.EQ.36) THEN
      GF(:,I)=GF(:,I)+SNGL(DAK(4+I*3:6+I*3))
    ELSEIF(NUMK.EQ.54) THEN
      GF(:,I)=GF(:,I)+SNGL(DAK(22+I*3:24+I*3))
    ENDIF
  ENDDO
  IF(NUMK.NE.54) THEN
    AK(4:9)=AK(4:9)+SNGL(DAK(1:6))
  ELSEIF(NUMK.EQ.54) THEN
    AK(4:5)=AK(4:5)+SNGL(DAK(1:2)); AK(8:9)=AK(8:9)+SNGL(DAK(3:4))
    DO IT=1,10
      TL1(IT)=TL1(IT)+SNGL(DAK(3+IT*2))
      TL2(IT)=TL2(IT)+SNGL(DAK(4+IT*2))
    ENDDO
  ENDIF
  ! AK(5)=AK(5)+SNGL(DAK(1)); AK(7:9)=AK(7:9)+SNGL(DAK(2:4))
ENDIF
EX=0.1
IF (IFLAGC.EQ.1) GOTO 3045

3025 CONTINUE

3045 CONTINUE

AK=SNGL(AKO)
TENLOOPS9: DO IT=1,NUMISO
call air(SREF(2,IT),APRESS(ICN(IT)),rho,volm,capp,rlam,qsat,epsi)
UHREF=UH(ICN(IT))/1.3
USTARR=US(ICN(IT))
SIGWR=SWR(ICN(IT))
AK(1:3)=GF(:,IT)
ZL=0.; ZREF=HCS
CALL CALCS(PARAM,FD(ICN(IT)),PAR(ICN(IT)),DEF,SWDREF(IT), &
LWDREF(IT),DTIME(ICN(IT)),APRESS(ICN(IT)), &
CKALL(:, :, IT),XPROF,SREF(1,IT),ESATL,thet1,RLAI,RC,RH,RNN,ak, &
hcs,cica,CSOURCE,esource,80,HSOURCE,C13SOURCE,O18SOURCE, &
H18SOURCE,UHREF,DRESP,DELTA,DEL18,DEL_E,ZSOU)
DO I=0,40
  SK(1,I)=CSOURCE(I*2)
  SK(2,I)=HSOURCE(I*2)
  SK(3,I)=ESOURCE(I*2)
  SK(4,I)=C13SOURCE(I*2)
  SK(5,I)=O18SOURCE(I*2)
  THETL(I)=THETL(I*2)
  RNN(I)=RNN(I*2)
  RLAI(I)=RLAI(I*2)
  RC(I)=RC(I*2)
  RH(I)=RH(I*2)
  DEF(I)=DEF(I*2)
  DELTA(I)=DELTA(I*2)

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CICA(I)=CICA(I*2)
DEL18(I)=DEL18(I*2)
DEL_E(I)=DEL_E(I*2)
ZSOU(I)=ZSOU(I*2)
ENDDO

CALL CALCE(APROFALL(:,3:4,IT),SPROFALL(:,7:9,IT),PARAM, &
FD(ICN(IT)),PAR(ICN(IT)),SWDREF(IT),LWDREF(IT), &
DTIME(ICN(IT)),APRESS(ICN(IT)),CKALL(:, :, IT),XPROF,SREF(1,IT), &
ak,hcs,CFLUX,eflux,80,ZL,ZREF,HFLUX, &
C13FLUX,O18FLUX,H18FLUX,UHREF,ZPR,0)
DO I=0,40
FK(3,I)=EFLUX(I*2)
FK(2,I)=HFLUX(I*2)
FK(1,I)=CFLUX(I*2)
FK(4,I)=C13FLUX(I*2)
FK(5,I)=O18FLUX(I*2)
ZPR(I)=ZPR(I*2)
ENDDO

DO I=1,40
ZI=ZSOU(I)
CALL INTVAL2(ZI,TEMP,NUML,XPROF(1:NUML),CKALL(2, :, IT))
CALL INTVAL2(ZI+0.1,TEMPD,NUML,XPROF(1:NUML),CKALL(2, :, IT))
TK=TEMP+273.15;TKD=TEMPD+273.15;DELT=(TEMPD-TEMP)/(0.1)
IF(NUMK.NE.54) THEN
CALL TURB2(USTARR,SIGWR,AK(6),AK(7),ZI,ZMON,SWZ,TLZ)
ELSEIF(NUMK.EQ.54) THEN
CALL TURB2(USTARR,SIGWR,TL1(IT),TL2(IT),ZI,ZMON,SWZ,TLZ)
ENDIF
TLPROF(I)=TLZ
ZOBUKHOV(I)=ZMON
ENDDO

CSUM1=0.;CSUM2=0.;CSUM3=0.;CSUM4=0.;CSUM5=0.
DO N=1,NUMLEV ! CALCULATE CHI-SQUARE = SUM (C_MODEL - C_MEAS)^2 / SIGMA^2
CSUM1=CSUM1+(CKALL(1,N,IT)-SPROFALL(N,1,IT))**2/SIG(1,N)**2
CSUM2=CSUM2+(CKALL(2,N,IT)-SPROFALL(N,2,IT))**2/SIG(2,N)**2
CSUM3=CSUM3+(CKALL(3,N,IT)-SPROFALL(N,3,IT))**2/SIG(3,N)**2
IF(ISOTOPE.S.GT.1) THEN
C13K=(CKALL(4,N,IT)/CKALL(1,N,IT)/RSTD-1.)*1000.
CSUM4 = CSUM4 + (C13K-APROFALL(N,1,IT))**2/SIG(4,N)**2
ENDIF
IF(ISOTOPE.S.GT.2) THEN
O18K=(CKALL(5,N,IT)/CKALL(1,N,IT)/R18STD-1.)*1000.
CSUM5 = CSUM5 + (O18K-APROFALL(N,2,IT))**2/SIG(5,N)**2
ENDIF
ENDDO
CHISQ1=CSUM1;CHISQ2=CSUM2;CHISQ3=CSUM3;CHISQ4=CSUM4;CHISQ5=CSUM5

WRITE(*,4036) CHISQ, (AK(K), K=1,9), dresp
do npr=1,3
IF(NPR.EQ.1) THEN
ICP=10; ISP=11; IFP=12; FREF=FC2(ICN(IT)); FAC=1./VOLM
PRINT *, 'CO2:'
ELSEIF(NPR.EQ.2) THEN
ICP=13; ISP=14; IFP=15; FREF=H(ICN(IT)); FAC=RHO*CAPP
WRITE(*,*) 'TEMPERATURE:'
ELSE
ICP=16; ISP=17; IFP=18; FREF=E(ICN(IT)); FAC=1./VOLM
WRITE(*,*) 'H2O:'
ENDIF
FKR=FK(NPR,40)*FAC
IF(IA.GE.ITER-1) THEN
WRITE(*,*) 'ITERATIONS FINISHED'
ELSE

```

```

WRITE(*,*) 'NO MORE IMPROVEMENT IN CHISQ AFTER ',IA,' ITERATIONS'
ENDIF
WRITE(*,*) 'FLUX= ',FKR,'EDDY FLUX= ',FREF
WRITE(TIMDAT,116) day(ICN(IT)),mon,Tthr(ICN(IT)),Ttmin(ICN(IT))
116      format(4x,a2,'-',a3,5x,i2.2,':',i2.2)
write(ICP,4021) timdat
4021  format(a32)
WRITE(ICP,4032) (AK(K),K=1,9)
WRITE(ICP,4034) CHISQ
write(ICP,4031) (xprof(n),cKall(NPR,n,IT),sprofall(n,NPR,IT), N=1, NUMLEV)
write(ICP,*)
4031  format(3f10.2)
4032  FORMAT(14F10.5)
WRITE(ISP,4021) TIMDAT
WRITE(ISP,4033) (ZSOU(I), SK(NPR,I)*FAC, FK(NPR,I)*FAC,THETL(I), I=1,40)
WRITE(ISP,*)
4033  FORMAT(4F10.3)
4034  FORMAT(' CHISQ = ',F8.3)
write(IFP,4035) timdat, FKR,fref,CHISQ
4035  format(a32,2f10.2,F8.2)
4036  FORMAT(' CHISQ = ',F8.3,' A = ',18F8.2)
4037  FORMAT(3F10.3,F10.5,2F10.7,F10.3,F10.2,F10.3,F10.2,F10.3,F10.3,ES10.3,6F10.3)
4038  format(a32)
4039  FORMAT(F10.2,2F10.3)
4040  FORMAT(3F10.3)
4041  FORMAT(A32, 5F10.2,7F8.3,9F10.2,F8.2,F8.3)
4042  FORMAT(20X,20F10.2)
4043  FORMAT(A20,20F10.2)
4044  FORMAT(A20,20F10.3)
4045  FORMAT(F10.2,2F10.5)
4046  FORMAT(2F10.3)
4047  FORMAT(9F10.3)
4048  FORMAT(36ES11.3)
4050  FORMAT(13A10)
IF(NPR.EQ.3) THEN
WRITE(19,4035) TIMDAT,FKR*RLAM*18.015*1.E-6,EREF,CHISQ*RLAM*18.015*1.E-6
ENDIF

ENDDO
write(20,4038) timdat
555 WRITE(20,4050) '      Z', ' LEAF TEMP', ' NET RAD', ' LEAF AREA', &
'      GSC', ' GBH', &
'      DA', ' DELTA', ' CI/CA', ' DELTA180', ' DELTA_E', &
'      TL', ' ZMON'
WRITE(20,4037) (ZSOU(I), THETL(I), RNN(I), RLAI(I),1./RC(I)/volm,1./RH(I),DEF(I), &
DELTA(I), CICA(I), DEL18(I), DEL_E(I),TLPROF(I)*SIGWR/1.27/HCS, &
ZOBUKHOV(I),SK(1,I)/VOLM,FK(1,I)/VOLM, &
SK(2,I)/VOLM,FK(2,I)/VOLM, SK(3,I)*RHO*CAPP,FK(3,I)*RHO*CAPP, I=0,40)
write(20,*)
IF(ISOTOPES.GE.1) THEN
WRITE(21,*)
WRITE(21,*)
WRITE(21,*)
WRITE(21,4021) TIMDAT
WRITE(21,4040) (XPROF(N), (CKALL(4,N,IT)/CKALL(1,N,IT)/RSTD-1.)*1000., &
APROFALL(N,1,IT),N=1,NUMLEV)
WRITE(22,4021) TIMDAT
WRITE(22,4039) (ZSOU(I), SK(4,I)/VOLM,FK(4,I)/VOLM, I=1,40)
WRITE(22,*)
WRITE(28,*)
WRITE(28,*)
WRITE(28,*)
WRITE(28,4021) TIMDAT
WRITE(28,4040) (XPROF(N), (CKALL(5,N,IT)/CKALL(1,N,IT)/R18STD-1.)*1000., &
APROFALL(N,2,IT),N=1,NUMLEV)
WRITE(29,4021) TIMDAT

```

```

WRITE(29,4045) (ZSOU(I), SK(5,I)/VOLM,FK(5,I)/VOLM, I=1,40)
WRITE(29,*)
WRITE(30,*)
WRITE(30,*)
WRITE(30,*)
WRITE(30,4021) TIMDAT
WRITE(30,4046) (XPROF(N), (CKALL(6,N,IT)/CKALL(3,N,IT)/SMOW-1.)*1000., N=1, NUMLEV)
ENDIF
WRITE(*,*) 'ZMON= ', ZMON
CALL INTVAL(28., 28., TEMP, CO2, H2O,NLEVL,ZZZ,PROF,28., 20, ICN(IT))
ESAT=6.1375*EXP(17.502*TEMP/(240.97+TEMP))
SL=17.502*240.97/(240.97+TEMP)**2*esat
s1=0.622*pmb/(pmb-0.378*esat)**2*s1
ep=rlam/cApp*s1
eqg=ep*rnn(0)*.9/(ep+1.)
WRITE(23, 4041) TIMDAT, AK(1)/VOLM, AK(2)*CAPP*RHO, AK(3)/VOLM, &
  eqg, AK(3)/VOLM*RLAM*18.015*1.E-6, EP, ak(4), AK(5), AK(6), AK(7), ak(8), ak(9), &
  CHISQ, CHISQ1, CHISQ2, CHISQ3, CHISQ4, CHISQ5, dresp, TL1(IT), TL2(IT)
IF (IX.EQ.1) THEN
  WRITE(24,4042) xprof
  WRITE(25,4042) XPROF
  WRITE(26,4042) XPROF
  WRITE(27,4042) XPROF
  IX=0
ENDIF
WRITE(24, 4043) TIMDAT, CK(1,1:NUMLEV)
WRITE(24, 4043) TIMDAT, SPROF(1:NUMLEV,1)
WRITE(25, 4043) TIMDAT, CK(2,1:NUMLEV)
WRITE(25, 4043) TIMDAT, SPROF(1:NUMLEV,2)
WRITE(26, 4043) TIMDAT, CK(3,1:NUMLEV)
WRITE(26, 4043) TIMDAT, SPROF(1:NUMLEV,3)
IF (ISOTOPES.GE.1) THEN
  WRITE(27, 4044) TIMDAT, ((CKALL(4,N,IT)/CKALL(1,N,IT)/RSTD-1.)*1000., N=1, NUMLEV)
  WRITE(27, 4044) TIMDAT, APROFALL(1:NUMLEV,1,IT)
ENDIF
ENDDO TENLOOPS9

WRITE(*,*) (ak(n), n=1,9)
IF (ICOSTFN.EQ.1) THEN
  WRITE(31, 4047) (COSTFN(ICOST-1,1,N), N=1,9)
  WRITE(31, 4047) (COSTFN(ICOST-1,2,N), N=1,9)
  WRITE(31, 4047) (COSTFN(ICOST-1,3,N), N=1,9)
ELSEIF (ICOSTFN.EQ.2) THEN
! INVERT HESSIAN MATRIX
CALL DLSGRR(NUMK, NUMK, HESS, NUMK, 1.E-12, IRANK, AINV, NUMK)
! INVERSE OF HESS BY SINGULAR VALUE DECOMPOSITION
DO K=1, numk
  WRITE(31, 4048) (AINV(J,K), J=1, numk)
ENDDO
  WRITE(31, *) IRANK
ENDIF

10000 end do !end reading control file

450 stop

460 stop 'error reading CO2 data'
480 stop 'error reading Temperature data'
490 stop 'error reading Vap press data'
500 stop 'error reading Flux data'
510 stop 'error reading SIGC data'
520 stop 'error reading SIGH data'
530 stop 'error reading SIGT data'

4 STOP
540 STOP 'CHISQ NaN'

```

END

G.1.2 Ground flux optimisation

The following Fortran 90 code is modified from that given in §G.1.1 to optimise only ground fluxes for the 10 day period from 21-30 May 2000.

```

PROGRAM GROUNDFLUX

! Modified from program CANMOD to optimise only ground fluxes
! Subroutines used
!   comskp      (sousub15.for) skip comments in data input file
!   air         (sousub15.for) calculate latent ht vap, RHO, CP, VOLM
!   turb2       (sousub15.for) calculate sigw and TL
!   dispm2      (sousub15.for) calculate dispersion matrix
!   integr      (sousub15.for) integrate a function
!   shsor2      (sousub15.for) sort profiles into ascending order
!   phi         (sousub15.for) calculate phi for stability correction
!   interp      (sousub15.for) interpolate concentration profiles
!   intval      (sousub15.for) calculate interpolated value
!   calce       (sousub15.for) calculate flux profiles
!   calcs       (sousub15.for) calculate source profiles
!   assim       (sousub15.for) calculate leaf level fluxes

PARAMETER(MMAX=20,NMAX=40,numfiles=308,NUML=20,NUMP=9,IFMAX=1000, ISMAX=1000, &
          NUMK=3,NISO=16,NUMAK=36,IDMAX=400)

! NUML=NUMBER OF CONCENTRATION LEVELS TO BE USED FROM SPLINE INTERPOLATION
! NUMP=NUMBER OF SCALAR INPUT PROFILES
! SOURCE ARRAYS, DIMENSION 0:M WHERE M IS NUMBER OF SOURCE LEVELS,
! Z=HEIGHT OF TOP OF SOURCE LAYERS; ZS=HEIGHT OF MIDDLE OF SOURCE LAYERS;
! DZ=WIDTH OF SOURCE LAYERS
! SA,SH,SE,SC = OUTPUT SOURCES; FA,FH,FE,FC = OUTPUT FLUXES
! DIS,DISN,DISF = DISPERSION MATRICES
! T,Q,EV,CC,CA,CH,CE = PROFILES INPUT TO MODEL (AFTER INTERPOLATION)
! ZC NO LONGER USED

      REAL, DIMENSION(:),ALLOCATABLE :: Z,ZS,DZ,FA,SA, &
          FH,SH,FE,SE,FC,SC,HH,BBADD
      REAL, DIMENSION(:,:), ALLOCATABLE :: DIS,DISN,DISF
      REAL, DIMENSION(:), ALLOCATABLE :: T,Q,EV,CC,CA,CH,CE,BB
      REAL*8, DIMENSION(:), ALLOCATABLE :: AA,AAL
      integer, dimension(:), allocatable :: IP
      REAL, DIMENSION(:,:), ALLOCATABLE :: ZC
      REAL A1,AH,AO,CCH,CCO,ALFAA,ALFAB,ALFAC,HC,SWREF,USREF
      COMMON /T/ ITURB,A1,AH,AO,CCH,CCO,alfaa,alfab,ALFAC, &
          HC,SWREF,USREF,IST_COR

      character mon*3,day(numfiles)*2,timdat*32
      character*60 exptnam,filenam,path_IP,path_OP
      character*90 path_file_IP,outfila,outfiles,outdmtx

!   arrays needed for profile and flux data for "numfiles" half-hrs
      character*8                                & !time & date
      Ttdate(numfiles),VPdate(numfiles),C2date(numfiles), &
      Fxdate(numfiles),SIGCDAT(NUMFILES),SIGHDAT(NUMFILES), &
      SIGTDAT(NUMFILES),D13DAT(NISO)

      integer Tthr(numfiles),Ttmin(numfiles),VPhr(numfiles), &

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        VPmin(numfiles),C2hr(numfiles),C2min(numfiles), &
        Fxhr(numfiles),Fxmin(numfiles),SIGCHR(NUMFILES),SIGCMIN(NUMFILES), &
        SIGHHR(NUMFILES),SIGHMIN(NUMFILES),SIGTHR(NUMFILES),SIGTMIN(NUMFILES),&
        D13HR(NISO),D13MIN(NISO),NLI(NISO),nday(numfiles),ISN(10),ICN(10)
common /timx/ Tthr,Ttmin,VPhr,VPmin,C2hr,C2min, Fxhr,Fxmin
integer timm(numfiles,10)
equivalence (timm,Tthr)

! Ttz,VPz,C2z = ORIGINAL HEIGHTS OF INPUT PROFILES
! ZZZ = INCORPORATES ORIGINAL HEIGHTS OF ALL SCALAR PROFILES INTO ONE MATRIX AFTER SORTING
! NLEVL = ORIGINAL NUMBER OF LEVELS FOR PROFILE DATA
! X,Y = HEIGHTS AND PROFILES AFTER INTERPOLATION
! XPROF=X
! Tt,VP,C2 = ORIGINAL INPUT PROFILES
! PROF = INCORPORATES ALL ORIGINAL PROFILES INTO ONE MATRIX AFTER SORTING
! PRAF = DUMMY MATRIX FOR SORTING
! SPROF = ALL PROFILES AFTER INTERPOLATION IN ONE MATRIX

        REAL, DIMENSION(:), ALLOCATABLE :: Ttz, VPz, C2z, za,B,C13Z,O18Z
        REAL, DIMENSION(:,:), ALLOCATABLE :: ZZZ,C13ZZ
        integer nlevl(11),nref(11)      !number of levels for each scalar
        REAL ZREF,Y(NUML),X(NUML),XPROF(NUML),NEWZ,NEWPROF

        REAL, DIMENSION(:,:), ALLOCATABLE :: Tt, VP, C2, PRAF,SPROF,F,SIGC,SIGH,SIGT,dcdt,&
        DHDT,DTDT,D13C,D18O
        REAL, DIMENSION(:,:,:), ALLOCATABLE :: PROF
        REAL*8 RL, DTIME(NUMFILES)

        real H(numfiles),E(numfiles),FC2(numfiles),zMonU(numfiles),us(numfiles),swr(numfiles), &
        LE(numfiles),RN(numfiles),Uh(numfiles), APRESS(NUMFILES),PAR(NUMFILES), fd(numfiles), &
        SWDR(NUMFILES),LWDR(NUMFILES),LZMON,LMON(NUMFILES)
        common /flxx/ H,E,FC2,sgw,us,ur
        real flxx(numfiles,7)
        equivalence (flxx,H)

! ARRAYS FOR ALTERNATIVE MODEL USING BETA FUNCTION TO CONSTRAIN SOURCE AND FLUX PROFILES
        REAL SK(6,0:ISMAX),FK(6,0:IFMAX),DSK(5,0:IDMAX+1,NUMAK),PARAM(5),&
        CD(NUML),SREF(6),THETL(0:ISMAX), ESATL(0:ISMAX),DUMMY(NUML),DEF(0:ISMAX), &
        DELTA(0:ISMAX),CICA(0:ISMAX),DEL18(0:ISMAX),RAIR(10), &
        SWDREF(10), LWDR(10),TLPROF(0:ISMAX),ZOBUKHOV(0:ISMAX)
        REAL AK(NUMAK),ake(NUMAK), AKO(NUMAK),GF(3,10),GFO(3,10),GFE(3,10)
        REAL CK(6,NUML),CKO(6,NUML), CKK(6,NUML),CKKK(6,NUML), CKE(6,NUML), &
        SIGCO2(NUML), SIGH20(NUML),SIGTEMP(NUML),SIG13C(NUML),SIG180(NUML), &
        SIG(5,NUML),SIGO(5,NUML)
        REAL SPROFALL(NUML,9,10),DCKALL(5,NUML,NUMAK,10),CKALL(6,NUML,10), &
        DCKEALL(5,NUML,NUMAK,10),DCKOALL(5,NUML,NUMAK,10),CKEALL(6,NUML,10), &
        CKOALL(6,NUML,10),CKKALL(6,NUML,10),DCKD(5,NUML,NUMAK),DFKTOP(3,NUMAK),FKTOP(3), &
        SPROFD(NUML),APROFC(NUML),APROFO(NUML), SPROFP(NUML), APROFCP(NUML), APROFOP(NUML)
        REAL DFK(5,0:IDMAX+1,NUMAK),DCK(5,NUML,NUMAK),FKS(6,0:ISMAX), &
        esource(0:ISMAX),ESOURCE2(0:ISMAX),&
        HSOURCE(0:ISMAX),HFLUX(0:IFMAX),HSOURCE2(0:ISMAX),eflux(0:IFMAX), CFLUX(0:IFMAX), &
        CFLUX1(NUMAK,0:IFMAX),CFLUX2(NUMAK,0:IFMAX),CSOURCE(0:ISMIX), &
        CSOURCE2(0:ISMIX),ZPR(0:IFMAX), &
        EFLUX1(NUMAK,0:IFMAX),EFLUX2(NUMAK,0:IFMAX), &
        HFLUX1(NUMAK,0:IFMAX),HFLUX2(NUMAK,0:IFMAX), EFLUXD(0:IFMAX), &
        CFLUXD(0:IFMAX),HFLUXD(0:IFMAX), &
        THETLE(0:ISMIX),ZOUT(IFMAX),C13FLUX(0:IFMAX),C13FLUXD(0:IFMAX),C13SOURCE(0:ISMIX), &
        RLAI(0:ISMIX),RC(0:ISMIX),RH(0:ISMIX),RNN(0:ISMIX),C13FLUX1(NUMAK,0:IFMAX), &
        C13FLUX2(NUMAK,0:IFMAX),RSUM13(5), RSUM14(5), RSUM15(5),RSUM18(5),RSUM10(5), &
        C13SOURCE2(0:ISMIX),rsum4(5),rsum5(5),rsum6(5),rsum7(5),rsum8(5), RSUM12(5), &
        DFKS(10,0:ISMIX), RSUM9(5),KBF,KDF, DCKO(5,NUML,NUMAK), DCKE(5,NUML,NUMAK), &
        O18SOURCE(0:ISMIX),O18FLUX(0:IFMAX),O18FLUXD(0:IFMAX),O18SOURCE2(0:ISMIX), &
        O18FLUX2(NUMAK,0:IFMAX),O18FLUX1(NUMAK,0:IFMAX), &
        H18SOURCE(0:ISMIX),H18FLUX(0:IFMAX),H18FLUXD(0:IFMAX),DEL_E(0:ISMIX),ZSOU(0:ISMIX)
        REAL*8 ALP(NUMK,NUMK), BET(NUMK),DAK(NUMK),AINV(NUMK,NUMK),DSUM
        REAL LSIGC(2),LSIGH(2),LSIGT(2),BINT(3),BINT2(3),IPN(NUMK), DCT(6,2),DCFT(5,2),&

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        DISC(NUML,0:ISMAX),DISCN(NUML,0:ISMAX),DISCF(NUML,0:ISMAX), &
        APROF(NUML,2), AZZ(NUML)
REAL*8 BETA12(3),costfn(10,3,9),HESS(NUMK,NUMK),&
        check(2,2),xxxx(numk)
EXTERNAL BETA, BETAI
DATA RSTD /0.011894/, R18STD /0.0020672/

! PRESET PARAMETERS:
    rmair = 0.02897      ! molecular weights (kg/mol) for air
    rmh2o = 0.018016    ! for H2O
    rmco2 = 0.044022    ! for CO2
    pmb   = 1000.       ! atmospheric pressure
    PI    = 3.14159
IWRITE=1          ! WRITE DISPERSION MATRIX
ICOST=1

! open and read control information from sourcfil.dat
    open(1,file='sourcfil_15d.dat')
2    call comskp(1)          !skip comments

    read(1,*,end=450) exptnam      !experiment name
    read(1,105,end=450) path_IP    !Input path name
    read(1,105,end=450) path_OP    !Output path name
105  format(a60)
    flen_IP=len_trim(path_IP)
    flen_OP=len_trim(path_OP)

    do 10000 iblk=1,300          !read up to 300 days' file names

        READ(1,*,end=450) (nlevl(I),I=1,3), (NREF(i),i=1,3),HC,PMB
        READ(1,*,err=450,END=450) ITURB,M0,M,A1,AH,A0,CCH,CCO,alfaa,alfab,ALFAC,ist_cor
        read(1,*,err=450,end=450) nfil

MN=MAXVAL(NLEVL)
ALLOCATE(Z(0:M),ZS(0:M),DZ(0:M),FA(0:M),SA(0:M),FH(0:M),SH(0:M), &
        FE(0:M),SE(0:M),FC(0:M),SC(0:M))
    ALLOCATE(AA((M+1)**2),BB(M+1),IP(M+1),AAL((M+1)**2),BBADD(M+1))
    ALLOCATE(T(NUML),Q(NUML),EV(NUML),CC(NUML), CA(NUML),CH(NUML),CE(NUML))
    ALLOCATE(ZC(NUMP,MN),HH((M+1)**2))
    ALLOCATE(Tt(MN,NUMFILES),C2(MN,NUMFILES),&
        VP(MN,NUMFILES),PROF(MN,NUMP,NUMFILES),SPROF(NUML,NUMP), &
        SIGC(MN,NUMFILES),SIGH(MN,NUMFILES),SIGT(MN,NUMFILES), &
        dcdt(mn,numfiles),DHDT(MN,NUMFILES),DTDT(MN,NUMFILES))
    ALLOCATE(PRAF(MN,NUMFILES),D13C(MN,NISO),D18O(MN,NISO))
    ALLOCATE(Ttz(MN),C2z(MN),VPz(MN),ZA(MN),ZZZ(MN,NUMP),B(MN),F(4,MN),C13Z(MN),O18Z(MN))
    ALLOCATE(DIS(NUML,0:M),DISN(NUML,0:M),DISF(NUML,0:M),C13ZZ(MN,NISO))

    do ifa=1,nfil              !read data for profiles and fluxes
        read(1,105) filenam
        path_file_IP=path_IP(1:flen_IP)//filenam

        open(10,file=path_file_IP,mode='read')

        select case(filenam(1:1))
            case('C','c')
                select case(filenam(2:2))
                    case('0','o')          !CO2
                        read(10,*)
                        read(10,200) (C2z(j),j=1,nlevl(1))          !read in CO2 heights
                        do i=1,numfiles          !read in CO2 data
                            read(10,210,end=100,err=460) &
                                C2date(i),C2hr(i),C2min(i),(C2(j,i),j=1,nlevl(1))
                            end do
                        continue
100                    nC2=i-1          !# CO2 records

```

```

        end select

case('T','t')
  read(10,*)                !skip one line
  read(10,200) (Ttz(j),j=1,nlevl(2))    !read in Temp heights
  do i=1,numfiles          !read in Temp data
    read(10,210,end=120,err=480) &
      Ttdate(i),Tthr(i),Ttmin(i),(Tt(j,i),j=1,nlevl(2))
  end do
120  continue
     nTt=i-1                !# Temp records

case('V','v')
  read(10,*)                !skip one line
  read(10,200) (VPz(j),j=1,nlevl(3))    !read in VP heights
  do i=1,numfiles          !read in VP data
    read(10,210,end=130,err=490) &
      VVdate(i),VPhr(i),VPmin(i),(VP(j,i),j=1,nlevl(3))
  end do
130  continue
     nVP=i-1                !# VP records

case('F','f')
  read(10,*,end=140,err=500)    !skip 1 lines
  do i=1,numfiles
    read(10,220,end=140) fxdate(i),fxhr(i),fxmin(i), &
      H(i),LE(i),E(i),FC2(i),us(i),swr(i),zMonU(i),Uh(i),rn(i), &
      PAR(I),fd(i),SWDR(I),LWDR(I)
  end do
140  continue
     nfx=i-1                !# flux records

CASE('A','a')
  READ(10,*)
  DO I=1,NUMFILES
    READ(10,270,END=141) DTIME(I), apress(i)
  ENDDO
141  CONTINUE
     apress=1000.

CASE('S','s')
  SELECT CASE(FILENAM(7:7))
  CASE('C')
    READ(10,*)
    READ(10,*)
    DO I=1,NUMFILES
      READ(10,230, END=150,ERR=510) nday(i),SIGCDAT(I),SIGCHR(I), &
        SIGCMIN(I),(SIGC(J,I),J=1,NLEVL(1))
    ENDDO
150  CONTINUE
  CASE('H')
    READ(10,*)
    READ(10,*)
    DO I=1,NUMFILES
      READ(10,231, END=160,ERR=520) SIGHDAT(I),SIGHHR(I), &
        SIGHMIN(I),(SIGH(J,I),J=1,NLEVL(3))
    ENDDO
160  CONTINUE
  CASE('T')
    READ(10,*)
    READ(10,*)
    DO I=1,NUMFILES
      READ(10,231, END=170,ERR=530) SIGTDAT(I),SIGTHR(I), &
        SIGTMIN(I),(SIGT(J,I),J=1,NLEVL(2))
    ENDDO

```

```

170      CONTINUE
        CASE('A')
          READ(10,*)
          READ(10,*)
          READ(10,232) (SIGCO2(J),J=1,NUML)
          READ(10,232) (SIGH20(J),J=1,NUML)
          READ(10,232) (SIGTEMP(J),J=1,NUML)
          READ(10,232) (SIG13C(J),J=1,NUML)
          READ(10,232) (SIG180(J),J=1,NUML)
        END SELECT

        CASE('D','d')
          SELECT CASE(FILENAM(2:2))
            CASE('C','c')
              READ(10,*)
              READ(10,*)
              DO I=1,NUMFILES
                READ(10,240,END=180) (DCDT(J,I),J=1,NLEVL(1))
              ENDDO
180          CONTINUE
            CASE('H','h')
              READ(10,*)
              READ(10,*)
              DO I=1,NUMFILES
                READ(10,240,END=190) (DHDT(J,I),J=1,NLEVL(1))
              ENDDO
190          CONTINUE
            CASE('T','t')
              READ(10,*)
              READ(10,*)
              DO I=1,NUMFILES
                READ(10,240,END=195) (DTDT(J,I),J=1,NLEVL(1))
              ENDDO
195          CONTINUE
            CASE('I','i')
              SELECT CASE(FILENAM(4:4))
                CASE('C','c')
                  READ(10,*)
                  READ(10,260,END=196) (C13z(j),j=1,6)          !read in C13 heights
                  DO I=1,NISO
                    READ(10,250) D13DAT(I),D13HR(I),D13MIN(I),(D13C(J,I),J=1,6)
                  ENDDO
196          CONTINUE
                CASE('O','o')
                  READ(10,*)
                  READ(10,200,END=197) (O18Z(J),J=1,6)
                  DO I=1,NISO
                    READ(10,260) (D180(J,I),J=1,6)
                  ENDDO
197          CONTINUE
              END SELECT
            END SELECT

          case default
            stop 'Incorrect profile or flux file type'

          end select

200      format(18x,10f8.2)
210      format(a8,i5,1x,i2,10f8.2)
220      format(a8,i5,1x,i2,6f8.2,f9.2,6f8.2)
230      format(I5,a8,i5,1x,i2,10f8.3)
231      format(a8,i5,1x,i2,10f8.3)
232      FORMAT(8X,20F8.2)
240      FORMAT(16X,10ES11.3)
250      FORMAT(A8,I5,1X,I2,6F9.3)

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```

260     FORMAT(16X,6F9.3)
270     FORMAT(F11.3,F8.2)

        end do                                !end reading block
!                                             of files

IX=1
RMSIGC=MAXVAL(SIGC)
RMSIGH=MAXVAL(SIGH)
RMSIGT=MAXVAL(SIGT)
LSIGC=MAXLOC(SIGC)
LSIGH=MAXLOC(SIGH)
LSIGT=MAXLOC(SIGT)
WRITE(*,*) RMSIGC, RMSIGH, RMSIGT
WRITE(*,*) LSIGC, LSIGH, LSIGT
! assume numfiles 1/2h records available each day
  nrec=numfiles
  PROF(:,1,:)=C2
  PROF(:,2,:)=TT
  PROF(:,3,:)=VP
  PROF(:,4,:)=SIGC
  PROF(:,5,:)=SIGT
  PROF(:,6,:)=SIGH
  PROF(:,7,:)=DCDT
  PROF(:,8,:)=DTDT
  PROF(:,9,:)=DHDT
  SIG(1,:)=SIGC02; SIG(2,:)=SIGTEMP; SIG(3,:)=SIGH20; SIG(4,:)=SIG13C; SIG(5,:)=SIG180
  SIG(1,:)=0.6*SIG(1,:);SIG(2,:)=0.2*SIG(2,:);SIG(3,:)=0.1*SIG(3,:)
  SIG(4,:)=0.3*SIG(4,:);SIG(5,:)=0.5*SIG(5,:) !WEIGHT TO EACH SPECIES
  ZZZ(:,1)=C2z
  ZZZ(:,2)=Ttz
  ZZZ(:,3)=VPz
  ZZZ(:,4)=C2z
  ZZZ(:,5)=Ttz
  ZZZ(:,6)=VPz
  ZZZ(:,7)=C2z
  ZZZ(:,8)=Ttz
  ZZZ(:,9)=VPz
  PROF(:,4,:)=0.3; PROF(:,5,:)=0.3      !CONSTANT SIGMA FOR EACH (10X ACTUAL)
! PROF(7:9,6,:)=0.3
  prof(:,6,:)=0.05
  DO I=4,9
    NLEVL(I)=NLEVL(I-3)
  ENDDO

! INTERPOLATE D13C, D180 PROFILES
  TH=28.0
  DO I=1,NISO
    NLI(I)=6;C13ZZ(:,I)=C13Z
    DO J=1,6      !CHECK FOR BAD DATA
      IF(ABS(D13C(J,I)).GT.100.) THEN
        NLI(I)=NLI(I)-1
        DO K=J,5
          D13C(K,I)=D13C(K+1,I)
          D180(K,I)=D180(K+1,I)
          C13ZZ(K,I)=C13Z(K+1)
        ENDDO
      ENDF
    ENDDO
    CALL INTERP(NLI(I),C13ZZ(:,I),D13C(:,I),X,Y,TH,NUML,NV,B,F)
    APROF(:,1)=Y; AZZ=X
    CALL INTERP(NLI(I),C13ZZ(:,I),D180(:,I),X,Y,TH,NUML,NV,B,F)
    APROF(:,2)=Y
  ENDDO

! sort profiles into ascending height order - assume order read in is sequential

```

```

!      but may be in descending order
!      utilise equivalence between zzz(nv,nf) & Ttz(nv),VPz(nv,nf)...
!      and between prof(nv,nf,nr) & Tt(nv,nr),VP(nv,nr)...
do nf=1,NUMP                                !profile files
  if(zzz(1,nf).gt. zzz(nlevl(nf),nf)) then    !need to reverse order
    do nv=1,nlevl(nf)                        !n levels
      za(nv)=zzz(nlevl(nf)-nv+1,nf)          !write to scratch array
      do nr=1,nrec                            !nrec records common to
!                                             all profile files
          praf(nv,nr)=prof(nlevl(nf)-nv+1,nf,nr) !write to scratch array
        end do                                !end record loop
      end do                                  !end level loop
!
!      now overwrite arrays in ascending order
do nv=1,nlevl(nf)
  zzz(nv,nf)=za(nv)
  do nr=1,nrec
    prof(nv,nf,nr)=praf(nv,nr)
  end do
end do
end do
end if
end do

DO II=1,NUMP
DO nv=1,MN
  zc(II,nv)=ZZZ(nv,II)
ENDDO
ENDDO

!      end data input section

!      *****

!      construct output file names from date info
mon=Ttdate(1)(6:8)
day(1)=Ttdate(1)(3:4)
if(day(1).eq.' ') day(1)='0'
!      *****

!      INTERPOLATE BETWEEN PROFILES
!
!      FOR TEMPERATURE ADD LINEARLY INTERPOLATED POINT BETWEEN TOP TWO
!      VALUES TO PREVENT LARGE DEVIATIONS OF THE SPLINE BETWEEN THESE TWO

NEWZ=(ZZZ(NLEVL(2),2)+ZZZ(NLEVL(2)-1,2))/2
ZZZ(NLEVL(2)+1,2)=ZZZ(NLEVL(2),2)
ZZZ(NLEVL(2),2)=NEWZ
NLEVL(2)=NLEVL(2)+1

do 3000 nr=1,nrec

!      ADD LINEARLY INTERPOLATED POINT BETWEEN TOP TWO VALUES FOR T AND SIGT

NEWPROF=(PROF(NLEVL(2)-1,2,NR)+PROF(NLEVL(2)-2,2,NR))/2
PROF(NLEVL(2),2,NR)=PROF(NLEVL(2)-1,2,NR)
PROF(NLEVL(2)-1,2,NR)=NEWPROF
NEWPROF=(PROF(NLEVL(2)-1,5,NR)+PROF(NLEVL(2)-2,5,NR))/2
PROF(NLEVL(2),5,NR)=PROF(NLEVL(2)-1,5,NR)
PROF(NLEVL(2)-1,5,NR)=NEWPROF

!      *****
!      Process all available records using MRR's program

!      check if turbulence data available (criterion: u* > 5 m/s)
if(us(nr).gt.5.) goto 3000                    !try next record

```

```

day(nr)=Ttdate(nr)(3:4)

!      assign fluxes at reference height
      Href=H(nr)                !heat
      Eref=LE(nr)               !LE
      F2ref=FC2(nr)             !CO2
      swref=swr(nr)             !sig_w above canopy
!      usref=swref/a1           !u* ref
      USREF=US(NR)
      tc=PROF(NLEVL(2),2,NR)    !ambient temp (deg C)
      Uhref=Uh(nr)/1.3

!      check if stability correction required
      if(ist_cor.eq.1) then
        IF(TTHR(NR).LT.5) ZMON=10.
        IF(TTHR(NR).GE.5.AND.TTHR(NR).LT.7) ZMON=50.
        IF(TTHR(NR).GE.7.AND.TTHR(NR).LT.8) ZMON=100.
        IF(TTHR(NR).GE.8.AND.TTHR(NR).LT.10) ZMON=500.
        IF(TTHR(NR).GE.10.AND.TTHR(NR).LT.17) ZMON=1000.
        IF(TTHR(NR).GE.17.AND.TTHR(NR).LT.18) ZMON=500.
        IF(TTHR(NR).GE.18.AND.TTHR(NR).LT.19) ZMON=100.
        IF(TTHR(NR).GE.19.AND.TTHR(NR).LT.22) ZMON=50.
        IF(TTHR(NR).GE.22) ZMON=10.
!      IF(TTHR(NR).LT.10.OR.TTHR(NR).GT.16) THEN
!      zMon=17./zMonU(nr)        !Monin Obukhov length
      else
        zMon=-1000.             !set to large -ve value
!                                  -> neutral
!      endif
!      end if

      call air(tc,pmb,rho,volm,capp,rlam,qsat,epsi)
      LMON(NR)=USREF**3*(TC+273.15)*RHO*CAPP/0.4/10./HREF !MONIN-OBUKHOV LENGTH

3000  continue

!*****
DO 4004 NR=1,NREC
write(timdat,116) day(nr),mon,Tthr(nr),Ttmin(nr)
WRITE(*,*) TIMDAT
NIS=3
! IF((DAY(NR).EQ.'25'.OR.DAY(NR).EQ.'27').AND.(TTHR(NR).GE.6.AND.TTHR(NR).LT.21)) THEN
IF(NR.GT.60.AND.TTHR(NR).GE.6.AND.TTHR(NR).LT.21) THEN !.AND. &
(DAY(NR).EQ.'28'.and.tthr(NR).EQ.6)) THEN
TH=28.0
DO II=1,3
CALL INTERP(NLEVL(II),ZZZ(:,II),PROF(:,II,NR),X,Y,TH,NUML,NV,B,F)
SPROF(:,II)=Y
CALL INTERP(NLEVL(II),ZZZ(:,II),PROF(:,II+6,NR),X,Y,TH,NUML,NV,B,F)
SPROF(:,II+6)=Y ! STORAGE
ENDDO
XPROF=X
202 IEDDY=0 ! USE EDDY FLUXES TO CONSTRAIN 1=YES, 0=NO
IDIS=0 ! USE DISPM SUBROUTINE FOR DERIV AND CONC CALC 1=YES, 0=NO
ICOSTFN=2 ! 1=calculate cost function (chisq) only, no optimisation,
! 2=output error covariance matrix
IFLAGC=0 ! exit after one iteration, including deriv calc
IOPT=0 ! 0=OPTIMISE ONLY GROUND FLUXES, 1=ALSO OTHER PARAMS
IPM=1
IN=1
open(unit=10, file='cprof')
OPEN(UNIT=11, FILE='SPROFC')
OPEN(UNIT=16, FILE='EPROF')
OPEN(UNIT=13, FILE='HPROF')
OPEN(UNIT=17, FILE='SPROFE')
OPEN(UNIT=14, FILE='SPROFH')

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open(unit=12, file='FLUXC')
OPEN(UNIT=15, FILE='FLUXH')
OPEN(UNIT=18, FILE='FLUXE')
OPEN(UNIT=19, FILE='FLUXLE')
OPEN(UNIT=20, FILE='MOREPROFS')
OPEN(UNIT=21, FILE='C13PROF')
OPEN(UNIT=22, FILE='SPROFC13')
OPEN(UNIT=23, FILE='GROUNDFLUX')
OPEN(UNIT=24, FILE='PROFC')
OPEN(UNIT=25, FILE='PROFE')
OPEN(UNIT=26, FILE='PROFH')
OPEN(UNIT=27, FILE='PROFC13')
OPEN(UNIT=28, FILE='O18PROF')
OPEN(UNIT=29, FILE='SPROFO18')
OPEN(UNIT=30, FILE='H18PROF')
OPEN(UNIT=31, FILE='CHISQ')
IWRITE=0
IFLAG=0
SWDREF=SWDR(NR); LWDREF=LWDR(NR)

NUMLEV=NUML          ! USE INTERPOLATED DATA
SPROF(:,1)=SPROF(:,1)+9.8 !CORRECT FOR OFFSET OF IRGA DATA FROM FLASK DATA

IS2=50      !NUMBER OF SEGMENTS FOR DC/DA INTEGRALS
IS3=100     !NUMBER OF POINTS WHERE SOURCE AND FLUX ARE EVALUATED
IS4=50      !NUMBER OF POINTS WHERE FLUX IS CALCULATED INITIALLY

FIS2=FLOAT(IS2)
FIS3=FLOAT(IS3)
FIS4=FLOAT(IS4)

HCS=23.     ! CANOPY HEIGHT
COUNT=0.
DO IK=1,NUMLEV      ! NUMBER OF HEIGHTS BELOW HC
  IF(XPROF(IK).LE.HCS) THEN
    COUNT=COUNT+1
  ENDIF
ENDDO

RL=0.001          ! INITIALISE RL (LEV-MARQ LAMBDA)

SLA1=5.; SLA2=4.  ! LEAF AREA PROFILE SHAPE
GHR=0.003        ! GH MULTIPLIER
WIND=3.          ! WIND EXTINCTION COEFFICIENT
CICA=0.6         ! INITIAL CI/CA
D13RESP=17.6     ! RESP. DISCR.
D18RESP=15.      ! RESP. DISCR.
SIG0=SIG        !RETAIN ORIGINAL SIGMAS FOR CONCENTRATIONS

VM=0.49         ! VMAX PARAMETER
SVMi=10.        ! SIGMA OF VMAX PARAMETER
ALAM=130.       ! LAMBDA FOR GS
SALAMi=2500.    ! SIGMA FOR LAMBDA
TLP1=23.        ! TL EXP COEFF
STLP1I=200.    ! SIGMA FOR TL EXP COEFF
TLP2=0.25      ! TL U*/H AT TOP OF CANOPY
STLP2I=3.      ! SIGMA FOR TL U*/H
KDF=0.20       ! DIFFUSE RADIATION EXTINCTION COEFFICIENT
SKDFI=8.       ! SIGMA FOR KDF
KBF=0.37       ! DIRECT RADIATION EXTINCTION COEFFICIENT
SKBFI=5.       ! SIGMA FOR KBF

AK(1:3)=(/0.05,-0.02,0.01/) ! CO2, HEAT AND H2O FLUX AT GROUND
AK(4)=VM       ! VMAX PARAMETER
AK(5)=ALAM     ! LAMBDA FOR GS
AK(6)=TLP1     ! TL EXP COEFF

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AK(7)=TLP2 ! TL U*/H AT TOP OF CANOPY
AK(8)=KDF ! DIRECT RADIATION EXTINCTION COEFFICIENT
AK(9)=KBF ! DIFFUSE RADIATION EXTINCTION COEFFICIENT

PARAM(1:2)=(/SLA1,SLA2/) ! SHAPE OF LEAF AREA PROFILE
PARAM(3)=GHR ! GH MULTIPLIER
PARAM(4)=4.3 ! TOTAL LEAF AREA INDEX
PARAM(5)=WIND ! WIND EXTINCTION COEFFICIENT

DO NPR=1,3
SREF(NPR)=SPROF(NUMLEV,NPR)
DO J=1,NUMLEV ! CHECK FOR BAD STD DEVIATION + BAD DC/DT
IF(SPROF(J,NPR+3).LT.0.001) SPROF(J,NPR+3)=1.
IF(ABS(SPROF(J,NPR+3)).GT.900.) SPROF(J,NPR+3)=1.
IF(ABS(SPROF(J,NPR+6)).GT.900.) SPROF(J,NPR+6)=0.
ENDDO
ENDDO
ZREF=XPROF(NUMLEV)
SMOW=0.0020052; DEL_S=-18.; ESTAR=9.2
D18VAP=-26.
SREF(6)=(1.+D18VAP/1000.)*SMOW*SREF(3)
SREF(4)=(-8./1000.+1)*RSTD*SREF(1)
SREF(5)=(-1./1000.+1)*R18STD*SREF(1)

DO N=1,NUMLEV
DO L=1,6
CKO(L,N)=SREF(L)
ENDDO
ENDDO
CK=CKO; CKK=CKO; AKO=AK; AKE=AK; IFLAGO=1

NC=0.;X2=0.
do i=0,IS3-1
ZAH=FLOAT(I)/FIS3*COUNT
J=NINT(ZAH)
IF(J.EQ.0)THEN; X1=0.;ELSE; X1=XPROF(J); ENDIF
IF(X1.EQ.X2) THEN; NC=0.; ELSE; NC=NC+1; ENDIF
IF(J.LT.20)THEN;IF(XPROF(J+1).GT.HCS) THEN; X2=HCS; ELSE; X2=XPROF(J+1); ENDIF;ENDIF
IF(J.GT.0)THEN;IF(XPROF(J).GT.HCS) THEN; X1=HCS; ENDIF;ENDIF
ZAH=NC/FIS3*COUNT
ZAL=X1+(X2-X1)*ZAH
ZAH=ZAL/HCS
ZSOU(I)=ZAL
ENDDO
ZSOU(IS3)=HCS

1122 AK=AKO
IF(ICOSTFN.EQ.1) THEN
IF(IPM.EQ.2) THEN
AK(IN)=AK(IN)+0.1*AK(IN)
ELSEIF(IPM.EQ.3) THEN
AK(IN)=AK(IN)-0.1*AK(IN)
ENDIF
ENDIF

ITER=200
3035 DO 3025 IA=1,ITER ! ITERATE FOR AK PARAMETERS

LIM=0
CKO=CK
DCKO=DCK

2121 CONTINUE

! check if stability correction required
if(ist_cor.eq.1) then

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      IF(TTHR(NR).LT.5) ZMON=10.
      IF(TTHR(NR).GE.5.AND.TTHR(NR).LT.7) ZMON=50.
      IF(TTHR(NR).GE.7.AND.TTHR(NR).LT.8) ZMON=100.
      IF(TTHR(NR).GE.8.AND.TTHR(NR).LT.10) ZMON=500.
      IF(TTHR(NR).GE.10.AND.TTHR(NR).LT.17) ZMON=1000.
      IF(TTHR(NR).GE.17.AND.TTHR(NR).LT.18) ZMON=500.
      IF(TTHR(NR).GE.18.AND.TTHR(NR).LT.19) ZMON=100.
      IF(TTHR(NR).GE.19.AND.TTHR(NR).LT.22) ZMON=50.
      IF(TTHR(NR).GE.22) ZMON=10.
      else
        zMon=-1000.                !set to large -ve value
!                                     -> neutral
      end if

      UHREF=UH(NR)/1.3
      USTARR=US(NR)
      SIGWR=SWR(NR)
      IFLAGO=1
      IF(IDIS.EQ.1) THEN
        call DISPM2(USTARR,SIGWR,AK(6),AK(7),timdat,NUMlev,NUMLEV,NUMLEV,0,IS3, &
          ZSOU,XPROF,zMon,DISC,DISCN,DISCF,IWRITE)
      ENDIF
      DO KK=1,3
! CALCULATE SOURCE AND FLUX PROFILES
      CALL CALCS(PARAM,FD(NR),PAR(NR),DEF,SWDREF,LWDREF,DTIME(NR),APRESS(NR),CK, &
        XPROF,SREF,ESATL,thet1,RLAI,RC,RH,RNN,ak, &
        hcs,cica,CSOURCE,esource,is3,HSOURCE,C13SOURCE,O18SOURCE,H18SOURCE, &
        UHREF,DRESP,DELTA,DEL18,DEL_E,ZSOU)
      SK(3,:)=ESOURCE ! THESE ARE THE SOURCE PROFILES FROM Z=0 TO Z=H
      SK(2,:)=HSOURCE
      SK(1,:)=CSOURCE
      SK(4,:)=C13SOURCE
      SK(5,:)=O18SOURCE
      SK(6,:)=H18SOURCE

      CALL INTVAL(28., 28., TEMP, CO2, H2O,NLEVL,ZZZ,PROF,28.,20,NR)
      ESAT=6.1375*EXP(17.502*TEMP/(240.97+TEMP))
      SL=17.502*240.97/(240.97+TEMP)**2*esat
      sl=0.622*pmb/(pmb-0.378*esat)**2*sl
      ep=rlam/cAPp*sl
      eqg=ep*rnn(0)*.9/(ep+1.)
! AK(3)=EQG*VOLM/RLAM/18.015/1.E-6
      CALL CALCE(SPROF(:,7:9),PARAM,FD(NR),PAR(NR),SWDREF,LWDREF,DTIME(NR),APRESS(NR), &
        CK,XPROF,SREF,ak,hcs,CFLUX,eflux,is4,0.,ZREF,HFLUX, &
        C13FLUX,O18FLUX,H18FLUX,UHREF,ZPR,0)
!WRITE TO DUMMY VARIABLES, FLUX PROFILES FROM Z=0 TO Z=H
      EFLUXD=EFLUX; HFLUXD=HFLUX; CFLUXD=CFLUX; C13FLUXD=C13FLUX; O18FLUXD=O18FLUX; H18FLUXD=H18FLUX

!
! IF(IST_COR.EQ.1) THEN
!   LZMON=USREF**3*(TC+273.15)*RHO*CAPP/0.4/10./HFLUX(IS4) !MONIN-OBUKHOV LENGTH
!   ZMON=LZMON
! ENDIF

      CKNR=0.;CKNR2=0.;CKNR3=0.;CKNR4=0.;CKNR5=0.;CKNR6=0. !CALCULATE NEAR FIELD CONC AT ZREF
      NC=0.;X2=0.
      DO I=0,IS3-1
        ZAH=FLOAT(I)/FIS3*COUNT
        J=NINT(ZAH)
        IF(J.EQ.0)THEN; X1=0.;ELSE; X1=XPROF(J); ENDIF
        IF(X1.EQ.X2) THEN; NC=0.; ELSE; NC=NC+1; ENDIF
        IF(J.LT.20)THEN;IF(XPROF(J+1).GT.HCS) THEN; X2=HCS; ELSE; X2=XPROF(J+1); ENDIF;ENDIF
        IF(J.GT.0)THEN;IF(XPROF(J).GT.HCS) THEN; X1=HCS; ENDIF;ENDIF
        ZAH=NC/FIS3*COUNT
        ZI=X1+(X2-X1)*ZAH
        ZID=ZI+(X2-X1)*COUNT/FIS3
        CALL TURB2(USTARR,SIGWR,AK(6),AK(7),ZI,zMon,SWO,TLO)

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CALL TURB2(USTARR,SIGWR,AK(6),AK(7),ZID,zMon,SWD,TLD)
RKN1=RKN((ZREF-ZI)/SWO/TLO)+RKN((ZREF+ZI)/SWO/TLO)
RKN2=RKN((ZREF-ZID)/SWD/TLD)+RKN((ZREF+ZID)/SWD/TLD)
  CKNR=CKNR+((SK(1,I))/SWO*RKN1+ (SK(1,I+1))/SWD*RKN2)/2./FIS3*HCS
  CKNR2=CKNR2+((SK(2,I))/SWO*RKN1+ (SK(2,I+1))/SWD*RKN2)/2./FIS3*HCS
  CKNR3=CKNR3+((SK(3,I))/SWO*RKN1+ (SK(3,I+1))/SWD*RKN2)/2./FIS3*HCS
  CKNR4=CKNR4+((SK(4,I))/SWO*RKN1+ (SK(4,I+1))/SWD*RKN2)/2./FIS3*HCS
  CKNR5=CKNR5+((SK(5,I))/SWO*RKN1+ (SK(5,I+1))/SWD*RKN2)/2./FIS3*HCS
  CKNR6=CKNR6+(SK(6,I)/SWO*RKN1+ SK(6,I+1)/SWD*RKN2)/2./FIS3*HCS
ENDDO
DO N=1,NUMLEV      ! CALCULATE NEAR FIELD CONC AT EACH Zi (MEASUREMENT HEIGHTS)
CKF1=0.;CKF2=0.;CKF3=0.;CKF4=0.; CKF5=0.; CKF6=0.
CKN=0.;CKN2=0.;CKN3=0.;CKN4=0.; CKN5=0.; CKN6=0.
ZL=XPROF(N)
NC=0.;X2=0.
DO I=0,IS3-1
  ZAH=FLOAT(I)/FIS3
  ZI=ZAH*HCS
  ZID=ZI+HCS/FIS3
  ZAH=FLOAT(I)/FIS3*COUNT
  J=NINT(ZAH)
  IF(J.EQ.0)THEN; X1=0.;ELSE; X1=XPROF(J); ENDIF
  IF(X1.EQ.X2) THEN; NC=0.; ELSE; NC=NC+1; ENDIF
  IF(J.LT.20)THEN;IF(XPROF(J+1).GT.HCS) THEN; X2=HCS; ELSE; X2=XPROF(J+1); ENDIF;ENDIF
  IF(J.GT.0)THEN;IF(XPROF(J).GT.HCS) THEN; X1=HCS; ENDIF;ENDIF
  ZAH=NC/FIS3*COUNT
  ZI=X1+(X2-X1)*ZAH
  ZID=ZI+(X2-X1)*COUNT/FIS3
  EPS=0.001*AK(6)
  EPS2=0.001*AK(7)
  CALL TURB2(USTARR,SIGWR,AK(6),AK(7),ZI,zMon,SWO,TLO)
  CALL TURB2(USTARR,SIGWR,AK(6),AK(7),ZID,ZMON,SWD,TLD)
  CALL TURB2(USTARR,SIGWR,AK(6)+EPS,AK(7),ZI,zMon,SWO,TLOE)
  CALL TURB2(USTARR,SIGWR,AK(6)+EPS,AK(7),ZID,ZMON,SWD,TLDE)
  CALL TURB2(USTARR,SIGWR,AK(6),AK(7)+EPS2,ZI,zMon,SWO,TLOB)
  CALL TURB2(USTARR,SIGWR,AK(6),AK(7)+EPS2,ZID,ZMON,SWD,TLDB)
  IF((ZL-ZI).NE.0.0.AND.(ZL-ZID).NE.0.0) THEN
    RKN1=RKN((ZL-ZI)/SWO/TLO)+RKN((ZL+ZI)/SWO/TLO)
    RKN2=RKN((ZL-ZID)/SWD/TLD)+RKN((ZL+ZID)/SWD/TLD)
  ELSEIF((ZL-ZI).EQ.0.0) THEN
    RKN1=RKN(HCS/FIS3/SWO/TLO)+RKN((ZL+ZI)/SWO/TLO)
    RKN2=RKN((ZL-ZID)/SWD/TLD)+RKN((ZL+ZID)/SWD/TLD)
  ELSEIF((ZL-ZID).EQ.0.0) THEN
    RKN1=RKN((ZL-ZI)/SWO/TLO)+RKN((ZL+ZI)/SWO/TLO)
    RKN2=RKN(HCS/FIS3/SWO/TLO)+RKN((ZL+ZID)/SWD/TLD)
  ENDIF
  CKN=CKN+((SK(1,I))/SWO*RKN1+ (SK(1,I+1))/SWD*RKN2)/2./FIS3*HCS
  CKN2=CKN2+((SK(2,I))/SWO*RKN1+ (SK(2,I+1))/SWD*RKN2)/2./FIS3*HCS
  CKN3=CKN3+((SK(3,I))/SWO*RKN1+ (SK(3,I+1))/SWD*RKN2)/2./FIS3*HCS
  CKN4=CKN4+((SK(4,I))/SWO*RKN1+ (SK(4,I+1))/SWD*RKN2)/2./FIS3*HCS
  CKN5=CKN5+((SK(5,I))/SWO*RKN1+ (SK(5,I+1))/SWD*RKN2)/2./FIS3*HCS
  CKN6=CKN6+(SK(6,I)/SWO*RKN1+ SK(6,I+1)/SWD*RKN2)/2./FIS3*HCS
ENDDO
DO I=0,IS3
  ZN=ZL+FLOAT(I)*(ZREF-ZL)/FIS3
  EPS=0.001*AK(6)
  EPS2=0.001*AK(7)
  CALL TURB2(USTARR,SIGWR,AK(6),AK(7),ZN,zMon,SWZ,TLZ)
  CALL TURB2(USTARR,SIGWR,AK(6)+EPS,AK(7),ZN,zMon,SWZ,TLZE)
  CALL TURB2(USTARR,SIGWR,AK(6),AK(7)+EPS2,ZN,zMon,SWZ,TLZB)
  ! GET FLUX PROFILES FROM Z=Zi TO Z=ZREF FOR CONCENTRATION INTEGRAL, WHERE Zi IS HEIGHT
  ! OF CONCENTRATION MEASUREMENT, FOR EACH Zi
  IF(ZN.EQ.ZPR(IS4)) THEN
    FK(3,I)=EFLUX(IS4); FK(2,I)=HFLUX(IS4); FK(1,I)=CFLUX(IS4); FK(4,I)=C13FLUX(IS4)
    FK(5,I)=O18FLUX(IS4); FK(6,I)=H18FLUX(IS4)
  ELSEIF(ZN.GT.ZPR(IS4).OR.ZN.LT.ZPR(0)) THEN

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      STOP 'ZN NOT IN RANGE FLUX CALC'
    ENDIF
  DO J=0,IS4-1
    IF(ZN.EQ.ZPR(J)) THEN !IF Zi COINCIDES WITH A HEIGHT AT WHICH WE ALREADY HAVE
      ! THE FLUX CALCULATION, TAKE THAT FLUX
      FK(3,I)=EFLUXD(J); FK(2,I)=HFLUXD(J); FK(1,I)=CFLUXD(J); FK(4,I)=C13FLUXD(J)
      FK(5,I)=O18FLUXD(J); FK(6,I)=H18FLUXD(J)
    ELSEIF(ZN.LT.ZPR(J+1).AND.ZN.GT.ZPR(J)) THEN ! OTHERWISE CALCULATE ADDITIONAL
      ! FLUX FROM HEIGHT WE HAVE TO HEIGHT WE WANT
      EADD=EFLUXD(J); HADD=HFLUXD(J); CADD=CFLUXD(J); C13ADD=C13FLUXD(J)
      O18ADD=O18FLUXD(J); H18ADD=H18FLUXD(J)
      ZR=ZPR(J)+(ZN-ZPR(J))*FIS4
      CALL CALCE(SPROF(: ,7:9),PARAM,FD(NR),PAR(NR),SWDREF,LWDREF,DTIME(NR),APRESS(NR), &
        CK,XPROF,SREF,ak,hcs,CFLUX,eflux,is4,ZPR(J),ZR,HFLUX, &
        C13FLUX,O18FLUX,H18FLUX,UHREF,ZOUT,1)
      FK(3,I)=EFLUX(1)+EADD
      FK(2,I)=HFLUX(1)+HADD
      FK(1,I)=CFLUX(1)+CADD
      FK(4,I)=C13FLUX(1)+C13ADD
      FK(5,I)=O18FLUX(1)+O18ADD
      FK(6,I)=H18FLUX(1)+H18ADD
    ENDIF
  ENDDO
  FKS(3,I)=FK(3,I)/SWZ**2/TLZ !DIVIDE BY SIGW^2 AND TL FOR INTEGRATION
  FKS(2,I)=FK(2,I)/SWZ**2/TLZ
  FKS(1,I)=FK(1,I)/SWZ**2/TLZ
  FKS(4,I)=FK(4,I)/SWZ**2/TLZ
  FKS(5,I)=FK(5,I)/SWZ**2/TLZ
  FKS(6,I)=FK(6,I)/SWZ**2/TLZ
ENDDO
DO I=0,IS3-1
  CKF1=CKF1+(FKS(1,I)+FKS(1,I+1))/2./FIS3*(ZREF-ZL) ! INTEGRATE FROM Zi TO ZREF
  CKF2=CKF2+(FKS(2,I)+FKS(2,I+1))/2./FIS3*(ZREF-ZL)
  CKF3=CKF3+(FKS(3,I)+FKS(3,I+1))/2./FIS3*(ZREF-ZL)
  CKF4=CKF4+(FKS(4,I)+FKS(4,I+1))/2./FIS3*(ZREF-ZL)
  CKF5=CKF5+(FKS(5,I)+FKS(5,I+1))/2./FIS3*(ZREF-ZL)
  CKF6=CKF6+(FKS(6,I)+FKS(6,I+1))/2./FIS3*(ZREF-ZL)
ENDDO
CK(1,N)=(CKN+CKF1-CKNR)+SREF(1) ! CONCENTRATION = NEAR-FIELD + FAR-FIELD -
CK(2,N)=(CKN2+CKF2-CKNR2)+SREF(2) ! NEAR-FIELD (ZREF) + CONC (ZREF)
CK(2,N)=MAX(CK(2,N),-2.); CK(2,N)=MIN(CK(2,N),25.)
CK(3,N)=(CKN3+CKF3-CKNR3)+SREF(3)
CK(3,N)=MAX(CK(3,N),0.); CK(3,N)=MIN(CK(3,N),15.)
CK(4,N)=(CKN4+CKF4-CKNR4)+SREF(4)
CK(5,N)=(CKN5+CKF5-CKNR5)+SREF(5)
CK(6,N)=(CKN6+CKF6-CKNR6)+SREF(6)
DO IK=1,6
  CK(IK,N)=MIN(CK(IK,N),1000.)
  CK(IK,N)=MAX(CK(IK,N),-1000.)
  IF(ABS(CK(IK,N)).EQ.1000.) THEN
    CK(IK,N)=SREF(IK)
    INAN=1
    GOTO 2122
  ENDIF
ENDDO
FKTOP(1)=CFLUXD(IS4)
FKTOP(2)=HFLUXD(IS4)
FKTOP(3)=EFLUXD(IS4)
IF(IDIS.EQ.1) THEN
DO NPR=1,5
ASUM=0.
DO I=1,IS3
ASUM=ASUM+DISC(N,I)*SK(NPR,I)*(ZSOU(I)-ZSOU(I-1))
ENDDO
ASUM=ASUM+DISC(N,0)*FK(NPR,0)*ZSOU(1)
CK(NPR,N)=ASUM+SREF(NPR)

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        ENDDO
      ENDF
    ENDDO
  ENDDO

2122  CSUM=0.
      DO N=1,NUMLEV          ! CALCULATE CHI-SQUARE = SUM (C_MODEL - C_MEAS)^2 / SIGMA^2
        DO NPR=1,3
          CSUM=CSUM+(CK(NPR,N)-SPROF(N,NPR))**2/SIG(NPR,N)**2
        ENDDO
      ENDDO
      IF (IEDDY.EQ.1) THEN
        SIGFC=ABS(0.05*FC2(NR)*VOLM)    ! SIGMA OF TOTAL C FLUX
        SIGFH=ABS(0.1*H(NR)/CAPP/RHO)  ! SIGMA OF TOTAL H FLUX
        SIGFE=ABS(0.1*E(NR)*VOLM)    ! SIGMA OF TOTAL E FLUX
        CSUM = CSUM + (FC2(NR)*VOLM-CFLUX(IS4))**2/SIGFC**2
        CSUM = CSUM + (H(NR)/CAPP/RHO-HFLUX(IS4))**2/SIGFH**2
        CSUM = CSUM + (E(NR)*VOLM-EFLUX(IS4))**2/SIGFE**2
      ENDF

      CHISQN=CSUM

      IF(ABS(CHISQN-CHISQ).LT.0.1) GOTO 3045  !EXIT LOOP IF NO IMPROVEMENT IN CHISQ
      CHISQNN=0.
      IF(IA.EQ.1.OR.IAC.EQ.1) THEN          ! 1ST ITERATION
        CHISQ=CHISQN
        IAC=0
        CKE=CK
      ELSEIF(IA.EQ.ITER-1.AND.CHISQN.LE.CHISQ) THEN  ! 2ND LAST ITERATION, EXIT IF CHISQ
        AKO=DBLE(AK)                          ! BETTER THAN PREVIOUS
        GOTO 3045
      ELSEIF(RL.GT.1.E+2) THEN              ! EXIT IF LAMBDA LARGE
        CK=CKO; AK=SNGL(AKO)
        GOTO 3045
      ELSEIF(INAN.EQ.1) THEN
        WRITE(*,*) 'CONC NAN, AK=',(AK(K),K=4,9)
        AK=SNGL(AKO)
        CK=CKO
        DCK=DCKO
        RL=MAX(RL*100.,0.1)
        INAN=0
        GOTO 808
      ELSE IF (CHISQN.GE.CHISQ) THEN        ! INCREASE LAMBDA IF CHISQ WORSE AND USE PREVIOUS PARAMS
        AK=SNGL(AKO)
        CK=CKO
        DCK=DCKO
        RL=MAX(RL*100.,0.1)
        GOTO 808
      ELSE IF (CHISQN.LT.CHISQ) THEN        ! DECREASE LAMBDA IF CHISQ BETTER, AND CONTINUE
        RL=RL/10.
        CHISQ=CHISQN
        AKE=AK; DCKE=DCK; CKE=CK
      ELSE
        STOP 'PROBLEM SOMEWHERE, MAYBE PARAMS OUT OF RANGE'
        AK=SNGL(AKO)
        CK=CKO
        DCK=DCKO
        RL=MAX(RL*100.,0.1)
        GOTO 808
      ENDF
      write(*,*) 'Chisq = ',chisq, 'Iterations:',ia, ' RL =',RL

1133  IF(ICOSTFN.EQ.1) THEN
        COSTFN(ICOST,IPM,IN)=CHISQ
      IF(IPM.EQ.1.OR.IPMEQ.2) THEN
        IPM=IPM+1

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      GOTO 1122
    ELSEIF(IPM.EQ.3.AND.IN.LT.9) THEN
      IN=IN+1
      IPM=2
      GOTO 1122
    ELSE
      ICOST=ICOST+1
      GOTO 3045
    ENDIF
  ENDIF

! CALCULATE DERIVATIVE OF SOURCE PROFILES WRT PARAMETERS
2022      ZL=0.

      SVM=SVMI;SALAM=SALAMI;STLP1=STLP1I;STLP2=STLP2I;SKDF=SKDFI;SKBF=SKBFI
!      check if stability correction required
      if(ist_cor.eq.1) then
        IF(TTHR(NR).LT.5) ZMON=10.
        IF(TTHR(NR).GE.5.AND.TTHR(NR).LT.7) ZMON=50.
        IF(TTHR(NR).GE.7.AND.TTHR(NR).LT.8) ZMON=100.
        IF(TTHR(NR).GE.8.AND.TTHR(NR).LT.10) ZMON=500.
        IF(TTHR(NR).GE.10.AND.TTHR(NR).LT.17) ZMON=1000.
        IF(TTHR(NR).GE.17.AND.TTHR(NR).LT.18) ZMON=500.
        IF(TTHR(NR).GE.18.AND.TTHR(NR).LT.19) ZMON=100.
        IF(TTHR(NR).GE.19.AND.TTHR(NR).LT.22) ZMON=50.
        IF(TTHR(NR).GE.22) ZMON=10.
!      ZMON=LZMON
      else
        zMon=-1000.          !set to large -ve value
!                               -> neutral
      end if

      UHREF=UH(NR)/1.3
      USTARR=US(NR)
      SIGWR=SWR(NR)
      DO N=1, NUMLEV
      do npr=1,5
      ZL=XPROF(N)
      NC=0.;X2=0.
      SUM1=0.; SUM2=0; SUM3=0.; SUM4=0.; SUM1A=0.; SUM5=0.; SUM8=0.; SUM9=0.; SUM1B=0.
      IF(IDIS.EQ.0) THEN
        DO NK=0,IS2-1
          ZN=ZL+FLOAT(NK)*(ZREF-ZL)/FIS2
          ZND=ZN+(ZREF-ZL)/FIS2
          CALL TURB2(USTARR,SIGWR,AK(6),AK(7),ZN,ZMON,SWZ,TLZ)
          CALL TURB2(USTARR,SIGWR,AK(6),AK(7),ZND,ZMON,SWZD,TLZD)
          IF(NK.LT.IS2) THEN      ! INTEGRATE FLUX DERIVS FROM Z=Zi TO Z=ZREF
            SUM1=SUM1+(1./SWZ**2/TLZ+1./SWZD**2/TLZD)/2./FIS2*(ZREF-ZL)
            SUM1A=SUM1A+(D13RESP/1000./SWZ**2/TLZ+D13RESP/1000./SWZD**2/TLZD)/2./FIS2*(ZREF-ZL)
            SUM1B=SUM1B+(D18RESP/1000./SWZ**2/TLZ+D18RESP/1000./SWZD**2/TLZD)/2./FIS2*(ZREF-ZL)
            SUM2=SUM2+(1./SWZ**2/TLZ+1./SWZD**2/TLZD)/2./FIS2*(ZREF-ZL)
            SUM3=SUM3+(1./SWZ**2/TLZ+1./SWZD**2/TLZD)/2./FIS2*(ZREF-ZL)
          ENDIF
        ENDDO
      ENDIF

      DCK(1,N,1)=SUM1      ! CONC DERIVS = INT(SOURCE DERIV) + INT (FLUX DERIV) - dc(ZREF)/da
      DCK(2,N,2)=SUM2
      DCK(3,N,3)=SUM3
      DCK(4,N,1)=SUM1A
      DCK(5,N,1)=SUM1B
      ENDDO
    ENDDO

    DO NPR=1,3
      DFK(NPR,:,NPR)=1.

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ENDDO
  DFK(4, :, 1)=D13RESP/1000.
  DFK(5, :, 1)=D18RESP/1000.

IF (IDIS.EQ.1) THEN
DO N=1, NUMLEV
DO NPR=1, 5
  DO L=1, 7
    K=L
    IF (L.EQ.6) K=8
    IF (L.EQ.7) K=9
    ASUM=0.
    DO I=1, IS3
      ASUM=ASUM+DISC(N, I)*DSK(NPR, I, K)*(ZSOU(I)-ZSOU(I-1))
    ENDDO
    ASUM=ASUM+DISC(N, 0)*DFK(NPR, 0, K)*ZSOU(1)
    DCK(NPR, N, K)=ASUM
  ENDDO
ENDDO
ENDDO
ENDDO
ENDIF

CALL TURB2(USTARR, SIGWR, AK(6), AK(7), ZREF, ZMON, SWTOP, TLTOP)
DCKD(:, :, 1:3)=DCK(:, :, 1:3)
DCK(:, :, 1:6)=DCK(:, :, 4:9)
DCK(:, :, 7:9)=0.
DCK(:, :, 3:4)=DCKD(:, :, 6:7)
  DCK(:, :, 7:9)=DCKD(:, :, 1:3)
  DFKTOP(:, 7:9)=1.
IF (IOPT.EQ.0) THEN
  DCK(:, :, 1:3)=DCK(:, :, 7:9)
ENDIF

IF (IA.EQ.1) DCKE=DCK

808 DO J=1, NUMK
  DO K=1, NUMK
    DSUM=0.
    DO N=1, NUMLEV
      DO NPR=1, 3
        DSUM=DSUM+DCK(NPR, N, J)*DCK(NPR, N, K)/SIG(NPR, N)**2
      ENDDO
    ENDDO
    HESS(J, K)=DSUM ! RETAIN HESSIAN MATRIX
    IF (IEDDY.EQ.1) THEN
      SIGFC=ABS(0.05*FC2(NR)*VOLM) ! SIGMA OF TOTAL C FLUX
      SIGFH=ABS(0.1*H(NR)/CAPP/RHO) ! SIGMA OF TOTAL H FLUX
      SIGFE=ABS(0.1*E(NR)*VOLM) ! SIGMA OF TOTAL E FLUX
      DSUM = DSUM + DFKTOP(1, J)*DFKTOP(1, K)/SIGFC**2
      DSUM = DSUM + DFKTOP(2, J)*DFKTOP(2, K)/SIGFH**2
      DSUM = DSUM + DFKTOP(3, J)*DFKTOP(3, K)/SIGFE**2
    ENDDO
    IF (J.EQ.K) THEN ! ALPHA(J, K) = SUM( dC/dAj * dC/dAk)/SIGMA^2
      ALP(J, K)=DSUM*(1.+RL) ! *(1 + LAMBDA) ON DIAGONALS
    ELSE
      ALP(J, K)=DSUM
    ENDDO
  ENDDO
  DSUM=0.
  DO NPR=1, 3
    DO N=1, NUMLEV
      IF (DCK(NPR, N, J).NE.0.) THEN
        DSUM=DSUM+(-CK(NPR, N)+SPROF(N, NPR))*DCK(NPR, N, J)/SIG(NPR, N)**2
      ENDDO
    ENDDO
  ENDDO

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      IF (IEDDY.EQ.1) THEN
        SIGFC=ABS(0.05*FC2(NR)*VOLM) ! SIGMA OF TOTAL C FLUX
        SIGFH=ABS(0.1*H(NR)/CAPP/RHO) ! SIGMA OF TOTAL H FLUX
        SIGFE=ABS(0.1*E(NR)*VOLM) ! SIGMA OF TOTAL E FLUX
        DSUM = DSUM + (-FKTOP(1)+FC2(NR)*VOLM)*DFKTOP(1,J)/SIGFC**2
        DSUM = DSUM + (-FKTOP(2)+H(NR)/CAPP/RHO)*DFKTOP(2,J)/SIGFH**2
        DSUM = DSUM + (-FKTOP(3)+E(NR)*VOLM)*DFKTOP(3,J)/SIGFE**2
      ENDIF
      BET(J)=DSUM ! BETA(J) = SUM (C_MOD - C_MEAS) * dC/dAj / SIGMA^2
    ENDDO

! SOLVE ALP*DAK=BET
  IF (IOPT.EQ.0) THEN
    DO J=1,NUMK
      DAK(J)=1./ALP(J,J)*BET(J)
    ENDDO
  ELSE

    CALL DLSGRR(NUMK,NUMK,ALP,NUMK,1.E-12,IRANK,AINV,NUMK)
    ! INVERSE OF ALP BY SINGULAR VALUE DECOMPOSITION
    DO K=1,NUMK
      DSUM=0.
      DO J=1,NUMK
        DSUM=DSUM+AINV(K,J)*BET(J)
      ENDDO
      DAK(K)=DSUM
    ENDDO

  ENDIF
  AKO=DBLE(AK) ! KEEP OLD PARAMETERS, ADJUST NEW PARAMS
  IF (IOPT.EQ.0) THEN
    AK(1:3)=AK(1:3)+SNGL(DAK(1:3))
  ELSE
    AK(4:9)=AK(4:9)+SNGL(DAK(1:6))
  ENDIF
  EX=0.1
  IF (IFLAGC.EQ.1) GOTO 3045

3025 CONTINUE

3045 CONTINUE

  AK=SNGL(AKO)
  UHREF=UH(NR)/1.3
  USTARR=US(NR)
  SIGWR=SWR(NR)
  ZL=0.; ZREF=HCS
  CALL CALCS(PARAM,FD(NR),PAR(NR),DEF,SWDREF,LWDREF,DTIME(NR),APRESS(NR),CK(:,:), &
    XPROF,SREF,ESATL,thet1,RLAI,RC,RH,RNN,ak, &
    hcs,cica,CSOURCE,esource,80,HSOURCE,C13SOURCE,O18SOURCE,H18SOURCE, &
    UHREF,DRESP,DELTA,DEL18,DEL_E,ZSOU)
  DO I=0,40
    SK(1,I)=CSOURCE(I*2)
    SK(2,I)=HSOURCE(I*2)
    SK(3,I)=ESOURCE(I*2)
    SK(4,I)=C13SOURCE(I*2)
    SK(5,I)=O18SOURCE(I*2)
    THETL(I)=THETL(I*2)
    RNN(I)=RNN(I*2)
    RLAI(I)=RLAI(I*2)
    RC(I)=RC(I*2)
    RH(I)=RH(I*2)
    DEF(I)=DEF(I*2)
    DELTA(I)=DELTA(I*2)
    CICA(I)=CICA(I*2)
    DEL18(I)=DEL18(I*2)
  
```

```

      DEL_E(I)=DEL_E(I*2)
      ZSOU(I)=ZSOU(I*2)
ENDDO

      CALL CALCE(SPROF(:,7:9),PARAM,FD(NR),PAR(NR),SWDREF,LWDREF,DTIME(NR),APRESS(NR), &
        CK(:,),XPROF,SREF,ak,hcs,CFLUX,eflux,80,ZL,ZREF,HFLUX, &
        C13FLUX,O18FLUX,H18FLUX,UHREF,ZPR,0)
DO I=0,40
  FK(3,I)=EFLUX(I*2)
  FK(2,I)=HFLUX(I*2)
  FK(1,I)=CFLUX(I*2)
  FK(4,I)=C13FLUX(I*2)
  FK(5,I)=O18FLUX(I*2)
  ZPR(I)=ZPR(I*2)
ENDDO

DO I=1,40
  ZI=ZSOU(I)
  CALL INTVAL2(ZI,TEMP,NUML,XPROF(1:NUML),CK(2,:))
  CALL INTVAL2(ZI+0.1,TEMPD,NUML,XPROF(1:NUML),CK(2,:))
  TK=TEMP+273.15;TKD=TEMPD+273.15;DELT=(TEMPD-TEMP)/(0.1)
  CALL TURB2(USTARR,SIGWR,AK(6),AK(7),ZI,ZMON,SWZ,TLZ)
  TLPROF(I)=TLZ
  ZOBUKHOV(I)=ZMON
ENDDO

  CSUM1=0.;CSUM2=0.;CSUM3=0.;CSUM4=0.;CSUM5=0.
  DO N=1,NUMLEV
    ! CALCULATE CHI-SQUARE = SUM (C_MODEL - C_MEAS)^2 / SIGMA^2
    CSUM1=CSUM1+(CK(1,N)-SPROF(N,1))**2/SIG(1,N)**2
    CSUM2=CSUM2+(CK(2,N)-SPROF(N,2))**2/SIG(2,N)**2
    CSUM3=CSUM3+(CK(3,N)-SPROF(N,3))**2/SIG(3,N)**2
  ENDDO
  CHISQ1=CSUM1;CHISQ2=CSUM2;CHISQ3=CSUM3;CHISQ4=CSUM4;CHISQ5=CSUM5

WRITE(*,4036) CHISQ, (AK(K), K=1,9), dresp
do npr=1,3
IF(NPR.EQ.1) THEN
  ICP=10; ISP=11; IFP=12; FREF=FC2(NR); FAC=1./VOLM
  PRINT *, 'CO2:'
ELSEIF(NPR.EQ.2) THEN
  ICP=13; ISP=14; IFP=15; FREF=H(NR); FAC=RHO*CAPP
  WRITE(*,*) 'TEMPERATURE:'
ELSE
  ICP=16; ISP=17; IFP=18; FREF=E(NR); FAC=1./VOLM
  WRITE(*,*) 'H2O:'
ENDIF
FKR=FK(NPR,40)*FAC
IF(IA.GE.ITER-1) THEN
  WRITE(*,*) 'ITERATIONS FINISHED'
ELSE
  WRITE(*,*) 'NO MORE IMPROVEMENT IN CHISQ AFTER ',IA,' ITERATIONS'
ENDIF
WRITE(*,*) 'FLUX= ',FKR,'EDDY FLUX= ',FREF
WRITE(TIMDAT,116) day(NR),mon,Tthr(NR),Ttmin(NR)
116   format(4x,a2,'-',a3,5x,i2.2,':',i2.2)
write(ICP,4021) timdat
4021   format(a32)
WRITE(ICP,4032) (AK(K),K=1,9)
WRITE(ICP,4034) CHISQ
write(ICP,4031) (xprof(n),cK(NPR,n),sprof(n,NPR), N=1, NUMLEV)
write(ICP,*)
4031   format(3f10.2)
4032   FORMAT(14F10.5)
WRITE(ISP,4021) TIMDAT
WRITE(ISP,4033) (ZSOU(I), SK(NPR,I)*FAC, FK(NPR,I)*FAC,THETL(I), I=1,40)
WRITE(ISP,*)

```

```

4033   FORMAT(4F10.3)
4034   FORMAT(' CHISQ = ',F8.3)
      write(IFP,4035) timdat, FKR,fref,CHISQ
4035   format(a32,2f10.2,F8.2)
4036   FORMAT(' CHISQ = ',F8.3,' A = ',18F8.2)
4037   FORMAT(3F10.3,F10.5,2F10.7,F10.3,F10.2,F10.3,F10.2,F10.3,F10.3,ES10.3,6F10.3)
4038   format(a32)
4039   FORMAT(F10.2,2F10.3)
4040   FORMAT(3F10.3)
4041   FORMAT(A32, 5F10.2,7F8.3,9F8.2)
4042   FORMAT(20X,20F10.2)
4043   FORMAT(A20,20F10.2)
4044   FORMAT(A20,20F10.3)
4045   FORMAT(F10.2,2F10.5)
4046   FORMAT(2F10.3)
4047   FORMAT(9F10.3)
4048   FORMAT(36ES11.3)
4050   FORMAT(13A10)
      IF(NPR.EQ.3) THEN
        WRITE(19,4035) TIMDAT,FKR*RLAM*18.015*1.E-6,EREF,CHISQ*RLAM*18.015*1.E-6
      ENDIF

      ENDDO
      write(20,4038) timdat
555   WRITE(20,4050) ' Z', ' LEAF TEMP', ' NET RAD', ' LEAF AREA', ' GSC', &
      ' GBH', ' DA', ' DELTA', ' CI/CA', ' DELTA180', ' DELTA_E', &
      ' TL', ' ZMON'
      WRITE(20,4037) (ZSOU(I), THETL(I), RNN(I), RLAI(I), 1./RC(I), 1./RH(I), DEF(I), &
      DELTA(I), CICA(I), DEL18(I), DEL_E(I), TLPROF(I), ZOBUKHOV(I), &
      SK(1,I)/VOLM,FK(1,I)/VOLM, &
      SK(2,I)/VOLM,FK(2,I)/VOLM, SK(3,I)*RHO*CAPP,FK(3,I)*RHO*CAPP, I=0,40)

      write(20,*)
      WRITE(*,*) 'ZMON= ', ZMON
      CALL INTVAL(28., 28., TEMP, CO2, H2O,NLEVL,ZZZ,PROF,28.,20,NR)
      ESAT=6.1375*EXP(17.502*TEMP/(240.97+TEMP))
      SL=17.502*240.97/(240.97+TEMP)**2*esat
      sl=0.622*pmb/(pmb-0.378*esat)**2*sl
      ep=rlam/cAPp*sl
      eqg=ep*rnn(0)*.9/(ep+1.)
      WRITE(23, 4041) TIMDAT, AK(1)/VOLM, AK(2)*CAPP*RHO, AK(3)/VOLM, &
      eqg,AK(3)/VOLM*RLAM*18.015*1.E-6,EP,ak(4),AK(5),AK(6),AK(7),ak(8),ak(9), &
      CHISQ,CHISQ1,CHISQ2,CHISQ3,CHISQ4,CHISQ5,dresp
      IF(IX.EQ.1) THEN
        WRITE(24,4042) xprof
        WRITE(25,4042) XPROF
        WRITE(26,4042) XPROF
        WRITE(27,4042) XPROF
        IX=0
      ENDIF
      WRITE(24, 4043) TIMDAT, CK(1,1:NUMLEV)
      WRITE(24, 4043) TIMDAT, SPROF(1:NUMLEV,1)
      WRITE(25, 4043) TIMDAT, CK(2,1:NUMLEV)
      WRITE(25, 4043) TIMDAT, SPROF(1:NUMLEV,2)
      WRITE(26, 4043) TIMDAT, CK(3,1:NUMLEV)
      WRITE(26, 4043) TIMDAT, SPROF(1:NUMLEV,3)

      WRITE(*,*) (ak(n), n=1,9)
      IF(ICOSTFN.EQ.1) THEN
        WRITE(31, 4047) (COSTFN(ICOST-1,1,N),N=1,9)
        WRITE(31, 4047) (COSTFN(ICOST-1,2,N),N=1,9)
        WRITE(31, 4047) (COSTFN(ICOST-1,3,N),N=1,9)
      ELSEIF(ICOSTFN.EQ.2) THEN
! INVERT HESSIAN MATRIX
      CALL DLSGRR(NUMK,NUMK,HESS,NUMK,1.E-12,IRANK,AINV,NUMK)
      ! INVERSE OF HESS BY SINGULAR VALUE DECOMPOSITION
      DO K=1,numk

```

```

        WRITE(31, 4048) (AINV(J,K), J=1,numk)
    ENDDO
        WRITE(31, *) IRANK
    ENDIF
    ENDIF
4004 CONTINUE

10000 end do                                !end reading control file

450  stop

460  stop 'error reading CO2 data'
480  stop 'error reading Temperature data'
490  stop 'error reading Vap press data'
500  stop 'error reading Flux data'
510  stop 'error reading SIGC data'
520  stop 'error reading SIGH data'
530  stop 'error reading SIGT data'

4    STOP
540  STOP 'CHISQ NaN'

    END

```

G.2 Subroutines

The following Fortran 90 code gives the subroutines and functions called in the programs CANMOD (§G.1.1) and GROUNDFLUX (§G.1.2) above.

```

$debug

!*****
    FUNCTION RKN(ZETA)
! NEAR-FIELD KERNEL FUNCTION IN LOCALIZED NEAR-FIELD THEORY
    DATA C1 /-0.39894/
    DATA C2 /-0.15623/
    IF (ZETA.EQ.0) STOP 'RKN: ZETA=0'
    EZ=EXP(-ABS(ZETA))
    RKN=C1*ALOG(1-EZ)+C2*EZ
    RETURN
    END

!*****
    FUNCTION RKNINT(ZETA)
! INTEGRAL OF NEAR-FIELD KERNEL FUNCTION: SMALL-ZETA APPROXIMATION
! VALID TO RELATIVE ERROR 0.001 AT ZETA=0.1
    DATA C3 /-0.39894/
    DATA C4 /-0.14127/
    DATA C5 /0.333333/
    ZA=ABS(ZETA)
    IF (ZA.EQ.0) THEN
        RKNINT=0
    RETURN
    END IF
    RKNINT=C3*ZA*(ALOG(ZA)-1)+C4*ZA+C5*(ZA**2)/2
    RETURN
    END

!*****

```

```

      SUBROUTINE INTEGR(X,Y,N,AREA)
! MRR, 26-NOV-80
! USES TRAPEZOIDAL RULE TO INTEGRATE FUNCTION Y(X), SPECIFIED AT N
! POINTS (X(I),Y(I),I=1,N). INTEGRAL GOES FROM X(1) TO X(N).
      DIMENSION X(N),Y(N)
      AREA=0
      IF (N.LE.0) STOP 'INTEGR: N<=0'
      IF (N.EQ.1) RETURN
      DO 1 I=2,N
      AREA=AREA+0.5*(Y(I)+Y(I-1))*(X(I)-X(I-1))
1      CONTINUE
      RETURN
      END

!*****
      SUBROUTINE SHSOR2(X,N,NMAX,NS)
! MRR, 03-APR-85 (ADAPTED FROM SHSORT)
! SORT (X(I,1),I=1,N) INTO ASCENDING ORDER WITH SHELL SORT. FORCE
! OTHER SERIES ((X(I,K),I=1,N),K=2,NS) TO HAVE SAME ORDER AS X(I,1).
      DIMENSION X(NMAX,NS),Y(10)
      IF (NS.GT.10) STOP 'SHSOR2: NS TOO BIG'
! M=INCREMENT=2**IM-1 (IM=LIM,...,1)
      LIM=ALOG(REAL(N+1))/ALOG(2.0)
! LOOP THROUGH VALUES OF M (SORTING INCREMENT)
      DO 1 IM=LIM,1,-1
      M=2**IM-1
! DO M DIFFERENT M-SORTS, STARTING AT IS
      DO 2 IS=1,M
! DO 1 M-SORT BY INSERTION
      DO 3 I=IS+M,N,M
      DO 7 K=1,NS
7      Y(K)=X(I,K)
      DO 4 J=I-M,IS,-M
      IF (X(J,1).GT.Y(1)) THEN
      DO 5 K=1,NS
5      X(J+M,K)=X(J,K)
      ELSE
      DO 6 K=1,NS
6      X(J+M,K)=Y(K)
      GOTO 3
      END IF
4      CONTINUE
      DO 8 K=1,NS
8      X(IS,K)=Y(K)
3      CONTINUE
2      CONTINUE
1      CONTINUE
      DO 10 I=2,N
      IF (X(I,1).LT.X(I-1,1)) WRITE(*,100) I
100  FORMAT(' SHELL SORT: OUT OF ORDER AT I =',I6)
10      CONTINUE
      RETURN
      END

!*****
      SUBROUTINE AIR(TC,PMB,RHO,VOLM,CAPP,RLAM,QSAT,EPSI)
! MRR, 09-NOV-88
! 23-OCT-91: MODIFIED TO USE BETTER GAS CONSTANT
!           MOLAR VOLUME VOLM INCLUDED IN ARGUMENT LIST
! AT TEMP T! (DEG C) AND PRESSURE PMB (MB), RETURN:
! RHO = AIR DENSITY (KG M-3)
! VOLM = MOLAR VOLUME (M3 MOL-1)
! CAPP = SPECIFIC HEAT OF AIR AT CONSTANT PRESSURE (J KG-1 K-1)
! RLAM = LATENT HEAT FOR WATER (J KG-1)
! QSAT = SATURATION SPECIFIC HUMIDITY (KG/KG) FROM TETEN FORMULA

```

```

! EPSI = (RLAM/CAPP)*D(QSAT)/DT
! A,B,C ARE TETEN COEFFS
! RGAS = UNIVERSAL GAS CONSTANT IN J/MOL/K = 8.3143
! RMAIR, RMH2O = KG-MOLECULAR WEIGHTS OF DRY AIR, WATER
! NUMERICAL VALUES FROM WALLACE AND HOBBS
  DATA A /6.106/
  DATA B /17.27/
  DATA C /237.3/
  DATA RGAS /8.3143/
  DATA RMAIR /0.02897/
  DATA RMH2O /0.018016/
! CAPP IN (J/KG/K), RLAM IN (J/KG), RHO IN (KG/M3), VOLM IN (M3/MOL)
  CAPP = 1004
  RLAM = (2501-2.38*TC)*1000
  TK = 273.16+TC
  PPA = 100*PMB
  RHO = RMAIR*PPA/(RGAS*TK)
  VOLM = RGAS*TK/PPA
! ES = SATURATION VAPOUR PRESSURE (MB), QSAT = SAT SPECIFIC HUM (KG/KG)
  ES=A*EXP(B*TC/(C+TC))
  QSAT=(RMH2O/RMAIR)*ES/PMB
  DESDT=ES*B*C/(C+TC)**2
  DQSDT=(RMH2O/RMAIR)*DESDT/PMB
  EPSI=(RLAM/CAPP)*DQSDT
  RETURN
  END

!*****
  SUBROUTINE COMSKP(IUNIT)
! MRR, 5-AUG-83
! SKIPS COMMENT LINES IN CONTROL DATA FILE, STOPS IF EOF FOUND
  CHARACTER*1 COM
1   READ(IUNIT,100,END=2) COM
100  FORMAT(A1)
     IF(COM.EQ.'C'.or.com.eq.'c') GOTO 1
     BACKSPACE IUNIT
     RETURN
2    STOP 'CONTROL FILE EOF'
     END

!*****
  subroutine phi(z,hc,zMon,phi_w,phi_h)
! calculates phi_w=sig_w/u*
! and phi_h=(k.z/T*)(dT/dz)
! assume z_ruff = 2.3*hc to obtain matching of T_L = 0.4 at z_ruff
! d = 0.75*hc
! z height above ground
! hc canopy height
! zMon Monin-Obukhov length

  if(abs(zMon).lt.0.001) then !check for L=0
    phi_w=1.25
    phi_h=1.0
    return
  end if

  z_ruff=2.3*hc
  z_d=0.75*hc

  if(z.ge.z_ruff) then
    zeta=(z-z_d)/zMon
  else
    zeta=hc/zMon
! zeta=(hc-z_d)/zMon
  end if

```

```

if(zMon.le.0.0) then
  phi_w=1.25*(1.0+3.0*abs(zeta)**0.333
  phi_h=(1.0+16*abs(zeta)**(-0.5)
else
  phi_w=1.25*(1.0+0.2*zeta)
  phi_h=1.0+5.0*zeta
end if

return
end
!*****

SUBROUTINE INTERP(NDATA,XDAT,FDATA,X,Y,TH,NUML,NINTV,BREAK,CSCOE)

! TH = TOP HEIGHT, LEVEL TO WHICH INTERPOLATION SHOULD BE TAKEN
INTEGER   NDATA

      INTEGER   NINTV, NOUT,N,L
      REAL      BREAK(NDATA), CSCOE(4,NDATA), CSVAL, &
              FDATA(NDATA), X(numl),XDATA(NDATA),XDAT(NDATA),Y(numl)
      EXTERNAL  CSAKM, CSVAL, UMACH

N=NDATA
XDATA=XDAT
!           Compute cubic spline interpolant
      CALL CSAKM (N, XDATA, FDATA, BREAK, CSCOE)
!           Get output unit number
      CALL UMACH (2, NOUT)

      NINTV = NDATA - 1
! calculate spline values between data
!   xd=TH/NUML
      xd=TH/(NUML-1)
      X(1)=0.7
      Y(1)=CSVAL(X(1),NINTV,BREAK,CSCOE)
!   X(2)=0.5
      Y(2)=CSVAL(X(2),NINTV,BREAK,CSCOE)
do l=2,NUML
!   do l=1,NUML
      X(L)=XD*(L-1)
!   X(L)=XD*L
      Y(L)=CSVAL(X(L),NINTV,BREAK,CSCOE)
ENDDO

RETURN
END

!*****

SUBROUTINE INTVAL(Z, DZ, TEMP, CO2, H2O,NLEVL,ZZZ,PROF,TH,NUML,NR)
! EVALUATE AVERAGE INTERPOLATED DATA FOR EACH SOURCE LAYER
REAL B(9),FS(4,9),X(NUML),Y(NUML),ZZZ(9,3),PROF(9,9,308)
INTEGER NLEVL(3),KK,I
EXTERNAL CSVAL

DO KK=1,3
CALL INTERP(NLEVL(KK),ZZZ(:,KK),PROF(:,KK,NR),X,Y,TH,NUML,NV,B,FS)
SUMV=0
DO I=1,40
XV=(Z-DZ)+I*DZ/40
SUMV=SUMV+CSVAL(XV,NV,B,FS)
ENDDO
IF (KK.EQ.1) THEN
CO2=SUMV/40
ELSEIF (KK.EQ.2) THEN

```

```

TEMP=SUMV/40
ELSEIF (KK.EQ.3) THEN
H2O=SUMV/40
ENDIF
ENDDO

RETURN
END

```

```
!*****
```

```

subroutine CALCE(DER2,DER,PARAM,FD,PAR,SWD,LWDR,DTIME,PA,CK,XPROF,SREF,ak, &
             hcs,CFLUX,eflux,is3,ZZL,ZREF,HFLUX,C13FLUX,O18FLUX,H18FLUX,UHREF, &
             ZPR,IFLAG)
PARAMETER ISMAX=1000, NUML=20
REAL PARAM(5), SREF(6),XPROF(100),DER(NUML,3),DER2(NUML,2),AK(18)
REAL eflux(0:ISMAX), &
     HFLUX(0:ISMAX),CFLUX(0:ISMAX),C13FLUX(0:ISMAX), &
     ZPR(0:ISMAX),O18FLUX(0:ISMAX), H18FLUX(0:ISMAX)
REAL CK(6,NUML),KBF,KDF,LWDR
REAL*8 DTIME
integer istop
external betai,BETA
data A /6.1375/
data B /17.502/
data C /240.97/
DATA RSTD /0.011894/, R18STD /0.0020672/, AB /7.4/, SMOW /0.0020052/

DEL_S=-18.
ISOTOPES=1
HA=PARAM(1);HB=PARAM(2); DL=0.001
BETLAI=BETA(HA,HB)
istop=IS3
fis3=float(istop)
is4=10.
fis4=float(is4)
IL=20
dz=(zref-zzl)/fis3/fis4
ST=1. ! STOMATA: 1=AMPHISTOMATOUS, 2=HYPOSTOMATOUS
ALAM=AK(5) !*100.
VFAC=AK(4)
KDF=AK(8)
KBF=AK(9)

EFLUX(0)=AK(3) !/10.
HFLUX(0)=AK(2) !/10.
CFLUX(0)=AK(1) !/10.
C13FLUX(0)=0.
DRESP=17.6; DAIR=-8.2
RAIR=(DAIR/1000.+1.)*RSTD
C13FLUX(0)=CFLUX(0)*RAIR/(DRESP/1000.+1.)
D18RESP=15.; D18AIR=-1.
R18AIR=(D18AIR/1000.+1.)*R18STD
O18FLUX(0)=CFLUX(0)*R18AIR/(D18RESP/1000.+1.)
H18FLUX(0)=EFLUX(0)*((DEL_S-ESTAR)/1000.+1.)*SMOW
ZPR(0)=0.
AV13C=0.; ASUM=0.
DO I=1,ISTOP
ESUM=0.
HSUM=0.
CSUM=0.
C13SUM=0.
O18SUM=0.
H18SUM=0.
DO N=1,is4
ZAH=ZZL/HCS+(FLOAT(N)/fis4*1./FIS3+FLOAT(I-1)/FIS3)*(ZREF-ZZL)/HCS

```

```

ZAN=ZAH+(1./FIS4*1./FIS3)*(ZREF-ZZL)/HCS
ZAL=ZAN*HCS
IF(ZAL.LE.HCS) THEN
  WI=EXP(PARAM(5)*(ZAH-1))*UHREF
  WIN=EXP(PARAM(5)*(ZAN-1))*UHREF
  RH=1./PARAM(3)*(DL/WI)**0.5
  RHN=1./PARAM(3)*(DL/WIN)**0.5
  RLAI=(ZAH**(HA-1.)*(1-ZAH)**(HB-1.))/BETLAI*PARAM(4)
  RLAIN=(ZAN**(HA-1.)*(1-ZAN)**(HB-1.))/BETLAI*PARAM(4)
  CLAI=BETAI(1.-ZAH,HB,HA)*PARAM(4)
  CLAIN=BETAI(1.-ZAN,HB,HA)*PARAM(4)

CALL INTVAL2(zah*HCS,co,NUML,XPROF(1:NUML),CK(1,:))
CALL INTVAL2(zah*HCS,TA,NUML,XPROF(1:NUML),CK(2,:))
CALL INTVAL2(zah*HCS,WAT,NUML,XPROF(1:NUML),CK(3,:))
CALL INTVAL2(ZAH*HCS,D13C,NUML,XPROF(1:NUML),CK(4,:))
CALL INTVAL2(ZAH*HCS,D18O,NUML,XPROF(1:NUML),CK(5,:))
CALL INTVAL2(ZAH*HCS,D18V,NUML,XPROF(1:NUML),CK(6,:))
  RAIR=D13C/CO
  R18AIR=D18O/CO
  R18VAP=D18V/WAT
  TK=TA+273.15
  ESTAR=2.644-3206./TK+1.5342E6/TK**2
CALL INTVAL2(ZAN*HCS,coN,NUML,XPROF(1:NUML),CK(1,:))
CALL INTVAL2(ZAN*HCS,TAN,NUML,XPROF(1:NUML),CK(2,:))
CALL INTVAL2(ZAN*HCS,WATN,NUML,XPROF(1:NUML),CK(3,:))
CALL INTVAL2(ZAH*HCS,D13CN,NUML,XPROF(1:NUML),CK(4,:))
CALL INTVAL2(ZAH*HCS,D18ON,NUML,XPROF(1:NUML),CK(5,:))
CALL INTVAL2(ZAH*HCS,D18VN,NUML,XPROF(1:NUML),CK(6,:))
  RAIRN=D13CN/CON
  R18AIRN=D18ON/CON
  R18VAPN=D18VN/WATN
  TKN=TAN+273.15
  ESTARN=2.644-3206./TKN+1.5342E6/TKN**2
CALL INTVAL2(ZAH*HCS,DC,NUML,XPROF(1:NUML),DER(:,1))
CALL INTVAL2(ZAH*HCS,DT,NUML,XPROF(1:NUML),DER(:,2))
CALL INTVAL2(ZAH*HCS,DE,NUML,XPROF(1:NUML),DER(:,3))
CALL INTVAL2(ZAN*HCS,DCD,NUML,XPROF(1:NUML),DER(:,1))
CALL INTVAL2(ZAN*HCS,DTD,NUML,XPROF(1:NUML),DER(:,2))
CALL INTVAL2(ZAN*HCS,DED,NUML,XPROF(1:NUML),DER(:,3))
CALL INTVAL2(ZAH*HCS,DCI,NUML,XPROF(1:NUML),DER2(:,1))
CALL INTVAL2(ZAN*HCS,DCID,NUML,XPROF(1:NUML),DER2(:,1))
CALL INTVAL2(ZAH*HCS,DOI,NUML,XPROF(1:NUML),DER2(:,2))
CALL INTVAL2(ZAN*HCS,DOID,NUML,XPROF(1:NUML),DER2(:,2))

CALL ASSIM(KBF,KDF,AG,ALAM,VFAC,FD,PAR,DTIME,SWD,LWDR,TA,PA,CO,WAT,CLAI, &
  RH,FC,FH,FE,TL,GSA,CI,DA,RNZ)
CC=CI-0.1*CO
HSOU=FH*RLAI/HCS-DT
CSOU=FC*RLAI/HCS-DC
ESOU=FE*RLAI/HCS-DE
DELTA=4.4+22.6*CI/CO
C13SOU=RAIR/(DELTA/1000.+1.)*CSOU-DCI
DEL_V=(R18VAP/SMOW-1.)*1000.
EK=(28./GSA/1.6+19.*RH*0.93*2.)/(1./GSA/1.6+RH*0.93*2.)
DEL_E = DEL_S + (EK+ESTAR) + (DEL_V-DEL_S-EK)*WAT/(DA+WAT)
DEL18 = AB + (DEL_E - (R18AIR/R18STD-1.)*1000.)*CC/(CO-CC)
O18SOU=R18AIR/(DEL18/1000.+1.)*CSOU-DOI
H18SOU=((DEL_E-ESTAR)/1000.+1.)*SMOW*ESOU
CALL ASSIM(KBF,KDF,AG,ALAM,VFAC,FD,PAR,DTIME,SWD,LWDR,TAN,PA,CON,WATN,CLAIN, &
  RHN,FC,FH,FE,TL,GSA,CIN,DA,RNZ)
CCN=CIN-0.1*CON
HSOUN=FH*RLAIN/HCS-DTD
CSOUN=FC*RLAIN/HCS-DCD
ESOUN=FE*RLAIN/HCS-DED
DELTAN=4.4+22.6*CIN/CON

```

```

C13SOUN=RAIRN/(DELTAN/1000.+1.)*CSOUN-DCID
DEL_VN=(R18VAPN/SMOW-1.)*1000.
EKN=(28./GSA/1.6+19.*RHN*0.93*2.)/(1./GSA/1.6+RHN*0.93*2.)
DEL_EN = DEL_S + (EKN+ESTARN) + (DEL_VN-DEL_S-EKN)*WATN/(DA+WATN)
DEL18N = AB + (DEL_EN - (R18AIRN/R18STD-1.)*1000.)*CCN/(CON-CCN)
O18SOUN=R18AIRN/(DEL18N/1000.+1.)*CSOUN-DOID
H18SOUN=((DEL_EN-ESTARN)/1000.+1.)*SMOW*ESOUN

```

```

HSUM=HSUM+(HSOU+HSOUN)/2. *DZ
CSUM=CSUM+(CSOU+CSOUN)/2. *DZ
ESUM=ESUM+(ESOU+ESOUN)/2. *DZ
C13SUM=C13SUM+(C13SOU+C13SOUN)/2. *DZ
O18SUM=O18SUM+(O18SOU+O18SOUN)/2. *DZ
H18SUM=H18SUM+(H18SOU+H18SOUN)/2. *DZ

```

```

AV13C=AV13C+RAIR/(DELTA/1000.+1.)*CSOU
ASUM=ASUM+CSOU

```

```

ENDIF
ENDDO
ZPR(I)=ZZL+FLOAT(I)/FIS3*(ZREF-ZZL)
IF(IFLAG.EQ.1) THEN
  EFLUX(I)=ESUM; HFLUX(I)=HSUM; CFLUX(I)=CSUM; C13FLUX(I)=C13SUM
  O18FLUX(I)=O18SUM; H18FLUX(I)=H18SUM; GOTO 100
ENDIF
EFLUX(I)=ESUM+EFLUX(I-1)
HFLUX(I)=HSUM+HFLUX(I-1)
CFLUX(I)=CSUM+CFLUX(I-1)
C13FLUX(I)=C13SUM+C13FLUX(I-1)
O18FLUX(I)=O18SUM+O18FLUX(I-1)
H18FLUX(I)=H18SUM+H18FLUX(I-1)
ENDDO
AV13C=AV13C/ASUM

```

```

100 return
end

```

```

!*****

```

```

subroutine CALCS(PARAM,FD,PAR,DEF,SWD,LWDR,DTIME,PA,CK,XPROF,SREF,ESATL,thet1,RLAI,RC, &
  RH,RN,ak,hcs,cica,csource,esource,is3,HSOURCE,C13SOURCE,O18SOURCE,H18SOURCE, &
  UHREF,DRESP,DELTA,DEL18,DEL_E,ZSOU)
PARAMETER ISMAX=1000, NUML=20
real PARAM(5),SREF(5),AK(18)
REAL esource(0:ISMAX),esatl(0:ISMAX),thet1(0:ISMAX), &
  csource(0:ISMAX),XPROF(100),C13SOURCE(0:ISMAX), &
  HSOURCE(0:ISMAX), RLAI(0:ISMAX), &
  RC(0:ISMAX),RN(0:ISMAX),RH(0:ISMAX), DEF(0:ISMAX),DELTA(0:ISMAX), &
  CICA(0:ISMAX),O18SOURCE(0:ISMAX),DEL18(0:ISMAX),H18SOURCE(0:ISMAX),DEL_E(0:ISMAX)
REAL CK(6,NUML),KBF,KDF,ZSOU(0:ISMAX),LWDR
REAL*8 DTIME
integer istop
external betai,BETA
data A /6.1375/
data B /17.502/
data C /240.97/
DATA RSTD /0.011894/, R18STD /0.0020672/, AB /7.4/, SMOW /0.0020052/

COUNT=0.
DO IK=1,NUML
  IF(XPROF(IK).LE.HCS) THEN
    COUNT=COUNT+1
  ENDIF
ENDDO

DEL_S=-18.

```

```

ISOTOPES=1
ST=1.      ! STOMATA: 1=AMPHISTOMATOUS, 2=HYPOSTOMATOUS
HA=PARAM(1);HB=PARAM(2); DL=0.001
BETLAI=BETA(HA,HB)
ALAM=AK(5) !*100.
VFAC=AK(4)
KDF=AK(8)
KBF=AK(9)

istop=is3
fis3=float(istop); DZ=1./FIS3
IL=20
  AVDEL=0.
  CSUM=0.
  NC=0.;X2=0.
do i=0,istop-1
  ZAH=FLOAT(I)/FIS3
  ZAL=ZAH*HCS
  ZAH=FLOAT(I)/FIS3*COUNT
  J=NINT(ZAH)
  IF(J.EQ.0)THEN; X1=0.;ELSE; X1=XPROF(J); ENDIF
  IF(X1.EQ.X2) THEN; NC=0.; ELSE; NC=NC+1; ENDIF
  IF(J.LT.20)THEN;IF(XPROF(J+1).GT.HCS) THEN; X2=HCS; ELSE; X2=XPROF(J+1); ENDIF;ENDIF
  IF(J.GT.0)THEN;IF(XPROF(J).GT.HCS) THEN; X1=HCS; ENDIF;ENDIF
  ZAH=NC/FIS3*COUNT
  ZAL=X1+(X2-X1)*ZAH
  ZAH=ZAL/HCS
  WI=EXP(PARAM(5)*(ZAH-1))*UHREF
  RH(I)=1./PARAM(3)*(DL/WI)**0.5
  RLAI(I)=(ZAH**(HA-1.)*(1-ZAH)**(HB-1.))/BETLAI*PARAM(4)
  CLAI=BETAI(1.-ZAH,HB,HA)*PARAM(4)

CALL INTVAL2(ZAL,CO,NUML,XPROF(1:NUML),CK(1,:))
CALL INTVAL2(ZAL,TA,NUML,XPROF(1:NUML),CK(2,:))
CALL INTVAL2(ZAL,WAT,NUML,XPROF(1:NUML),CK(3,:))
CALL INTVAL2(ZAL,D13C,NUML,XPROF(1:NUML),CK(4,:))
CALL INTVAL2(ZAL,D18O,NUML,XPROF(1:NUML),CK(5,:))
CALL INTVAL2(ZAL,D18V,NUML,XPROF(1:NUML),CK(6,:))
RAIR=D13C/CO
R18AIR=D18O/CO
R18VAP=D18V/WAT
TK=TA+273.15
ESTAR=2.644-3206./TK+1.5342E6/TK**2

CALL ASSIM(KBF,KDF,AG,ALAM,VFAC,FD,PAR,DTIME,SWD,LWDR,TA,PA,CO,WAT,CLAI, &
  RH(I),FC,FH,FE,TL,GSA,CI,DA,RNZ)
CC=CI-0.1*CO
HSOURCE(I)=FH*RLAI(I)/HCS
CSOURCE(I)=FC*RLAI(I)/HCS
ESOURCE(I)=FE*RLAI(I)/HCS
DELTA(I)=4.4+22.6*CI/CO
CICA(I)=CI/CO
C13SOURCE(I)=RAIR/(DELTA(I)/1000.+1.)*CSOURCE(I)
DEL_V=(R18VAP/SMOW-1.)*1000.
EK=(28./GSA/1.6+19.*RH(I)*0.93*2.)/(1./GSA/1.6+RH(I)*0.93*2.)
DEL_E(I) = DEL_S + (EK+ESTAR) + (DEL_V-DEL_S-EK)*WAT/(DA+WAT)
DEL18(I) = AB + (DEL_E(I) - (R18AIR/R18STD-1.)*1000.)*CC/(CO-CC)
O18SOURCE(I)=R18AIR/(DEL18(I)/1000.+1.)*CSOURCE(I)
H18SOURCE(I)=(DEL_E(I)-ESTAR)/1000.+1.)*SMOW*ESOURCE(I)

DEF(I)=DA
THETL(I)=TL
RC(I)=1./GSA
AVDEL=AVDEL+DELTA(I)*CSOURCE(I)
CSUM=CSUM+CSOURCE(I)
! RN(O)=AG

```

```

      RN(I)=RNZ
      ZSOU(I)=ZAL
      CONTINUE
    enddo
  AVDEL=AVDEL/CSUM
  DRESP=AVDEL
  WI=UHREF;
  RH(ISTOP)=1./PARAM(3)*(DL/WI)**0.5; RLAI(ISTOP)=0.;
  CALL INTVAL2(HCS,TE,NUML,XPROF(1:NUML),CK(2,:))
  CALL INTVAL2(HCS,WAT,NUML,XPROF(1:NUML),CK(3,:))
  CALL INTVAL2(HCS,CO,NUML,XPROF(1:NUML),CK(1,:))
  CALL INTVAL2(HCS,D180,NUML,XPROF(1:NUML),CK(5,:))
  CALL INTVAL2(HCS,D18V,NUML,XPROF(1:NUML),CK(6,:))
  R18AIR=D180/CO
  R18VAP=D18V/WAT
  TK=TA+273.15
  ESTAR=2.644-3206./TK+1.5342E6/TK**2
  CALL ASSIM(KBF,KDF,AG,ALAM,vfac,FD,PAR,DTIME,SWD,LWDR,TA,PA,CO,WAT,CLAI, &
    RH(I),FC,FH,FE,TL,GSA,CI,DA,RNZ)
  CC=CI-0.1*CO
  RN(ISTOP)=RNZ
  DELTA(ISTOP)=4.4+22.6*CI/CO
  CICA(ISTOP)=CI/CO
  DEL_V=(R18VAP/SMOW-1.)*1000.
  EK=(28./GSA/1.6+19.*RH(ISTOP)*0.93*2.)/(1./GSA/1.6+RH(ISTOP)*0.93*2.)
  DEL_E(ISTOP) = DEL_S + (EK+ESTAR) + (DEL_V-DEL_S-EK)*WAT/(DA+WAT)
  DEL18(ISTOP) = AB + (DEL_E(ISTOP) - (R18AIR/R18STD-1.)*1000.)*CC/(CO-CC)
  THETL(ISTOP)=TL
  DEF(ISTOP)=DA
  RC(ISTOP)=1./GSA
  ESATL(ISTOP)=A*EXP(B*(THETL(ISTOP)))/(C+THETL(ISTOP))
  ESOURCE(istop)=0.
  HSOURCE(ISTOP)=0.
  CSOURCE(ISTOP)=0.
  C13SOURCE(ISTOP)=0.
  O18SOURCE(ISTOP)=0.
  H18SOURCE(ISTOP)=0.
  ZSOU(ISTOP)=HCS
  ESOURCE(0)=0.
  HSOURCE(0)=0.
  CSOURCE(0)=0.
  C13SOURCE(0)=0.
  O18SOURCE(0)=0.
  H18SOURCE(0)=0.
  ZSOU(0)=0.
222 RETURN
END

```

!*****

```

      SUBROUTINE INTVAL2(Z, INTV, NDATA, XDAT, FDATA)
! EVALUATE AVERAGE INTERPOLATED DATA FOR EACH SOURCE LAYER
      INTEGER      NINTV, N, NDATA
      REAL         BREAK(NDATA), CSCOE(4,NDATA), CSVAL, &
                  XDATA(NDATA), XDAT(NDATA), INTV
      REAL         FDATA(NDATA)
      EXTERNAL    CSAKM, CSVAL

      N=NDATA
      XDATA=XDAT
!
      Compute cubic spline interpolant
      CALL CSAKM (N, XDATA, FDATA, BREAK, CSCOE)

      NINTV = NDATA - 1

```

```

INTV=CSVAL(Z,NINTV,BREAK,CSCOE) ! GET INTERPOLATED VALUE AT Z

RETURN
END

!*****

SUBROUTINE ASSIM(KBF,KDF,AG,ALAM,vfac,FRACD,PAR,DTIME,SWD,LWDR,TEMP,PA,CA,WAT,CLAI,RBH, &
FC,FH,FE,TL,GS,CI,DA,RNZ)
IMPLICIT REAL(A-Z)
PARAMETER (NALPHA=9)
INTEGER I, ITER
REAL*8 TIME, DTIME
REAL ILSUN(NALPHA), ILSUNR(NALPHA), COSALPHA(NALPHA), ILSUNE(NALPHA), JLSUN25(NALPHA), &
JLSUNT(NALPHA), CISU(NALPHA), AVLSU25(NALPHA), AJLSU25(NALPHA), AVLSUT(NALPHA), &
AJLSUT(NALPHA), ALSUN(NALPHA), FALPHA(NALPHA), ALPHA(O:NALPHA), &
ALSU25(NALPHA), GSCSU(NALPHA), GCSU(NALPHA), RSCSU(NALPHA), RSESU(NALPHA), TLSUN(NALPHA), &
ESATLSU(NALPHA), FHSUN(NALPHA), FESUN(NALPHA), DOSUN(NALPHA)

LAT=60.5
PI = 3.1415926
KC25=40.4*10.;KO25=24800. ! MICHAELIS-MENTON CONSTANTS OF RUBISCO FOR CO2 AND O2
EAKC=59400.;EAKO=36000.;EAVCMX=64800.
PCD=0.036 !CANOPY REFLECTION COEFFICIENT FOR DIFFUSE PAR
PCDR=0.2 ! CANOPY REFLECTION COEFFICIENT FOR DIFFUSE NIR
KD1=0.719 !diffuse and scattered diffuse PAR extinction coefficient (radians)
KD=KDF
! KD=KBF*1.56
! KDF=KBF*1.56
FA=0.426 ! FORWARD SCATTERING COEFFICIENT OF PAR IN THE ATMOSPHERE
NO=150. ! NITROGEN CONC AT CANOPY TOP (148 FROM WALCROFT ET AL. 1997, 250 from measured
! N conc and SLA=2.5 from Bergh et al. 1998, 280 from Kellomaki+Wang)
KN=0.7 ! NITROGEN EXTINCTION COEFF (DE P + F)
NB=0. ! NITROGEN NOT USED IN PHOTOSYNTH (25 FROM DE P + F, -8 from Kellomaki+Wang)
O2=20900. ! OXYGEN CONCENTRATION
SJ=625.9;HJ=256000.;EJ=48000. !parameter for electron transport(SJ,JK-1mol-1;HJ,Jmol-1;EJ is
!* activation energy, Jmol-1)
THETA=0.7 ! CURVATURE OF ELECTRON TRANSPORT WITH IRRADIANCE, DAVID 0.7, WALCROFT 0.9
GSTR25=3.69*10. ! GAMMA STAR, CO2 COMPENSATION POINT, DAVID GIVES 3.69, WALCROFT 4.27
ERKC=66400. ! EFFECT OF TEMP ON RESP
PO=1013 ! ATM PRESSURE AT SEA LEVEL
SIGMA=0.15 ! LEAF SCATTERING COEFFICIENT OF PAR
ALPHA_L=PI/3. !AVERAGE LEAF ANGLE
AA=6.1375 ! CONSTANTS FOR SATURATION VAPOUR PRESSURE
BB=17.502
CC=240.97
PAS=PA*100. ! PRESSURE IN PASCALS
TK=TEMP+273.15 ! TEMPERATURE IN K
CP=1005.+(TEMP+23.15)**2/3364. ! SPECIFIC HEAT CAPACITY OF AIR AT CONSTANT PRESSURE
RLAM=(2501.-2.38*TEMP)*1000. ! LATENT HEAT OF VAPOURISATION
RMH2O=0.018 ! MOLECULAR WEIGHT OF WATER
RMAIR=0.028965 ! AVERAGE MOLECULAR WEIGHT OF AIR
RGAS=8.3143 ! IDEAL GAS CONSTANT
RHO=RMAIR*PAS/RGAS/TK ! AIR DENSITY
VOLM=RGAS*TK/PAS ! MOLAR VOLUME OF AIR
EMISS=0.98 ! LEAF EMISSIVITY
STEFBOL=5.67E-8 ! STEFAN-BOLTZMANN CONSTANT
TIME=DTIME-36891. ! TIME IN DAY OF YEAR PLUS FRACTIONAL HOUR
CA=CA ! CO2 IN UMOL/MOL
CICA=0.6 ! INITIAL CI/CA
CI=CICA*CA ! INTERCELLULAR CO2
CISUV=CI; CISUJ=CI; CISDJ=CI
LAI=CLAI ! CUMULATIVE LEAF AREA INDEX AT THIS LEVEL
LC=4.3 ! TOTAL CANOPY LEAF AREA INDEX
A2=0.425 ! FRACTION OF PAR ABSORBED BY PSII, TANIA USES 0.3, WALCROFT 0.2

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GO=0.01      ! INTERCEPT OF GC RELATION (MOL/M2/S) FROM LEUNING 1995
A1=4.4       ! SLOPE OF GC RELATION LEUNING 1995
DO=15.       ! VAPOUR PRESSURE DEFICIT PARAMETER FOR GC RELATION LEUNING 1995
LAMBDA=ALAM ! GS MODEL LAMBDA
FAC=vfac     ! FACTOR TO TWEAK VCMAX
SWABS=0.2    ! ABSORPTION COEFF FOR NEAR IR
KCOR=SWABS**0.5 ! K CORRECTION FOR SWABS
KLW=KDF      ! EXT. COEFF. FOR DOWNWARD LW
KL=KDF
LWG=EXP(-KL*(LC-LAI))*EMISS*STEFBOL*273.15**4
LWGA=KL*LWG
LWD=-EMISS*STEFBOL*TK**4*(EXP(-KL*LAI)-1.)
LWDA=-KL*EMISS*STEFBOL*TK**4*EXP(-KL*LAI)
LWU=-EMISS*STEFBOL*TK**4*(EXP(-KL*(LC-LAI))-1.)
LWUA=-KL*EMISS*STEFBOL*TK**4*EXP(-KL*(LC-LAI))
LWL=EMISS*STEFBOL*TK**4*0.5 ! FACTOR 0.5 FOR PROJECTED LA
! LWDR=EMISS*STEFBOL*(TK-20.)**4

! LEAF ANGLES
ALPHA(0)=0.
DO I=1,NALPHA
  ALPHA(I)=PI/2./NALPHA*FLOAT(I)
  FALPHA(I)=-COS(ALPHA(I))+COS(ALPHA(I-1))
  COSALPHA(I)=0.5*(SIN(ALPHA(I))**2-SIN(ALPHA(I-1))**2)/FALPHA(I)
ENDDO

!*RAD converts degrees into radians:
RAD = PI/180.

!*Sine and cosine of latitude:
SINLAT = SIN(RAD*LAT)
COSLAT = COS(RAD*LAT)

!*Maximal sine of declination:
SINDCM = SIN(RAD*23.4)

!*Sine and cosine of declination
SINDEC = -SINDCM*COS(2.*PI*(TIME+10.)/365.)
COSDEC = SQRT(1.-SINDEC*SINDEC)

!*The terms A and B
A = SINLAT*SINDEC
B = COSLAT*COSDEC

!*Daylength
DAYL = 12.*(1.+(2./PI)*ASIN(A/B) )

!*Generating hour from day
HOUR = (TIME-IDINT(TIME))*24.

!*Determining solar noon (Iqbal, 1983) (TOO) and
!* hour angle of sun (H) for specified location
! PARAMETER LS=150.;LES=147.34
GAD=2.*PI*(TIME-1.)/365.
ET=0.017+0.4281*COS(GAD)-7.351*SIN(GAD)- &
  3.349*COS(2.*GAD)-9.371*SIN(2.*GAD)
! TOO=12.+(4.*(LS-LES)-ET)/60.
TOO=12.97
H=PI*(HOUR-TOO)/12.

!*Sine of solar height:
SINB=A+B*COS(H)

!*Solar constant fluctuations (W/m2):
SC = 1367. *(1.+0.033*COS(2.*PI*(TIME-10.)/365.))

!! INTEGRAL OF SINE OF SOLAR HEIGHT OVER THE HOUR OF THIS PROFILE
SININT = A + B*12./PI*(SIN(PI/12.*(HOUR-TOO))-SIN(PI/12.*(HOUR-1.-TOO)))

!! RADIATION IN KJ/M2/HR FROM THAT IN W/M2
RDD=max(SWD*3.6,0.)

!! HOURLY AVERAGE ATMOS. TRANS.
ATMTR = RDD/(SININT*3.6*SC)

!*diurnal radiation on top of canopy(micromol m-2s-1)
S = MAX(0.,ATMTR*SC*SINB*0.5*4.55)

! RADIATION AT TOP OF CANOPY FROM MEASURED PAR (MICROMOL/M2/S)
S = MAX(0.,PAR)

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```

SR=MAX(0.,SWD)
SLW=MAX(0.,LWDR)
!*beam radiation extinction coefficient of canopy(radians)
KB=0.5/SINB
KB=KBF/SINB
PSWH=(1.-SWABS**0.5)/(1.+SWABS**0.5)
PSWB=1.-EXP(-2.*PSWH*KB/(1.+KB))
PSWD=0.38
!*beam and scattered beam PAR extinction coefficient (radians)
KB1=0.46/SINB
KB1=KBf*(1.-SIGMA)**0.5/SINB
KD1=KDF*(1.-SIGMA)**0.5
!*canopy reflection coefficient for beam PAR
PCB=1.-EXP(-2.*0.041*KB/(1.+KB))
PCBR=1.-EXP(-2.*0.382*KB/(1.+KB))
PCDR=1.-EXP(-2.*0.382*KD/(1.+KD))
!*the optical air mass
M=(PA/PO)/SINB
!*fraction of diffuse radiation
FD=(1.-ATMTR**M)/(1.+ATMTR**M*(1./FA-1.))
FD=MIN(FRACD,1.)
!*Diffuse PAR per unit ground area (umolm-2s-1)
ID=FD*S
IDR=FD*(SR-S/4.55)
!*Beam PAR per unit ground area (umolm-2s-1)
IB=(1.-FD)*S
IBR=(1.-FD)*(SR-S/4.55)
! DIFFUSE PAR AT LEAF LEVEL
IDL=(1.-pcd)*KD1*ID*EXP(-KD1*LAI)
IDLR=(1.-pcdr)*KD*KCOR*IDR*EXP(-KD*KCOR*LAI)
IDLW=KLW*SLW*EXP(-KLW*LAI)
! REFLECTED PAR AND NIR
IDPAR=0.5*KL*(1.-sigma)**0.5*IB*EXP(-KB1*LC)*EXP(-KL*(1.-sigma)**0.5*(LC-LAI))
IDNIR=0.5*KL*(swabs)**0.5*IBR*EXP(-KB*KCOR*LC)*EXP(-KL*(swabs)**0.5*(LC-LAI))
! SCATTERED PAR AT LEAF LEVEL
IBS=IB*((1.-pcd)*KB1*EXP(-KB1*LAI)-(1.-sigma)*KB*EXP(-KB*LAI))
IBSR=IBR*(KB*KCOR*EXP(-(1.-pcdr)*KB*KCOR*LAI)-swabs*KB*EXP(-KB*LAI))
!*Total canopy absorption
IC=(1.-PCB)*IB*(1.-EXP(-KB1*LAI))+ &
(1.-PCD)*ID*(1.-EXP(-KD1*LAI))
!*PAR absorbed by the sunlit leaves FOR WHOLE CANOPY
ICSUN=IB*(1.-0.15)*(1.-EXP(-KB*LAI))+ &
ID*(1.-PCD)*(1.-EXP(-(KD1+KB)*LAI))*KD1/(KD1+KB) &
+IB*((1.-PCB)*(1.-EXP(-(KB1+KB)*LAI))*KB1/(KB1+KB) &
-(1.-0.15)*(1.-EXP(-2.*KB*LAI))/2.)
! PAR ABSORBED BY SUNLIT LEAVES FOR INDIVIDUAL LEVELS
DO I=1,NALPHA
ILSUN(I)=(1.-SIGMA)*IB*COSALPHA(I)/SINB+IDL+IBS+IDPAR
ILSUNR(I)=SWABS*IBR*COSALPHA(I)/SINB+IDLR+IBSR
ENDDO
!*PAR absorbed by the shaded leaves
ICSHD=IC-ICSUN
! PAR ABSORBED BY SHADED LEAVES FOR INDIVIDUAL LEAVES
ILSHD=(IDL+IBS+IDPAR)
ILSHDR=(IDLR+IBSR)
!*PAR effectively absorbed by the sunlit and shaded leaves
ICSUNE=ICSUN*A2
ICSHDE=ICSHD*A2
ILSUNE=ILSUN*A2
ILSHDE=ILSHD*A2
!*Total PAR effectively absorbed by the canopy
ICTOTE=ICSUNE+ICSHDE
!*CANOPY NITROGEN DISTRIBUTION AND PHOTOSYNTHETIC CAPACITY
!*leaf nitrogen concentration per unit leaf area (mmolm-2)
!*for soybean
NL= 148.

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!*CANOPY PHOTOSYNTHETIC CAPACITY (at 25 oC)
!*photosynthetic rubisco capacity per unit leaf area (umolm-2s-1) 116 FOR SOYBEAN
! value of 32.7 from Walcroft et al. 1997 for Pinus radiata PER TOTAL LEAF AREA
! (20 AT 20 DEG C CONVERTS TO 32.7 AT 25 DEG C ACCORDING TO THEIR EQUATION)
! but this is 98 on a projected leaf area basis OR 65 PER ONE-SIDED LA
! WHICH IS ~ THE SAME AS PROJECTED LA FOR FIR AND SPRUCE COMPARED TO PINE
! KELLOMAKI+WANG 2000 GET XN25=0.18 AT 20 DEG, FOR N IN MMOL/PROJECTED LA
! REGRESSION IN WALCROFT HAS SLOPE 0.212
! factor 0.5 for post-winter recovery (rough guess from Bergh et al. 1998)
  VL25=65*0.5 ! this value not used - see below
!*ratio of measured Rubisco capacity to leaf N, 0.21 FROM WALCROFT ET AL. 1997
  XN25=VL25/(NL-NB)
  XN25=0.2*1.64*FAC ! 1.64 FACTOR TO CONVERT TO 25 DEG
                    ! FACTOR FAC FOR POST-WINTER RECOVERY
!*photosynthetic capacity of sunlit and shaded leaves
EK=MAX(0.,(1.-EXP(-KN-KB*LAI)))
VC25=LAI*XN25*(NO-NB)*(1.-EXP(-KN))/KN
VCSU25=LAI*XN25*(NO-NB)*EK/(KB*LAI+KN)
VCS25=VC25-VCSU25
NL=(NO-NB)*EXP(-KN*LAI/LC)+NB
! NL=NO*EXP(-KN*LAI/LC)
NL=NO
VL25=XN25*(NL-NB)
!*maximum rate of electron transport per unit leaf area (umolm-2s-1)
  JMSU25=2.1*VCSU25
  JMSD25=2.1*VCS25
! MAX ELECTRON TRANSPORT AT LEAF LEVEL AT 25 DEG ratio from Walcroft et al. 1997
  JML25=2.1*VL25
!*CANOPY PHOTOSYNTHESIS
!*The Farquhar et al.(1980.1982) equations
!*Effect of temperature on VL(leaf) AND VC(canopy)
!   VCT=VC25*EXP((1./298.-1./(TEMP+273.))*EAVCMX/8.314)
  VLT=VL25*EXP((1./298.-1./(TEMP+273.))*EAVCMX/8.314)
  VLT=VL25*EXP(26.35-65330/8.314/(TEMP+273.15)) !NEW PHOTOSYNTH PARAMS BERNACCHI ET AL. 2001
!   VCSUNT=VCSU25*EXP((1./298.-1./(TEMP+273.))*EAVCMX/8.314)
!   VCSHDT=VCS25*EXP((1./298.-1./(TEMP+273.))*EAVCMX/8.314)
!*Effect of temperature on Michaelis-Menten constant of rubisco
!*   for O2 and CO2 (Pa)
  KO=KO25*EXP((1./298.-1./(TEMP+273.))*EAKO/8.314)
  KC=KC25*EXP((1./298.-1./(TEMP+273.))*EAKC/8.314)
  KO=100.*EXP(20.3-36380/8.314/(TEMP+273.15)) !NEW PHOTOSYNTH PARAMS BERNACCHI ET AL. 2001
  KC=EXP(38.05-79430/8.314/(TEMP+273.15)) !NEW PHOTOSYNTH PARAMS BERNACCHI ET AL. 2001
!*Effect of temperature on gammastar
  GMSTAR=GSTR25+(0.188*(TEMP-25.)+0.0036*(TEMP-25.))**2.)*10.
  GMSTAR=EXP(19.02-37830/8.314/(TEMP+273.15)) !NEW PHOTOSYNTH PARAMS BERNACCHI ET AL. 2001
! MAX ELECTRON TRANSPORT AT LEAF LEVEL AND TEMP
  JMLT=JML25*EXP((((TEMP+273.2)/298.2-1.)*EJ)/(8.3144*( &
    TEMP+273.2)))*(1.+EXP((298.2*SJ-HJ)/(298.2*8.3144)))/ &
    (1.+EXP((SJ*(TEMP+273.2)-HJ)/(8.3144*(TEMP+273.2))))
! ELECTRON TRANSPORT AT LEAF LEVEL AND TEMP
  DO I=1,NALPHA
    JLSUNT(I)=(ILSUNE(I)+JMLT-SQRT(((ILSUNE(I)+JMLT)**2.)-(4.*THETA* &
      ILSUNE(I)*JMLT)))/(2.*THETA)
  ENDDO
  JLSHDT=(ILSHDE+JMLT-SQRT(((ILSHDE+JMLT)**2.)-(4.*THETA* &
    ILSHDE*JMLT)))/(2.*THETA)
!*Assimilation rate limited by rubisco (Av) and
!*limited by electron transport (Aj) at 25 oC
  K25=40.4*(1.+02/24800.)
  CISU(1:NALPHA)=CI
  CISD=CI
! FRACTION OF LEAVES IN SUN
  FSUN=EXP(-KB*LAI)
!*RESPIRATION (at 25 oC)
!*Leaf and canopy respiration (at 25 oC),umolm-2s-1
!*for soybean

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      RL25=VL25*0.0089
!      RC25=(VC25*RL25/VL25)
!*Effect of temperature on respiration
!      PARAM ERKC=66400.
      RLT=RL25*EXP((1./298.-1./(TEMP+273.))*ERKC/8.314)
      RLT=RL25*EXP(18.73-46390/8.314/(TEMP+273.15)) !NEW PHOTOSYNTH PARAMS BERNACCHI ET AL. 2001
!      RCT=RC25*EXP((1./298.-1./(TEMP+273.))*ERKC/8.314)
      K=KC*(1.+O2/KO)
! FIND VAPOUR PRESSURE DEFICIT
      ESAT=AA*EXP(BB*TEMP/(CC+TEMP))
      DA=ESAT-WAT
! SLOPE OF VP WITH TEMP
      SL=BB*CC/(CC+TEMP)**2*ESAT
! CHANGE OF LATENT HEAT WITH SENSIBLE HEAT
      EPSILON=SL*RLAM/CP/PA
! GAMMA AT TEMP
      GMT=(RLT/VLT*K+GMSTAR)/(1.-RLT/VLT)
! EFFECTIVE BOUNDARY LAYER RESISTANCE FOR HEAT
      RBHSTAR=1./(1./(RBH*VOLM)+4.*STEFBOL*EMISS*TK**3/(CP*RHO*VOLM))
      H=1./(RBH*0.93*2.*VOLM+EPSILON*RBHSTAR)
! LEAF TO AIR VPD WHEN STOMATA ARE FULLY CLOSED
      DO I=1,NALPHA
        DOSUN(I)=DA+EPSILON*RBHSTAR/RLAM*(ILSUN(I)/4.55+ILSUNR(I)+ &
          IDLW+LWGA+(LWDA+LWUA)+IDPAR/4.55+IDNIR)
        DOSUN(I)=DOSUN(I)*1000.
      ENDDO
      DOSHD=DA+EPSILON*RBHSTAR/RLAM*(ILSHD/4.55+ILSHDR+ &
        IDLW+LWGA+(LWDA+LWUA)+IDPAR/4.55+IDNIR)
      DOSHD=DOSHD*1000.
! IF(ITER.GT.0) THEN
  IF(DA.LT.0.) THEN
    DA=1. !; WAT=ESAT
  ENDIF

!ANALYTICAL SOLUTION FOR ASSIMILATION
  RBC=RBH*1.3*2.*VOLM
  DO I=1,NALPHA
    DSQRT=SQRT(1.6*DOSUN(I)*(CA-GMT)/LAMBDA)
    AAV=RBC-1.6/H
    BBV=DSQRT-CA-K+(RLT-VLT)*(RBC-1.6/H)
    CCV=(RLT-VLT)*(DSQRT-CA)-VLT*GMSTAR-K*RLT
    SQV=BBV**2-4.*AAV*CCV
    IF(SQV.LT.0) THEN
      AJLSUT(I)=0.
    ELSE
      AVLSUT(I)=(-BBV-SQRT(BBV**2-4.*AAV*CCV))/2./AAV
    ENDIF
    AAJ=4.*(RBC-1.6/H)
    BBJ=4.*(DSQRT-CA-2.*GMSTAR)+(4.*RLT-JLSUNT(I))*(RBC-1.6/H)
    CCJ=(4.*RLT-JLSUNT(I))*(DSQRT-CA)-8.*RLT*GMSTAR-JLSUNT(I)*GMSTAR
    SQJ=BBJ**2-4.*AAJ*CCJ
    IF(SQJ.LT.0) THEN
      AJLSUT(I)=0.
    ELSE
      AJLSUT(I)=(-BBJ-SQRT(BBJ**2-4.*AAJ*CCJ))/2./AAJ
    ENDIF
    ALSUN(I)=MIN(AVLSUT(I),AJLSUT(I))
  ENDDO
  DSQRT=SQRT(1.6*DOSHD*(CA-GMT)/LAMBDA)
  AAV=RBC-1.6/H
  BBV=DSQRT-CA-K+(RLT-VLT)*(RBC-1.6/H)
  CCV=(RLT-VLT)*(DSQRT-CA)-VLT*GMSTAR-K*RLT
  SQV=BBV**2-4.*AAV*CCV
  IF(SQV.LT.0.) THEN
    AVLSDT=0.
  ELSE

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    AVLSDT=(-BBV-SQRT(BBV**2-4.*AAV*CCV))/2./AAV
ENDIF
AAJ=4.*(RBC-1.6/H)
BBJ=4.*(DSQRT-CA-2.*GMSTAR)+(4.*RLT-JLSHDT)*(RBC-1.6/H)
CCJ=(4.*RLT-JLSHDT)*(DSQRT-CA)-8.*RLT*GMSTAR-JLSHDT*GMSTAR
SQJ=BBJ**2-4.*AAJ*CCJ
IF(SQJ.LT.0) THEN
    AJLSDT=0.
ELSE
    AJLSDT=(-BBJ-SQRT(BBJ**2-4.*AAJ*CCJ))/2./AAJ
ENDIF
ALSHD=MIN(AVLSDT,AJLSDT)

DO I=1,NALPHA
    GCSU(I)=(ALSUN(I))/(SQRT(MAX(1.6/LAMBDA*DOSUN(I)*(CA-GMT),0.))-1.6*(ALSUN(I))/H)
    GCSU(I)=1./(1./(GCSU(I))+RBC)
    IF(GCSU(I).GT.0.) THEN
        CISU(I)=CA-ALSUN(I)/GCSU(I)
    ELSE
        CISU(I)=CA
    ENDIF
ENDIF
ENDDO
GSCSD=(ALSHD)/(SQRT(MAX(1.6/LAMBDA*DOSH*(CA-GMT),0.))-1.6*(ALSHD)/H)
GCSU(I)=1./(1./(GSCSD)+RBC)
IF(GCSD.GT.0.) THEN
    CISD=CA-ALSHD/GCSD
ELSE
    CISD=CA
ENDIF

! NET ASSIMILATION
SUM=0.
DO I=1,NALPHA
    SUM=SUM+ALSUN(I)*FALPHA(I)
ENDDO
ALTNET=SUM*FSUN+ALSHD*(1.-FSUN)

! BOUNDARY LAYER AND STOMATAL RESISTANCE FOR CO2 IN S/M
GSUM=0.; CISUM=0.
DO I=1,NALPHA
    GSUM=GSUM+GCSU(I)*FALPHA(I)*VOLM
    RSCSU(I)=1./(GCSU(I)*VOLM)
    CISUM=CISUM+CISU(I)*FALPHA(I)
    RSESU(I)=RSCSU(I)/1.6
ENDDO
AVGSCSU=GSUM
RBC=RBH*1.3*2.; RSCSD=1./(GSCSD*VOLM)
GS=AVGSCSU*FSUN+1./RSCSD*(1.-FSUN)
CI=CISUM*FSUN+CISD*(1.-FSUN)
IF(DA.EQ.0.) THEN
    RSCSU=0.; RSCSD=0.
ENDIF

! BOUNDARY LAYER AND STOMATAL RESISTANCE FOR H2O
RBE=RBH*0.93*2.; RSESD=RSCSD/1.6

! SATURATION VAPOUR DENSITY AT AIR TEMP + SLOPE WITH TEMP
ESAT=AA*EXP(BB*TEMP/(CC+TEMP))*rmh2o/VOLM/1000.
SL=BB*CC/(CC+TEMP)**2*esat

! LEAF TEMPERATURE FOR SHADE LEAVES
LWL=EMISS*STEFBOL*(TLSHD+273.15)**4*0.5 !FACTOR 0.5 FOR PROJECTED LA
TLSHD=TEMP + (ILSHD/4.55+ILSHDR+IDLW+LWGA+(LWDA+LWUA)+IDPAR/4.55+IDNIR - &
    RLAM*(ESAT-WAT*rmh2o/volm/1000.)/(RBE+RSESD))/ &
    (RLAM*SL/(RBE+RSESD) + RHO*CP/RBH + 4.*EMISS*STEFBOL*TK**3)
TLSHD=MAX(TLSHD,0.); TLSHD=MIN(TLSHD,30.)

! SAT VAPOUR DENS AT LEAF TEMP FOR SHADE LEAVES
ESATLSD=AA*EXP(BB*TLSHD/(CC+TLSHD))*rmh2o/VOLM/1000.
TLSHD=TEMP + (ILSHD/4.55+ILSHDR+IDLW+LWGA+(LWDA+LWUA)+IDPAR/4.55+IDNIR - &

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      RLAM*(ESATLSD-WAT*rmh2o/volm/1000.)/(RBE+RSESD))/ &
      (RHO*CP/RBH + 4.*EMISS*STEFBOL*TK**3)
      TLSHD=MAX(TLSHD,0.); TLSHD=MIN(TLSHD,30.)
! LEAF TEMPERATURE FOR SUN LEAVES
      DO I=1,NALPHA
      LWL=EMISS*STEFBOL*(TLSUN(I)+273.15)**4*0.5 !FACTOR 0.5 FOR PROJECTED LA
      TLSUN(I)=TEMP + (ILSUN(I)/4.55+ILSUNR(I)+IDLW+LWGA+(LWDA+LWUA)+IDPAR/4.55+IDNIR - &
      RLAM*(ESAT-WAT*rmh2o/volm/1000.)/(RBE+RSESU(I)))/ &
      (RLAM*SL/(RBE+RSESU(I)) + RHO*CP/RBH + 4.*EMISS*STEFBOL*TK**3)
      TLSUN(I)=MAX(TLSUN(I),0.); TLSUN(I)=MIN(TLSUN(I),30.)
! SAT VAPOUR DENS AT LEAF TEMP FOR SUN LEAVES
      ESATLSU(I)=AA*EXP(BB*TLSUN(I)/(CC+TLSUN(I)))*rmh2o/VOLM/1000.
      TLSUN(I)=TEMP + (ILSUN(I)/4.55+ILSUNR(I)+IDLW+LWGA+(LWDA+LWUA)+IDPAR/4.55+IDNIR - &
      RLAM*(ESATLSU(I)-WAT*rmh2o/volm/1000.)/(RBE+RSESU(I)))/ &
      (RHO*CP/RBH + 4.*EMISS*STEFBOL*TK**3)
      TLSUN(I)=MAX(TLSUN(I),0.); TLSUN(I)=MIN(TLSUN(I),30.)
      ENDDO
! AVERAGE LEAF TEMPERATURE
      TLSUM=0.
      DO I=1,NALPHA
      TLSUM=TLSUM+TLSUN(I)*FALPHA(I)
      ENDDO
      TL=TLSUM*FSUN+TLSHD*(1.-FSUN)
! HEAT FLUX (K M/S) AND WATER FLUX (MMOL/MOL M/S) FOR SUN LEAVES
      DO I=1,NALPHA
      FHSUN(I)=1./RBH*(TLSUN(I)-TEMP)
      FESUN(I)=1./(RBE+RSESU(I))*(ESATLSU(I)/RMH20*VOLM*1000.-WAT)
      ENDDO
! HEAT FLUX (K M/S) AND WATER FLUX (MMOL/MOL M/S) FOR SHADE LEAVES
      FHSHD=1./RBH*(TLSHD-TEMP)
      FESHSD=1./(RBE+RSESD)*(ESATLSD/RMH20*VOLM*1000.-WAT)
! TOTAL HEAT (K M/S), WATER (MMOL/MOL M/S) AND CO2 (MICROMOL/MOL M/S) FLUX AT LEAF LEVEL
      HSUM=0.; ESUM=0.
      DO I=1,NALPHA
      HSUM=HSUM+FHSUN(I)*FALPHA(I)
      ESUM=ESUM+FESUN(I)*FALPHA(I)
      ENDDO
      FH=HSUM*FSUN+FHSHD*(1.-FSUN)
      FE=ESUM*FSUN+FESHSD*(1.-FSUN)
      FC=-ALTNET*VOLM
! AVAIL ENERGY AT GROUND ASSUMING ALL PAR INTERCEPTED AND ALL ELSE NOT
      AG=SWD-PAR/4.55
! AVAIL ENERGY AT LEVEL Z
      ID=FD*S
      IB=(1.-FD)*S
      IDL=(1.-pcd)*ID*EXP(-KD1*LAI)
      IBS=IB*((1.-pcd)*EXP(-KB1*LAI)-(1.-sigma)*EXP(-KB*LAI))
      IDPAR=0.5*IB*EXP(-KB1*LC)*EXP(-KL*(1.-sigma)**0.5*(LC-LAI))
      ISUN=((1.-PCB)*IB+IDL+IBS-IDPAR)
      ISHD=(IDL+IBS-IDPAR)
      FSUN=EXP(-KB*LAI)
      IDR=FD*(SR-S/4.55)
      IBR=(1.-FD)*(SR-S/4.55)
      IDLR=(1.-pcdr)*IDR*EXP(-KD*KCOR*LAI)
      IBSR=IBR*((1.-pcdr)*EXP(-KB*KCOR*LAI)-swabs*EXP(-KB*LAI))
      IDLW=SLW*EXP(-KLW*LAI)
      IDNIR=0.5*IBR*EXP(-KB*KCOR*LC)*EXP(-KL*(swabs)**0.5*(LC-LAI))
      ISUNR=((1.-PCDR)*IBR+IDLR+IBSR+IDLW-IDNIR)
      ISHDR=(IDLR+IBSR+IDLW-IDNIR)
      FSUNR=EXP(-KB*LAI)
      RNZ=FSUNR*(ISUNR-LWU+LWD-LWG)+(1.-FSUNR)*(ISHDR-LWU+LWD-LWG)+ &
      (FSUN*ISUN+(1.-FSUN)*ISHD)/4.55

      RETURN
      END

```

```

!*****
      subroutine TURB2 (UST,SWR,A6,B,Z,ZMON, sw,TL)
!-----
! Find turbulence statistics sw and TL at height z
! For sw, use aa = sw/ustar:
!   when zhc > zhc1:   aa = aa1
!   when 1 < zhc < zhc1: aa varies linearly between aah and aa1
!   when 0 < zhc < 1:   aa varies exponentially with coefficient csw
! For TL, use cc = TL*ustar/hc
!   when zhc > 1:     cc = max (vonk*(z-disp)/(hc*aa1**2), cch)
!   when zhc0 < zhc < 1: cc = cch
!   when 0 < zhc < zhc0: cc varies linearly from 0 to cch
! 22-oct-99 (MRR): rewritten from version in SOURCE10
!-----
      REAL AA1,AAH,AO,CCH,CCO,CSW,ALFAB,ALFAC,HC,SWREF,USTAR
      common /t/ ITURE,AA1,AAH,AO,CCH,CCO,CSW,ALFAB,ALFAC, &
             HC,SWREF,USTAR,IST_COR
      vonk = 0.4                      ! von Karman constant
      DISP = 0.75
      ZHC1 = 1.0
      ZHC0 = 0.15
      ZHC2 = -0.1
      ZHC3 = 0.1
      zhc = z/hc
      ustar = swr/aa1
      c1 = vonk/aa1
      c0 = 0.3
      C00 = 0.0
      A=A6 !*100.
      if (zhc.lt.0) stop 'TURB: zhc < 0'
      call phi(z,hc,zMon,phi_w,phi_h)      !stability function
! Find sw:
      if(iturb.eq.1) then      ! exponential profile
         if (zhc.gt.zhc1) then
            aa = aa1                      ! well above hc
         else if (zhc.ge.DISP) then
            aa = aah + (zhc-DISP)*(aa1-aah)/(zhc1-DISP)  ! just above hc
         else
            aa = aah * exp(csw*(zhc-DISP))      ! below hc
         end if
         sw = aa * ustar
      elseif (iturb.eq.2) then  !linear profile
         if (zhc.gt.zhc1) then
            aa = aa1
         elseif (ZHC.GT.ZHC2) THEN
            aa = a0 + (aa1-a0)*(zhc/zhc1)
         ELSEIF (ZHC.GT.ZHC3) THEN
            AA = 0.1 + (ZHC2*AA1+(1.-ZHC2)*A0-0.1)*(ZHC-ZHC3)/ZHC2
         ELSE
            AA = 0.00001 + (0.1 - 0.00001)*ZHC/ZHC3
         !
            AA = 0.01
         endif
         sw = aa*ustar
      elseif (iturb.eq.3) then  ! polynomial profile
         if(zhc.lt.1.05) then
            aa = -1.2344*zhc**3 + 1.698*zhc**2 + 0.6938*zhc + 0.099
         else
            aa = aa1
         endif
         sw = aa*ustar
      elseif(iturb.eq.4) then  ! cosine profile
         if(zhc.gt.1) then
            aa = aa1
         else
            aa = (aa1+a0)/2 + (aa1-a0)/2*cos(3.14159*(1-zhc))
         end if
      end if

```

```

        endif
        sw = aa*ustar
    else
        stop 'incorrect iturb'
    endif
    if(ist_cor.eq.1)    SW = ustar*aa*phi_w/1.25
! Find TL:
    if (zhc.gt.2) then
        cc1 = vonk*(zHC-disp)/(aa1**2)           ! above z=hc
        cc = max(cc1,cch)
    else
        cc = cch * min(1.0,zhc/zhc0)           ! below z=hc
    end if
    if(iturb.eq.5) then
        cc = c1*(zhc-disp) + (c0+c1*disp)*exp(-c1*zhc/(c0+c1*disp))
    elseif(iturb.eq.0) then
        cc = cc0 + (cch-cc0)*(zhc-zhc0)/(1.-zhc0)
        if(zhc.lt.zhc0) then
            cc = C00+(cc0-C00)*zhc/zhc0
        endif
    ELSEIF(ITURB.EQ.3) THEN
        IF(A.GT.100.) THEN
            IF(ZHC.EQ.0) THEN
                CC=0.
            ELSE
                CC=B
            ENDIF
        ELSE
            CC = B*(1.-EXP(-A*ZHC))/(1.-EXP(-A))
        ENDIF
    endif
    if(ist_cor.eq.1)    cc=cc*1.25**2/(phi_w**2 * phi_h)
    TL = cc * (hc/ustar)

    return
end

!*****

SUBROUTINE DISPM2(US,SW,A,B,timdat,NMAX,nlevl,NREF,M0,M,Z,ZC,zMon, &
DIS,DISN,DISF,IWRITE)

! CALCULATE DISPERSION MATRIX DIS(I,J), SUCH THAT:
! C(I)-C(NREF) = SUM (J=M0,M) (DIS(I,J)*S(J)*DZ(J))
! NEAR-FIELD AND FAR-FIELD PARTS OF DIS RETURNED SEPARATELY IN ARRAYS
! DISN AND DISF. PARAMETER NMAX SETS FIRST DIMENSION OF DIS ARRAYS.
! ARRAY ZC(N): HOLDS HEIGHTS AT WHICH CONCENTRATIONS C(I) ARE GIVEN.
! REFERENCE LEVEL IS I=NREF, SO ZREF=ZC(NREF).
! ARRAY Z(0:M): HOLDS HEIGHT LIMITS OF SOURCE LAYERS, WITH Z(M)=HC.
! CALCULATIONS EXTEND ONLY OVER SOURCES (J=M0,M), WHERE M0 IS 0 OR 1.
! ELEMENT J=0 CORRESPONDS TO GROUND-LEVEL SOURCE. FOR J>=1, UNIT SOURCE
! UNIFORMLY FILLS LAYER J, BETWEEN Z(J-1 AND Z(J)

integer nint
PARAMETER(NINT=50)
REAL DIS(NMAX,0:M),DISN(NMAX,0:M),DISF(NMAX,0:M), &
Z(0:M),ZC(nlevl),RINT(nint),ZI(nint), &
zs(-1:nint),dz(-1:nint)
character timdat*32
HC=Z(M)
ZREF=ZC(NREF)

! LOOP THROUGH INDICES OF ARRAY DIS(I,J)
DO 1 J=M0,M           ! LEVEL OF UNIT SOURCE
IF(J.EQ.0) THEN
    ZS(J)=0

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      DZ(J)=0
    ELSE
      zs(j)=(Z(J)+Z(J-1))/2
      dz(j)=Z(J)-Z(J-1)
    ENDIF
    call turb2(US,SW,A,B,zs(j),Zmon,swj,tlj)
    RLJ=SWJ*TLJ
    DO 2 I=1,nlevl                ! LEVEL OF CONCENTRATION
! FIRST GET FAR-FIELD PART DISF, ASSUMING ZREF>HC
      IF (ZC(I).LT.ZREF) THEN      ! ZC(I) BELOW ZREF
        DO K=1,nint
          ZI(K) = ZC(I) + (ZREF-ZC(I))*FLOAT(K-1)/FLOAT(NINT-1)
          CALL TURB2(US,SW,A,B,ZI(K),zMon,SW,TL)
          RKF=SW**2*TL            ! FAR-FIELD DIFFUSIVITY
        IF(J.GT.0) THEN
          IF (ZI(K).LE.Z(J-1)) THEN ! GET FLUX FROM UNIT SOURCE
            FLUX=0                ! FLUX BELOW SOURCE LAYER
          ELSE IF (ZI(K).LE.Z(J)) THEN
            FLUX=(ZI(K)-Z(J-1))/dz(j) ! FLUX WITHIN SOURCE LAYER
          ELSE
            FLUX=1                ! FLUX ABOVE SOURCE LAYER
          END IF
        ELSE
          FLUX=1
        ENDIF
        RINT(K)=FLUX/RKF
      END DO
      CALL INTEGR(ZI,RINT,NINT,AREAF)
    ELSE IF (ZC(I).EQ.ZREF) THEN   ! ZC(I) AT ZREF
      AREAF=0
    ELSE                            ! ZC(I) ABOVE ZREF
      DO K=1,NINT
        ZI(K) = ZREF + (ZC(I)-ZREF)*FLOAT(K-1)/FLOAT(NINT-1)
        CALL TURB2(US,SW,A,B,ZI(K),zMon,SW,TL)
        RKF=SW**2*TL            ! FAR-FIELD DIFFUSIVITY
        FLUX=1                  ! ALWAYS TRUE SINCE ZREF>=HC
        RINT(K)=FLUX/RKF
      END DO
      CALL INTEGR(ZI,RINT,NINT,AREAF)
      AREAF=-AREAF              ! SIGN CHANGE BECAUSE ZREF BELOW
    END IF
    DISF(I,J)=AREAF
! NOW GET NEAR-FIELD PART DISN
    IF (J.EQ.0) THEN              ! GROUND SOURCE: NO NEAR FIELD
      DISN(I,J)=0
    ELSE                            ! ELEVATED SOURCE
      T2=RKN((ZC(I)+zs(j))/RLJ)/SWJ ! C AT IMAGE Z
      T3=RKN((ZREF-zs(j))/RLJ)/SWJ ! C AT ZREF
      T4=RKN((ZREF+zs(j))/RLJ)/SWJ ! C AT IMAGE ZREF
      IF (ZC(I).GT.Z(J-1).AND.ZC(I).LE.Z(J)) THEN
!
        ZJI=(Z(J-1)+ZC(I))/2      ! JI IS MEAN OF Z(J-1),ZC(I)
        ZIJ=(ZC(I)+Z(J))/2        ! IJ IS MEAN OF ZC(I),Z(J)
        CALL TURB2(US,SW,A,B,ZJI,zMon,SWJI,TLJI)
        CALL TURB2(US,SW,A,B,ZIJ,zMon,SWIJ,TLIJ)
        T1JI=TLJI*RKNINT((ZC(I)-Z(J-1))/(SWJI*TLJI))
        T1IJ=TLIJ*RKNINT((Z(J)-ZC(I))/(SWIJ*TLIJ))
        T1=(T1JI+T1IJ)/dz(j)
      ELSE
        T1=RKN((ZC(I)-zs(j))/RLJ)/SWJ ! C AT Z: ZC(I) OUTSIDE SOURCE
      END IF
      DISN(I,J)=T1+T2-T3-T4
    END IF

! ADD DISF AND DISN TO GET DIS(I,J)
    DIS(I,J)=DISF(I,J)+DISN(I,J)

```

```

2   CONTINUE
1   CONTINUE

! WRITE DISPERSION MATRIX
  IF(IWRITE.EQ.1) THEN
    WRITE(4,300) timdat
300  FORMAT(1x,a32,' ARRAY ((DIS(I,J),J=M0,M),I=1,nlevl-1),  zc')
    write(4,310) nlevl,m
310  FORMAT(2i5)
    DO I=1,nlevl
      WRITE(4,330) (DIS(I,J),J=M0,M), zc(i)
    END DO
    write(4,320) m-m0+1
320  format(' M levels for source mid-heights with thickness:-'/i4)
    do j=1,m
      write(4,330) zs(j), dz(j)
    end do
    write(4,*)
330  FORMAT(1X,100F8.3)
  ENDIF

  RETURN
  END

!*****

```

Appendix H

Regional model source code

H.1 Correction of CO₂ profiles

The following Fortran 77 code applies a correction to the CO₂ concentration data according to the calibration gases (interpolated between heights at which calibration occurs).

```
c Program to correct aircraft Licor CO2 data for drift in calibration
c gas, using both 340ppm and 380ppm calibrations.
c Written by Jon Lloyd early 1999, altered by Julie Styles for use
c with uneven numbers of 340 and 380ppm calibrations 25/2/99.
c First the csv file from the flight needs to be set up with time in
c general format, and 34 in the time field before each set of five
c 340ppm calibration values, and 38 before each set of 380ppm
c calibration values, and 99 before the sample values. Rows should be
c deleted to leave only the last five valid calibration values, and to
c allow time for the sample values to be valid (about twenty rows)
c The file should be saved as csv, and the name should be altered
c below to call the correct file.
program flights
  implicit doubleprecision (a-h,o-z)
  real*8 co2cal(20000), co2raw,flow,press(20000),pirga(20000)
  real*8 praw, rh(20000),tair(20000), tirga(20000)
  real*8 cal(2,100), digtime(20000), ctime(2,100), cvalue(2)
  real*8 time,pr,dens,te,pt,virpt,wat,elev
  open (unit=11,file=
x 'c:\siberia\flight data\Corrected data\z240798f6.intf')
  open (unit=16,file=
x 'c:\siberia\flight data\corrected data\z240798f6.corr')
  open (unit=12, file=
x 'c:\siberia\flight data\corrected data\temperature
x\z240798f6.tempout')
  j = 1
  ical1 = 0
  ical2 = 0
  read (12,*,end=45) time,pr,dens,te,pt,virpt,wat,elev
  close (unit=12)
45  continue
130  do 30 i = 1,20000
  read (11,*,end=40) digtime(j), co2cal(j), co2raw, flow,
x  press(j), pirga(j), praw, rh(j), tair(j), tirga(j),
x  traw

1234  format (3x,6(i2,x),7x,f7.3,2x,f7.2,2x,f9.6,2x,f7.2,2x,f6.2,2x,
x  f7.2,2x,3(f7.4,2x),f7.2)
```

```

    goto 51
131 continue
51   intday = int(digtime(j))
    if (intday.lt.100.and.intday.gt.30) goto 50
    digtime(j) = (digtime(j)-float(intday))*24.
    if (digtime(j).lt.1) then
        digtime(j)=digtime(j)+24
    endif
    j = j+ 1
30   continue
    do i=1,20000
        tair(i)=tair(i+60)
    enddo
50   continue
    if (intday.eq.38) then
        ical2 = ical2 + 1
        do 60 k = 1,4
            read (11,*) digtim , co2ca, co2ra, flow,
x   pres, pirc, pra, rhum, ta, tirc,
x   traw
            cal(2,ical2) = co2ca/4. + cal(2,ical2)
            if (k.eq.3) then
                intday = int(digtim)
                ctime(2,ical2) = (digtim-float(intday))*24.
            endif
60   continue
        write (6,*) ctime(2,ical2), cal(2,ical2)
        goto 130
        else if (intday.eq.34) then
            ical1 = ical1 + 1
            do 70 k = 1,4
                read (11,*) digtim , co2ca, co2ra, flow,
x   pres, pirc, pra, rhum, ta, tirc,
x   traw
                cal(1,ical1) = co2ca/4. + cal(1,ical1)
                if (k.eq.3) then
                    intday = int(digtim)
                    ctime(1,ical1) = (digtim-float(intday))*24.
                endif
70   continue
                write (6,*) ctime(1,ical1), cal(1,ical1)
                goto 130
                else if (intday.eq.99) then
                    goto 130
                else
                    close (unit = 11)
                    pause
                endif
40   continue
        nobs = j
        numcals: if (ical1.eq.ical2) then
            ncal = ical1
            if (ctime(1,ical1).lt.1) then
                ctime(1,ical1)=ctime(1,ical1)+24
            endif
            if (ctime(2,ical2).lt.1) then
                ctime(2,ical2)=ctime(2,ical2)+24
            endif
            do 10 i = 1,nobs
                do 10 iseg = 2,ncal
                    timesegments: if (digtime(i).lt.ctime(2,iseg).and.digtime(i).gt.
x   ctime(2,iseg-1)) then
                    do ispan = 1,2
                        cvalue(ispan) = cal(ispan,iseg-1) + (cal(ispan,iseg) -
x   cal(ispan,iseg-1))/(ctime(ispan,iseg) - ctime(ispan,iseg-1))*
x   (digtime(i) - ctime(ispan,iseg-1))

```

```

        enddo
        call calculate
        else if (digtime(i).gt.ctime(2,ical2)) then timesegments
            if (iseg.eq.2) then
                cvalue(1) = cal(1,ical1)
                cvalue(2) = cal(2,ical2)
            call calculate
            endif
        endif timesegments
10    continue
c the above only works if there are an equal number of 340ppm and 380ppm
c calibrations - the next sequence does it if there are more 340ppm
c calibrations than 380ppm ones
        else if (ical1.gt.ical2) then numcals
            ncal = ical1
            do 20 i = 1,nobs
            do 20 iseg = 2,ncal
                timesegs: if (digtime(i).lt.ctime(2,iseg).and.digtime(i).gt.
x         ctime(2,iseg-1).and.iseg.le.ical2) then
                do ispan = 1,2
                    cvalue(ispan) = cal(ispan,iseg-1) + (cal(ispan,iseg) -
x         cal(ispan,iseg-1))/(ctime(ispan,iseg) - ctime(ispan,iseg-1))*
x         (digtime(i) - ctime(ispan,iseg-1))
                enddo
                call calculate
            else if (digtime(i).gt.ctime(2,ical2).and.digtime(i).lt.
x         ctime(1,ical1).and.digtime(i).lt.ctime(1,iseg)
x         .and.digtime(i).gt.ctime(1,iseg-1)) then timesegs
                cvalue(1) = cal(1,iseg-1) + (cal(1,iseg) -
x         cal(1,iseg-1))/(ctime(1,iseg) - ctime(1,iseg-1))*
x         (digtime(i) - ctime(1,iseg-1))
                cvalue(2) = cal(2,ical2)
            call calculate
            else if (digtime(i).gt.ctime(1,ical1)) then timesegs
                if (iseg.eq.ncal) then
                    cvalue(1) = cal(1,ical1)
                    cvalue(2) = cal(2,ical2)
                call calculate
                endif
            endif timesegs
20    continue
        write (6,*) ical1, ical2
        endif numcals
        stop
contains
subroutine calculate
        co2new1 = co2cal(i) + 340. - cvalue(1)
        co2new2 = co2cal(i) + 380 - cvalue(2)
        co2new = (co2new1 + co2new2)/2.
        height = (1 - (press(i)/(pr*10))**(1/5.2568))*44308
        tk = tair(i) + 273.15
        abshum = 2.17/tk**rh(i)/100*613.75*exp(17.502*tair(i)/
x         (240.97 + tair(i)))
        rho = press(i)/10/0.287/tk
        pottemp = tk*(1000./press(i))*0.286
        spechum = abshum/(rho*1000 + abshum)
        vpt = pottemp*(1 + 0.61*spechum)
        airmol = press(i)*100./ (8.314*tk)
        watervap = abshum/18./airmol*1e3
c         write (6,1345) digtime(i), cvalue(1),cvalue(2),co2cal(i)
c         x         , co2new,tair(i),pottemp-273.15,vpt-273.15,watervap, height
        write (16,1345) digtime(i), cvalue(1),cvalue(2),co2cal(i)
x         , co2new, tair(i),pottemp-273.15,vpt-273.15,watervap, height
1345    format (f9.5, 4f8.3,3f8.2,f8.3, f9.2)
c         write (6,*) i, iseg,nobs, ical1, ical2
        end subroutine calculate

```

```
end program flights
```

H.2 Interpolation and smoothing of CO₂ profiles

The following Fortran 77 code linearly interpolates CO₂ concentrations at heights where data are missing, and average concentrations are calculated for each 25-metre interval up to the highest measured height.

```

program co2
implicit none
real(8) hourtime(20000), cal1(20000),cal2(20000)
real(8) halftime,maxheight,height(20000),
x   co2uncorr(20000),co2corr(20000)
real(8) temp(20000),ptemp(20000),vpt(20000)
real(8) h2o(20000),co2down(120,9000)
real(8) co2up(120,9000),sumco2up(120),avco2up(120)
real(8) avco2down(120),sumco2down(120)
integer i,j,k,l,ni,nj,m,nk,nup,mi,num(120),numd(120),
x   n,nm,ij,ik,il
open (unit=10, file=
x'c:\siberia98\flight data\corrected data\
xz240798f6.corr')
open (unit=20, file=
x'c:\siberia98\flight data\corrected data\co2\
xz240798f6.co2')

sumco2up=0
sumco2down=0
num=1
numd=1
do i=1,20000
read (10,*,end=30) hourtime(i),cal1(i),cal2(i),co2uncorr(i)
x   ,co2corr(i),temp(i),ptemp(i),vpt(i),h2o(i),height(i)
enddo
30 continue

c ditch bad data before finding maximum height
do mi=1,20000
if (height(mi).gt.3500) then
height(mi)=0
endif
enddo
maxheight=maxval(height)

do m=1,20000
if (height(m).eq.maxheight) then
halftime=hourtime(m)
write(6,*) hourtime(m),maxheight
endif
enddo

do nk=1,20000
upflight: if (hourtime(nk).lt.halftime) then
do nup=1,120
if (height(nk).lt.nup*25.and.height(nk).ge.(nup-1)*25.and.
x   height(nk).ne.0.and.co2corr(nk).ne.0) then
co2up(nup,num(nup))=co2corr(nk)
num(nup)=num(nup)+1

```

```

        endif
    enddo
endif upflight
downflight: if (hourtime(nk).ge.halftime) then
    do ni=1,120
        if (height(nk).lt.ni*25.and.height(nk).ge.(ni-1)*25.and.
x        height(nk).ne.0) then
            co2down(ni,numd(ni))=co2corr(nk)
            numd(ni)=numd(ni)+1
        endif
    enddo
endif downflight
    enddo

    do j=1,9000
        do k=1,120
            sumco2up(k)=sumco2up(k)+co2up(k,j)
            sumco2down(k)=sumco2down(k)+co2down(k,j)
        enddo
    enddo
    do nj=1,120
        avco2up(nj)=sumco2up(nj)/(num(nj)-1)
        avco2down(nj)=sumco2down(nj)/(numd(nj)-1)
        if (num(nj).eq.1) then
            avco2up(nj)=0
        endif
        if (numd(nj).eq.1) then
            avco2down(nj)=0
        endif
    enddo
    call interpolate

    do l =1,120
        write(6,*) (l-1)*25, ' to' ,l*25, avco2up(l)
x        ,avco2down(l),num(l),numd(l)
        write(20,1111) (l-1)*25,l*25,avco2up(l),
x        avco2down(l)
    enddo
1111    format (2i10,2f10.4)

contains
subroutine interpolate
c Interpolate linearly between heights for missing data
do n=2,120
    nm=1
    ij=1
upzeros: if (avco2up(n).eq.0.and.avco2up(n-1).ne.0) then
    do ik=1,120-n
        if (avco2up(n+nm).eq.0) then
            nm=nm+1
        endif
        if ((n+nm+1).eq.120) then
            goto 24
        else if (avco2up(n+nm).ne.0) then
            avco2up(n)=(avco2up(n+nm)-avco2up(n-1))/(nm+1)
x            +avco2up(n-1)
24    endif
        enddo
    endif upzeros
downzeros: if (avco2down(n).eq.0.and.avco2down(n-1).ne.0) then
    do il=1,120-n
        if (avco2down(n+ij).eq.0) then
            ij=ij+1
        endif
        if ((n+ij+1).eq.120) then
            goto 26

```

```

        else if (avco2down(n+ij).ne.0) then
          avco2down(n)=(avco2down(n+ij)-avco2down(n-1))/(ij+1)
x      + avco2down(n-1)
26    endif
        enddo
      endif downzeros
    enddo
  end subroutine interpolate
end program co2

```

H.3 Virtual potential temperature and height calculation

The following Fortran 77 code applies a correction to the temperature and humidity data due to sensor response lag. It calculates virtual potential temperature using humidity and pressure data and height using pressure data as described in Appendix E.

```

program TEMPERATURE

! program to calculate potential temperature, vpt, h2o conc and
! elevation ! for the full flight profile - the CO2 calibration
! program "flights" ! cuts out times when calibration was occurring.

implicit doubleprecision (a-h,o-z)
real*8 co2cal(20000), co2raw,flow,press(20000),pirga(20000)
real*8 praw, rh(20000),tair(20000), tirga(20000),height(20000),difftemp(20000)
real*8 cal(2,100), digtime(20001), ctime(2,100), cvalue(2),maxtime(1)
open (unit=11,file='Z230798f2.TEMPIN')
open (unit=16,file='z230798f2.tempout')
130 do i = 1,20000
  read (11,*,end=40) digtime(i), co2cal(i), co2raw, flow, &
    press(i), pirga(i), praw, rh(i), tair(i), tirga(i), &
    traw
  enddo
40  continue
  do i=1,20000
    digtime(i)=(digtime(i)-int(digtime(i)))*24
    height(i) = (1 - (press(i)/(press(1)))*(1/5.2568))*44308
  enddo
do 50 i=1,20000
if(digtime(i).eq.0) goto 50
  if (tair(i+64).ne.0.and.i.gt.64) then
    sumt=0.
    sumrh=0.
    do k=56,64
      sumt=tair(i+k)+sumt
      sumrh=rh(i+k)+sumrh
    enddo
    avt=sumt/9
    avrh=sumrh/9
    sumt=0
    sumrh=0
    do k=56,64
      sumt=tair(i-k)+sumt
      sumrh=rh(i-k)+sumrh
    enddo
    tav=sumt/9
    rhav=sumrh/9
    difftemp(i)=avt-tav
  endif
enddo

```

```

    diffrh=avrh-rhav
    difftime=(digtime(i+60)-digtime(i-60))*3600
    tav2=(tair(i-1)+tair(i)+tair(i+1))/3
    rhav2=(rh(i-1)+rh(i)+rh(i+1))/3
    tempcorr = tav2+273.15 + difftemp(i)/difftime*60
    rhcorr = rhav2 + diffrh/difftime*90
elseif(i.le.64) then
    tempcorr=tair(i+60)+273.15
elseif(tair(i+64).eq.0) then
    tempcorr=tair(i)+273.15-0.6
endif
    if (tempcorr.ne.0) then
    tk = tair(i) + 273.15
    abshum = 2.17/tk*rh(i)/100*613.75*exp(17.502*tair(i)/ &
        (240.97 + tair(i)))
    abshum2 = 2.17/tempcorr*rh(i)/100*613.75* &
        exp(17.502*(tempcorr-273.15)/ &
        (240.97 + tempcorr-273.15))
    rho = press(i)/10./0.287/tk
    rho2 = press(i)/10./0.287/tempcorr
    pottemp = tk*(1000./press(i))*0.286
    pottemp2 = tempcorr*(1000./press(i))*0.286
    spechum = abshum/(rho*1000 + abshum)
    spechum2 = abshum2/(rho2*1000 + abshum2)
    virttemp=tk*(1.+0.61*spechum)
    virttemp2=tempcorr*(1.+0.61*spechum)
    vpt = pottemp*(1 + 0.61*spechum)
    vpt2 = pottemp2*(1 + 0.61*spechum)
    airmol = press(i)*100./ (8.314*tk)
    airmol2=press(i)*100./(8.314*tempcorr)
    watervap = abshum/18./airmol*1e3
    watervap2 = abshum2/18./airmol2*1e3
    cp = 1005+((virttemp2-250.)**2)/3364
    height2 = cp*vpt2/9.81* &
        (1-(press(i)/press(1))**(287.05/cp))
if(press(i).gt.0) then
    height3 = -287.05*virttemp2/9.81*log(press(i)/press(1))
endif
    write (16,1345) digtime(i),press(i)/10.,rho,tair(i), &
        pottemp-273.15, &
        vpt-273.15,watervap, &
        tempcorr-273.15, pottemp2-273.15, vpt2-273.15, &
        height(i),height2,height3,rho2
    endif
50 continue
    rmaxdifftemp=maxval(difftemp)
    write(*,*) rmaxdifftemp
1345    format (f9.5, f9.3,f10.5,4f8.3,1x,f8.3,1x,f8.3,1x,f8.3,
&
        3f8.2,f10.5)

end program TEMPERATURE

```

H.4 Density profiles

The following Fortran 77 code calculates average density for each 25-metre interval up to the highest measurement height, using density output from the code in §H.3 above.

```

program density

```

```

implicit none
real(8) hourtime(20000), press(20000),rho(20000)
real(8) halftime,maxheight,height(20000)
real(8) temp(20000),ptemp(20000),vpt(20000),
x   ctemp(20000),cptemp(20000),cvpt(20000),
x   height2(20000),height3(20000),ch2o(20000),rho2(20000)
real(8) h2o(20000),densdown(120,9000)
real(8) densup(120,9000),sumdensup(120),avdensup(120),num(120)
real(8) avdensdown(120),sumdensdown(120),numd(120)
integer i,j,k,l,ni,nj,m,nk,nup,mi
open (unit=10, file=
x'c:\siberia98\flight data\corrected data\temperature\
xz240798f6.tempout')
open (unit=20, file=
x'c:\siberia98\flight data\corrected data\temperature\
xz240798f6.rho')

sumdensup=0
sumdensdown=0
num=1
numd=1
do i=1,20000
read (10,*,end=30) hourtime(i),press(i),rho(i),
x temp(i),ptemp(i),vpt(i),h2o(i),ctemp(i),cptemp(i),
x cvpt(i),height(i),height2(i),height3(i),rho2(i),ch2o(i)
enddo
30 continue

c ditch bad data before finding maximum height
do mi=1,20000
if (height(mi).gt.3500) then
height(mi)=0
endif
enddo
maxheight=maxval(height)

do m=1,20000
if (height(m).eq.maxheight) then
halftime=hourtime(m)
write(6,*) hourtime(m),maxheight
endif
enddo

do nk=1,20000
upflight: if (hourtime(nk).lt.halftime) then
do nup=1,120
if (height(nk).lt.nup*25.and.height(nk).ge.(nup-1)*25.and.
x height(nk).ne.0) then
densup(nup,num(nup))=rho2(nk)
num(nup)=num(nup)+1
endif
enddo
endif upflight
downflight: if (hourtime(nk).ge.halftime) then
do ni=1,120
if (height(nk).lt.ni*25.and.height(nk).ge.(ni-1)*25.and.
x height(nk).ne.0) then
densdown(ni,numd(ni))=rho2(nk)
numd(ni)=numd(ni)+1
endif
enddo
endif downflight
enddo

do j=1,9000
do k=1,120

```

```

sumdensup(k)=sumdensup(k)+densup(k,j)
sumdensdown(k)=sumdensdown(k)+densdown(k,j)
enddo
enddo
do nj=1,120
avdensup(nj)=sumdensup(nj)/(num(nj)-1)
avdensdown(nj)=sumdensdown(nj)/(numd(nj)-1)
if (num(nj).eq.1) then
avdensup(nj)=0
endif
if (numd(nj).eq.1) then
avdensdown(nj)=0
endif
enddo

do l =1,120
write(6,*) (l-1)*25, ' to' ,l*25, avdensup(l)
x   ,avdensdown(l),num(l),numd(l)
write(20,1111) (l-1)*25,l*25,avdensup(l),
x   avdensdown(l)
enddo
1111 format (2i10,2f8.4)
end program density

```

H.5 Virtual potential temperature profiles

The following Fortran 77 code calculates average virtual potential temperature for each 50-metre interval up to the highest measurement height using the virtual potential temperature output from §H.3 above.

```

$debug
program avtemp
implicit none
real(8) hourtime(20000), press(20000),rho(20000)
real(8) halftime,maxheight,height(20000)
real(8) temp(20000),ptemp(20000),vpt(20000),
x   ctemp(20000),cptemp(20000),cvpt(20000),height2(20000),
x   height3(20000)
real(8) h2o(20000),tempdown(2,60,9000)
real(8) tempup(2,60,9000),sumtempup(2,60),avtempup(2,60),
x   num(60)
real(8) avtempdown(2,60),sumtempdown(2,60),numd(60)
integer i,j,k,l,ni,nj,m,nk,nup,mi
open (unit=10, file=
x'c:\siberia98\flight data\corrected data\temperature\
xz220798f1.tempout')
open (unit=20, file=
x'c:\siberia98\flight data\corrected data\temperature\
xz220798f1.pt')

sumtempup=0
sumtempdown=0
num=1
numd=1
do i=1,20000
read (10,*,end=30) hourtime(i),press(i),rho(i),
x   temp(i),ptemp(i),vpt(i),h2o(i),ctemp(i),cptemp(i),
x   cvpt(i),height(i),height2(i),height3(i)

```

```

        enddo
30    continue

c    ditch bad data before finding maximum height
    do mi=1,20000
      if (height(mi).gt.3500) then
        height(mi)=0
      endif
    enddo
    maxheight=maxval(height)

    do m=1,20000
      if (height(m).eq.maxheight) then
        halftime=hourtime(m)
write(6,*) hourtime(m),maxheight
      endif
    enddo

    do nk=1,20000
      if (cptemp(nk).gt.-50) then      !ditch bad data
upflight: if (hourtime(nk).lt.halftime) then
      do nup=1,60
        if (height(nk).lt.nup*50.and.height(nk).ge.(nup-1)*50.and.
x      height(nk).ne.0) then
          tempup(1,nup,num(nup))=cptemp(nk)
          tempup(2,nup,num(nup))=cvpt(nk)
          num(nup)=num(nup)+1
        endif
      enddo
endif upflight
downflight: if (hourtime(nk).ge.halftime) then
      do ni=1,60
        if (height(nk).lt.ni*50.and.height(nk).ge.(ni-1)*50.and.
x      height(nk).ne.0) then
          tempdown(1,ni,numd(ni))=cptemp(nk)
          tempdown(2,ni,numd(ni))=cvpt(nk)
          numd(ni)=numd(ni)+1
        endif
      enddo
endif downflight
      endif
    enddo

    do j=1,9000
      do k=1,60
        do l=1,2
          sumtempup(1,k)=sumtempup(1,k)+tempup(1,k,j)
          sumtempdown(1,k)=sumtempdown(1,k)+tempdown(1,k,j)
        enddo
      enddo
      do nj=1,60
        do l=1,2
          avtempup(1,nj)=sumtempup(1,nj)/(num(nj)-1)
          avtempdown(1,nj)=sumtempdown(1,nj)/(numd(nj)-1)
          if (num(nj).eq.1) then
            avtempup(1,nj)=0
          endif
          if (numd(nj).eq.1) then
            avtempdown(1,nj)=0
          endif
        enddo
      enddo

      do l =1,60
write(6,*) (l-1)*50, ' to' ,l*50, avtempup(1,l)

```

```
x      ,avtempdown(1,1),num(1),numd(1)
write(20,1111) (1-1)*50,1*50,avtempup(1,1),
x      avtempdown(1,1),avtempup(2,1),avtempdown(2,1)
enddo
1111   format (2i10,4f8.4)
end program avtemp
```