

# THE MET INPUT MODULE

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*In this document 'ADMS' refers to ADMS 6.0. Where information refers to other models, the model name is given in full.*

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## **Summary**

This paper describes the specification of the met input module, together with a description of data requirements for running the module.

### **1. Introduction and Overview**

Meteorological data are principally input to the model via the met file which is supplied by the user. The met input module reads the data from the met file and uses these data to estimate values of the various meteorological quantities required for running the dispersion model. The data required in the met file are data describing the conditions for one or more hours, the conditions being assumed to remain fixed in each hour. These data might be statistical (in which a succession of cases are given, each having a certain frequency or 'weight' associated with it) or sequential (in which a chronological succession of hours are treated) or some more general collection of one or more (non-weighted) hours.

The module is called once for each hour's data which requires processing. The inputs to the module consist of a number of variables passed through the module's argument list (most of these variables originate from the user via the menu system and input (e.g. apl) file) and the data from the met file itself. The module checks that the input data are sensible and not missing when needed, uses these data to estimate the meteorological quantities required, and, if the met site is not representative of the dispersion area, corrects for differences between the locations due to, e.g., differences in roughness length or precipitation characteristics. All output from the module is through the argument list.

There are a large number of variables which can be provided in the met file, although normally only a small number would be used. The possible types of data in the met file are (i) met data proper (including sea surface temperature information), (ii) information on the site

characteristics at the met site or in the dispersion area (e.g. albedo), (iii) time information, and (iv) data on the frequency with which a specific set of conditions occurs. The met data are all assumed to be measured at one location, the ‘met site’, which need not be in the ‘dispersion area’. If the observations come from a number of different sites (e.g. wind from an on site anemometer, precipitation from a nearby rain gauge site and some other data from a more distant met station) the user needs to decide which location should be regarded as the ‘met site’. In many cases the site of the wind measurement would be the most appropriate choice. The met site and dispersion area are assumed to be over land, unless the marine boundary layer option is chosen by the user.

If a variable required is present in the met file, then the output value will normally be identical to the met file value. However the module may sometimes change the value. This might be because the input values are not consistent with the physics assumed in the module and/or the values obtained through the argument list, or because of corrections for differences between the met site and the dispersion area.

In addition to the met file, the user may provide measurements of vertical profiles of some of the meteorological data required as input to the model (specifically, wind speed, temperature and specific humidity). If valid vertical profile data are supplied, these data override the values in the met file.

Many of the schemes used to estimate unknown quantities have limitations. These can however often be overcome by providing more input variables in the met file. The main limitations are described in §5.1.

SI units are used except where stated.

## 2. Input and output

### Met file input

A complete list of variables which can be input through the met file is as follows. The minimum and maximum allowed values for each of these variables are given in the relevant model's User Guide.

#### List (1)

$U$	wind speed at measurement height (assumed to be friction velocity if measurement height set to 0.0, or geostrophic wind if measurement height set to 1000.0)
$U_g^*$	geostrophic wind speed normalised by friction velocity
$\phi$	wind direction (angle wind is coming from in degrees clockwise from north) at measurement height (surface wind direction if measurement height set to 0.0; geostrophic wind direction if measurement height set to 1000.0)
$\Delta\phi$	geostrophic wind direction minus surface wind direction (both directions measured in degrees clockwise from north)
$F_{\theta_0}$	surface sensible heat flux
$1/L_{MO}$	1/Monin-Obukhov length
$h$	boundary layer depth
$c_L$	cloud amount (oktas)
$K^+$	incoming solar radiation
$T_0^C$	near surface temperature (°C)
$N_u$	buoyancy frequency above the boundary layer
$\Delta\theta$	temperature jump across the boundary layer top
$P$	precipitation rate (mm/hour)
$T_{sea}$	sea surface temperature (°C)
$\Delta T$	near surface temperature over land minus sea surface temperature
$\sigma_{\theta}^{deg}$	standard deviation of changes in mean wind direction (degrees)
$q_0$	near surface specific humidity
$r_{h0}$	near surface relative humidity (percent)
$r_{hu}$	relative humidity just above the boundary layer (percent)
$(dr_h/dz)_u$	$d(\text{relative humidity})/dz$ above the boundary layer (percent/m)
$\lambda E$	surface latent heat flux
$z$	wind measurement height* (m)
$z_0$	roughness length at met site* (m)

$z_{0d}$	roughness length in dispersion area* (m)
$r$	surface albedo at met site*
$r_d$	surface albedo in dispersion area*
$\alpha$	modified Priestley-Taylor parameter* (as defined in Holtslag and van Ulden, 1983, J. Clim. Appl. Met., <u>22</u> , 517-529 and see equation (6)) at met site
$\alpha_d$	modified Priestley-Taylor parameter* in dispersion area
$hour$	hour of day (e.g. 5.30am = 5.5). The value should be in local solar time.
$day$	day of year (e.g. 1 <sup>st</sup> Jan =1.0)
$year$	year (full 4 digit number, e.g. 1999.0)
$f$	frequency with which a given set of met conditions occurs (arbitrary units, e.g. percentage of occasions or number of hours per year)
<i>Detailed frequency data</i>	– detailed frequency information giving the frequency with which a given set of met conditions occurs for certain months of the year or times of day (same units as for $f$ ).

\*These data can alternatively be input via the argument list.

The input wind speed and direction might be a geostrophic wind, surface layer wind or friction velocity. Geostrophic wind is used here to denote any one of the geostrophic wind, the gradient wind or the wind at the boundary layer top. At the level of modelling adopted here, we do not distinguish between these quantities. An exception to this is when the model is applied in low latitudes; here the geostrophic wind is not a useful concept and the phrase ‘geostrophic wind’ should be interpreted as ‘wind at boundary layer top’.

The format of the met file consists of two parts. Firstly a list of  $m$  variable names is provided. These would usually be drawn from those in List (1) but need not all be (if a variable is not in (1) the corresponding data are ignored). Normally only a small subset of the variables in (1) would be input, the majority of the variables being unknown. A sequence of records follows, one for each hour of data, with each record giving the values of the  $m$  variables. Missing values are indicated by –999.0. For further details, please refer to the example met file in the appendix.

### **Argument list input**

The following data are input through the argument list:

$R_{lat}$	latitude (degrees, north positive)
$T_{sample}$	sampling time (hours)

$z$	height of the wind measurement at met site (1,000.0 is used to indicate geostrophic wind, 0.0 to indicate friction velocity)
$z_0$	roughness length at met site*
$z_{0d}$	roughness length in dispersion area*
$r$	surface albedo at met site*
$r_d$	surface albedo in dispersion area*
$\alpha$	modified Priestley-Taylor parameter at met site*
$\alpha_d$	modified Priestley-Taylor parameter in dispersion area*
$1/L_{MOmax}$	maximum value of $1/L_{MO}$ at met site
$1/L_{MOmaxd}$	maximum value of $1/L_{MO}$ in dispersion area
$P_{corr}$	precipitation correction factor (ratio of average rainfall in dispersion area to that at the measurement site)

#### *Name of met file*

*Sequential-data flag* – indicates that the data provided in the met file are hourly sequential

*Site-representative flags* – indicate whether various quantities (roughness length, albedo, Priestley-Taylor parameter, minimum Monin-Obukhov length, rainfall rate) are the same at the met site and dispersion area

*First-time flag* – indicates that the met input module is being called for the first time

*Message flag* – indicates that the met input module is to issue a message giving statistics of errors and warnings, but is not to process any hours of data.

\*These data can alternatively be input via the met file.

Apart from *first-time flag* and *message flag*, these variables only need to be specified the first time the module is called and indeed are ignored on subsequent calls. Even on the first call, it is not essential to provide values of  $r$ ,  $r_d$ ,  $\alpha$ ,  $\alpha_d$ ,  $1/L_{MOmax}$ ,  $1/L_{MOmaxd}$  or  $P_{corr}$ , with -999.0 being used to indicate missing data - values of  $r$ ,  $r_d$ ,  $\alpha$ ,  $\alpha_d$  may be obtained from the met file, and if any of the variables are missing, defaults are adopted.

#### **Argument list output**

We will now describe the data output through the argument list. This consists of two structures containing the ‘met-as-read’ and the ‘processed-met’ for one hour (but without any of the

frequency information), a structure containing the frequency information, a number of flags, and a number of variables concerned with counting the met data.

The met data structures consist of all the variables in List (1) except for the frequency information, with the addition of the following variables:

### List (2)

$u_*$	friction velocity
$U_g$	geostrophic wind speed
$\phi_0$	surface wind direction (angle wind is coming from in degrees clockwise from north)
$\phi_g$	geostrophic wind direction (angle wind is coming from in degrees clockwise from north)
$\theta_*$	temperature scale (positive for $F_{\theta_0} < 0$ )
$w_*$	convective velocity scale if $F_{\theta_0} > 0$ , zero if $F_{\theta_0} \leq 0$
$s$	sine of solar elevation
$T_0^K$	near surface temperature (K)
$\sigma_\theta^{rad}$	standard deviation of changes in mean wind direction (radians)

Missing data is denoted by -999.0. The met-as-read structure will always have missing entries. However, if none of the flags are set, the processed-met-data structure will contain values of all structure elements with the exception of  $U$ ,  $\phi$ ,  $T_{sea}$  and  $r_{h0}$  (other modules in ADMS should use values calculated from  $u_*$ ,  $\phi_0$ ,  $\Delta T$ ,  $q_0$  etc.), with the possible exception of  $s$ ,  $c_l$ ,  $K^+$ ,  $P$ ,  $\Delta T$ ,  $q_0$ , *hour*, *day* and *year* (it is not always possible to calculate these quantities and it is still possible to do a basic dispersion calculation without them; other modules which need them should check whether they are present).

The structure containing the frequency information consists of the variable  $f$  and variables containing the detailed frequency information. Provided the *fatal-error* and *no-more-data* flags (see below) are not set,  $f$  will always have a valid value. If it is not present in the met file, it is set to 1.0. However the detailed frequency information will be present only if it is present in the met file.

The flags are as follows. If a fatal error occurs then the *fatal-error* flag is set. This indicates a serious error and the main control program should then halt the computation. When the end of the met file is reached the *no-more-data* flag is set. Also, if the data in the met file for a particular hour are inadequate or not sensible, the *inadequate-data* flag is set. In addition, in ADMS 6 if  $U = 0$  the *calm-conditions* flag is set, as ADMS 6 does not by default calculate dispersion for hours with calm conditions. These flags enable the main control program to proceed appropriately.

The met-data counting variables are  $n_{inad}$ ,  $f_{inad}$ ,  $n_{calm}$ ,  $f_{calm}$ ,  $n_{total}$ ,  $f_{total}$ , and  $i_{hour}$ .  $n_{inad}$  indicates the cumulative number of hours' data for which the *inadequate-data flag* has been set while  $f_{inad}$  indicates the cumulative frequency of occasions for which the flag has been set (these differ only if the input data are statistical).  $n_{calm}$ ,  $f_{calm}$ ,  $n_{total}$  and  $f_{total}$  give similar information for calm conditions and those occasions when neither flag is set.  $i_{hour}$  indicates that the data being considered are the  $i_{hour}$ -th hour's data from the met file.

### 3. Guidance on input

In this section we give some guidance on which met variables to input and we discuss appropriate values of some of the input variables.

First we discuss the question of which variables to include in the met file. For a successful dispersion calculation, the variables  $U$  and  $\phi$  must be given. In ADMS 6 if the calm conditions option is not being used then  $U$  must be such that the wind speed at a height of 10 m is greater than or equal to 0.75 m/s, while in ADMS-Roads, ADMS-Urban and ADMS-Airport the wind speed is increased to ensure it is above 0.75 m/s at 10 m. In addition,  $F_{\theta_0}$  or  $1/L_{MO}$  or sufficient data to estimate  $F_{\theta_0}$  must be given.  $F_{\theta_0}$  can be estimated if *day* and *hour* and either  $c_l$  or  $K^+$  (or both) are given; however, although  $c_l$  is not needed when  $K^+$  is given, we would recommend that  $c_l$  is provided if possible whenever  $F_{\theta_0}$  needs to be estimated as this is likely to improve the estimate. Also specifying  $T_0^C$  is advisable for daytime hours ( $s > 0$ ) whenever  $F_{\theta_0}$  needs to be estimated.

Specifying  $h$  is advisable if you think you can provide a better estimate than the met input module. In mid latitudes with (a) sequential data which includes *day* and *hour* stretching back at least till an hour before dawn ( $s = 0$ ) and either  $s > 0$  or  $F_{\theta_0}$  in the previous hour is  $> 0$ , or (b)  $s \leq 0$  and  $F_{\theta_0}$  in the previous hour is  $\leq 0$ , then you're unlikely to be able to provide a better estimate unless you have measurements aloft. In other situations the module's estimate will be less reliable. If neither (a) nor (b) applies and you don't specify  $h$ , then it is advisable to specify the variables needed to estimate  $F_{\theta_0}$  as described in the previous paragraph, even if  $F_{\theta_0}$  and/or  $1/L_{MO}$  is provided – this may help in estimating  $h$  by enabling the module to estimate the values of  $F_{\theta_0}$  occurring prior to the current hour.

In addition  $P$  is needed if wet deposition is to be calculated and  $\Delta T$  (or  $T_{sea}$  and  $T_0^C$ ) are needed if the coastline module is to be used. For visible plume calculations, it is essential that  $q_0$  or sufficient data to estimate it (i.e.  $r_{h0}$  and  $T_0^C$ ) are given. For chemistry calculations  $K^+$  is needed or the means to estimate it (i.e.  $c_l$ , *hour* and *day*). For some time dependent source calculations it is necessary to specify *day* and *hour* (and *year* is also desirable in such cases),

while for others the input data must be statistical with  $f$  and *detailed frequency data* provided. For statistical input data, information on  $f$  is of course always needed.

There are a number of other variables which can be input, but these would not normally be given unless the user wished to alter the defaults within the model. If  $F_{\theta_0}$  needs to be estimated for daytime hours (either for the current hour or for earlier times in connection with estimating  $h$  for the current hour), values of  $r$  and  $\alpha$  may improve the estimates. If  $h$  needs to be estimated, providing  $N_u$  may improve the estimate of  $h$  when  $F_{\theta_0} > 0$ . Also providing  $N_u$ ,  $\Delta\theta$  and  $T_0^C$  may perhaps improve the accuracy of the dispersion calculation a little and  $T_0^C$  would also improve the accuracy of the relation between temperature and buoyancy which is assumed by the met input module. For daytime conditions with  $h$  not given in the met file, the most important role of the variable  $N_u$  is perhaps in estimating  $h$ , and in such cases the module's estimate of  $h$  can depend on the history of  $N_u$ ; hence, if the input data are not sequential, the value of  $N_u$  in such situations should represent an average over values since dawn (defined here as the last time the heat flux changed from negative to positive).  $U_{g*}$  and  $\Delta\phi$  would not normally be given but could be useful in situations where the assumptions that the module would normally use to estimate the relation between the geostrophic wind and surface stress break down (see §5.1). For a full understanding of the importance of each of the various variables it is necessary to understand how they are used and how they are estimated when absent (see below and the documentation of the other modules).

It should be noted that, if  $F_{\theta_0}$  or  $1/L_{MO}$  is input, then  $r$  and  $\alpha$  are not used. (Actually this is a slight over-simplification as  $r$  and  $\alpha$  might affect estimates of  $F_{\theta_0}$  for previous hours, which in turn could affect  $h$  in the current hour.) Similarly, if  $U_{g*}$  and  $\Delta\phi$  are specified in the met file, then these are assumed to apply at both the met site and in the dispersion area; as a result no allowance for differences in roughness is made within the met input module when both  $U_{g*}$  and  $\Delta\phi$  are given in the met file. However, if (i)  $U_{g*}$  and  $\Delta\phi$  are given, (ii) the *roughness-representative flag* is not set, and (iii) a surface layer wind speed is given in the met file, this wind speed is interpreted in the met input module using the met site roughness length, while the wind speed profile computed in the boundary layer structure module is calculated from  $u_*$  using the dispersion area roughness length. The use of a different value of roughness length in the boundary layer structure module can produce inconsistencies and so it is recommended that  $z_0$  and  $z_{0d}$  are set equal to each other for this case.

It seems likely the two most common types of met file will be those containing statistical data consisting of  $U$ ,  $\phi$ ,  $F_{\theta_0}$ ,  $h$  and  $f$  with the possible addition of  $P$  and *detailed frequency data* (such data is supplied by the Met Office for the main UK met stations), and those containing sequential data (or a single hour's data) giving  $U$ ,  $\phi$ ,  $c_l$ , *hour, day*,  $T_0^C$  and possibly  $P$ ,  $r_{h0}$ ,  $T_{sea}$  and/or *year*.



If there are a large number of hours of statistical data, the order in which the sequence of records are arranged in the met file can be important for computational efficiency (depending on the design of the main control program). For example it may assist the code to be computationally efficient if  $P$  and  $\phi$  change faster than the other variables (if there are no buildings, terrain features etc. which could cause the dispersion properties to be different for different wind directions, then there is no need to recalculate the dispersion if only  $P$  and/or  $\phi$  have changed).

We include here some guidance on values of certain parameters. For the surface albedo  $r$  we suggest the following values, based on values given by Oke (1987, p12):

Snow-covered ground	0.6
Non snow-covered ground	0.23 (the default).

The value 0.23 is an average albedo for a range of non snow-covered surfaces. It does not seem worthwhile giving more detailed advice for different surfaces (desert, forest etc.) since the values for each of these surface types show considerable variability. The albedo of snow covered surfaces also shows considerable variability, and the given value is again an average value.

For the modified Priestley-Taylor parameter  $\alpha$  (which reflects the amount of available moisture) Holtslag and van Ulden (1983) give the following values:

Dry bare earth	0.0
Dry grassland	0.45
Moist grassland	1.0 (the default).

Further discussion of the value of  $\alpha$  is given by Beljaars and Holtslag (1990, 1991) and Hanna and Chang (1992).

For roughness length Oke (1987, pp57 and 298) recommends ranges of values for many surface types. Some suggested values based on these recommendations are given here:

Sea	0.0001 m
Short grass	0.005 m
Open grassland	0.02 m
Root crops	0.1 m
Agricultural areas (min)	0.2 m
Agricultural areas (max)	0.3 m
Parkland, open Suburbia	0.5 m

Cities, woodlands	1.0 m
Large urban areas	1.5 m

The choice of an effective  $z_0$  in heterogeneous terrain is a complex matter which is not discussed here (see e.g. Fiedler and Panofsky 1972, Wieringa 1986).

The variable  $1/L_{MOmax}$  is used to limit how stable the flow can get, reflecting the idea that in urban areas the flow is only rarely very stable because of anthropogenic heat sources and heat storage in the fabric of buildings etc. Stability in urban areas is not well understood, but the following minimum values for  $L_{MO}$  (corresponding to the reciprocal  $1/L_{MOmax}$ ) should provide reasonable results:

Large conurbations (population > 1 million)	100 m
Cities and large towns	30 m
Mixed urban/industrial	30 m
Small towns (population < 50,000)	10 m
Rural	1 m (the default).

If  $1/L_{MOmax}$  is not specified by the user, the minimum value of  $L_{MO}$  is estimated by the model to be the maximum of 10 times the roughness length and 1 m.

The factor  $P_{corr}$  is intended to take account of the fact that rainfall conditions in the dispersion area may vary systematically from those at the site where  $P$  is measured, for example because the altitude differs between the locations. Unless there are reasons to think the rainfall is systematically different at the two locations,  $P_{corr}$  should be set to 1 or not input at all.

#### 4. Messages

Whenever the *fatal-error* flag, the *inadequate-data* flag or the *calm-conditions* flag is set, a message is issued to explain what has happened. If the list of variables which is read from the met file contains a variable which does not occur in List (1), a message is issued to warn of this and the corresponding data are ignored. A warning message is also issued if the list of variables is too long. In this case the data corresponding to the variables at the end of the list are ignored. Messages are also issued to warn that a particular estimate which has been made is unreliable.

## 5. Processing the met data

This met input module estimates, where possible, the values of the met variables required. In section 5.1 below we describe the physical assumptions made and in section 5.2 the structure of the computation is described. To fully understand what is done, it is necessary to understand the structure as well as the physics; this is because the way the physics is applied varies according to which variables are input and which variables are deemed to take precedence if conflicting data are input. As noted in Section 1 it is possible that, for variables which are input through the met file, the output from the met input module will differ from the input. This is so even if no corrections for differences in site characteristics between the met site and the dispersion area are being made. The situations where this can occur are as follows. (1) When  $L_{MO}$  and  $F_{\theta_0}$  are both input – here  $L_{MO}$  takes precedence and  $F_{\theta_0}$  is ignored. (2) When  $F_{\theta_0}$  is input but implies conditions are stable and violates the bound on the heat flux in stable conditions which follows from the assumed physics (see below). Here  $F_{\theta_0}$  is replaced by a value consistent with the physics. (3) When  $L_{MO}$  and/or  $F_{\theta_0}$  is input, but implies that conditions are more stable than allowed by the variable  $1/L_{MOmax}$ . Here  $L_{MO}$  is set to the limiting value. If  $h$  is not input, then the new value of  $L_{MO}$  is used in estimating  $h$  (as one would expect). However if  $h$  is input, then  $h$  is recalculated using the new value of  $L_{MO}$ , and the recalculated value of  $h$  is used if it is larger. This is done primarily to enable datasets with  $h$  values which were calculated without any limit on  $L_{MO}$  to benefit from the option to limit  $L_{MO}$ . However this could be awkward if one wanted to fix  $h$  to a particular value – here one would have to ensure that the limit on  $L_{MO}$  wasn't violated in order to avoid  $h$  being altered. (4) If  $q_0$  and  $r_{h0}$  are both input,  $q_0$  takes precedence.

### 5.1 Physics

When items in List (2) are not in the met file and need to be estimated, the met input module makes use of a number of physical assumptions, approximations and models. Most of these assumptions are inexact and suffer from some limitations and uncertainties. Some specific difficulties are noted below, but we note here some general issues. Firstly the effects of topography and non-uniformities in the surface properties are neglected. Secondly it is generally assumed that the boundary layer parameters at any one time can be expressed in terms of the values of surface variables at the same time. In reality however the boundary layer is influenced by the history of the air mass and such things as synoptically induced vertical motions, static stability aloft and baroclinicity. These difficulties are most serious with respect to the assumptions made for the relation between the geostrophic wind and surface stress and for  $h$ . In general these problems cannot be overcome without much greater complexity and, in any case, the adoption of any such improved scheme would need much more information than would generally be available. An

exception is the prediction of  $h$  in a growing daytime boundary layer where some account of the history effects and static stability aloft can be taken. Thirdly there is a general difficulty with describing the boundary layer structure in stable conditions. This is because under such conditions the flow is very sensitive to small slopes, topography and details of surface properties.

(a)  $\kappa, \rho_a, c_p, g, f, L_{MO}$  and  $w_*$ : Von Karman's constant,  $\kappa$ , is taken to be 0.4 (Pasquill and Smith 1983, pp42-43). The air density,  $\rho_a$ , the air specific heat capacity,  $c_p$ , and the gravitational acceleration,  $g$ , are taken to be  $1.225 \text{ kg/m}^3$ ,  $1012.0 \text{ J/kg}^\circ\text{C}$  and  $9.807 \text{ m/s}^2$  respectively. The Coriolis parameter, Monin-Obukhov length and convective velocity scale are defined in the usual way by  $\omega = (4\pi/86400)\sin(2\pi R_{lat}/360)$ ,  $L_{MO} = -u_*^3 \rho_a c_p T_0^\kappa / \kappa F_{\theta_0} g$  and  $w_*^3 = -u_*^3 h / \kappa L_{MO}$  (Pasquill and Smith 1983, pp39, 41 and 70). However, near the equator where the magnitude of the Coriolis parameter is small, the schemes described below for estimating the geostrophic wind from the friction velocity (or vice versa) and for estimating the boundary layer depth are not soundly based and can give absurd results. As a result a lower limit of  $5 \times 10^{-5}$  (the value at a latitude of about  $20^\circ$ ) is adopted for the magnitude of the Coriolis parameter. Although this fix-up improves the situation, the results obtained using  $\omega$  must be regarded as unreliable when the fix-up is called into play.

(b) Surface layer wind profile: We assume the surface layer wind  $U_s$  is given as a function of height  $z$  by

$$\frac{\kappa U_s}{u_*} = \log\left(\frac{z + z_0}{z_0}\right) + \Psi\left(\frac{z + z_0}{L_{MO}}\right) - \Psi\left(\frac{z_0}{L_{MO}}\right) \quad (1)$$

For stable conditions ( $F_{\theta_0} \leq 0$ ),  $\Psi$  is assumed to be given by

$$\Psi(\zeta) = a\zeta + b(\zeta - c/d)\exp(-d\zeta) + bc/d \quad (2)$$

with  $a = 0.7$ ,  $b = 0.75$ ,  $c = 5$  and  $d = 0.35$  (Holtslag and de Bruin 1988), while for unstable conditions ( $F_{\theta_0} > 0$ ) we assume

$$\Psi(\zeta) = 2 \tan^{-1} x - \log((1 + x)^2(1 + x^2)) \quad (3)$$

where  $x = (1 - 16\zeta)^{1/4}$  (Dyer and Hicks 1970, Benoit 1977). Note that in (3) we adopt the convention that  $z = 0$  corresponds to the height where  $U_s = 0$  (or, more precisely, the height where  $U_s$  would equal zero if the surface layer form held right down to the ground).

(c) Relation between geostrophic wind and surface stress: Let  $(U_{gx}, U_{gy})$  be the geostrophic wind in coordinates for which  $(1,0)$  is aligned with the surface stress. Then  $U_g^2 = U_{gx}^2 + U_{gy}^2$  and

$\Delta\phi = \arctan(-U_{gy}/U_{gx})$ . For stable conditions ( $F_{\theta_0} \leq 0$ ) we assume

$$\begin{aligned}\frac{\kappa U_{gx}}{u_*} &= 2.2 \frac{h}{L_{MO}} + \log\left(\frac{h + 30z_0}{z_0}\right) + 0.19 \\ \frac{\kappa U_{gy}}{u_*} &= -\max\left(\left(3.55 \frac{h}{L_{MO}} + 1.87\right), 5.14\right) \text{sign}(\omega)\end{aligned}\quad (4a)$$

with  $h$  being determined from

$$\frac{h}{L_{MO}} = \frac{0.3u_*/|\omega|L_{MO}}{1 + 1.9h/L_{MO}}$$

which gives

$$h = \frac{0.6u_*}{|\omega|(1 + \sqrt{1 + \alpha})}\quad (4b)$$

where

$$\alpha = \frac{2.28u_*}{|\omega|L_{MO}}$$

These formulae are based on the theory of Brost and Wyngaard (1978) and the boundary layer depth formula of Nieuwstadt (1981) (see also Derbyshire 1990). In Brost and Wyngaard's formulae, one of the constants has been changed and the max function has been added. This is to ensure a smooth match to the unstable formulae. Note also that the value of  $h$  given by (4b) is used in (4a) even if  $h$  is available from the met file.

For unstable conditions ( $F_{\theta_0} > 0$ ) we assume

$$\begin{aligned}\frac{\kappa U_{gx}}{u_*} &= \log\left(\frac{u_*/|\omega| + 100z_0}{z_0}\right) - A(\mu) \\ \frac{\kappa U_{gy}}{u_*} &= -B(\mu) \text{sign}(\omega)\end{aligned}\quad (4c)$$

with

$$A(\mu) = \begin{cases} 1.01 - 0.105 \mu - 9.9 \times 10^{-4} \mu^2 + 8.1 \times 10^{-7} \mu^3 & \mu > -50 \\ 3.69 & \mu \leq -50 \end{cases}$$

$$B(\mu) = \begin{cases} 5.14 + 0.142 \mu + 1.17 \times 10^{-3} \mu^2 - 3.3 \times 10^{-6} \mu^3 & \mu > -50 \\ 1.38 & \mu \leq -50 \end{cases}$$

and  $\mu = \kappa u_* / |\omega| L_{MO}$ . These expressions are based on the Rossby number similarity formulation of Arya (1975).

Some changes have been made to the log terms in the expressions of Brost and Wyngaard (1978) and Arya (1975).  $h$  has been replaced by  $h + 30z_0$  in the log term in (4a) while  $u_* / |\omega|$  has been replaced by  $u_* / |\omega| + 100z_0$  in the log term in (4c). These corrections are negligible in the regime where Rossby number similarity theory is formally valid, but are included to ensure the formulae are well behaved for large values of  $z_0$  and light winds. The modifications preserve the smooth transition from stable to unstable conditions. The formulae are not however to be considered reliable in situations where these alterations are important as the whole basis for the approach is invalid when the friction Rossby number  $u_* / |\omega| z_0$  is not large.

(d) Solar elevation: The sine of the solar elevation,  $s$ , is assumed to be given by

$$s = \sin\left(\frac{2\pi R_{lat}}{360}\right) \sin\left(\frac{2\pi A}{360}\right) + \cos\left(\frac{2\pi R_{lat}}{360}\right) \cos\left(\frac{2\pi A}{360}\right) \cos\left(\frac{2\pi(hour - 12.5)}{24}\right)$$

where  $A$ , the solar declination (in degrees), equals  $23.45 \sin(2\pi(day + 284)/365)$  (Ratto 1988). More accurate formulae exist (e.g. Holtslag and van Ulden (1983), Nielsen et al (1981), Ratto (1988)) but are unnecessarily complicated for our purposes. This expression calculates the solar elevation at the middle of the hour being modelled, an option is available to calculate solar elevation at the time entered instead. If this options is used the  $hour - 12.5$  term is replaced with  $hour - 12$ .

(e)  $K^+$  and  $F_{\theta_0}$  at night: For  $s \leq 0$ ,  $K^+$  is zero and  $F_{\theta_0}$  (over land) is assumed to be given by

$$F_{\theta_0} = -\rho_a c_p u_* \theta_* \quad (5a)$$

with

$$\theta_* = 0.09(1 - 0.5(c_L/8)^2) \quad (5b)$$

(Holtslag and van Ulden 1982; van Ulden and Holtslag 1983). For very large  $u_*$  this formula clearly over-estimates  $F_{\theta_0}$ . However this is not a serious problem because  $F_{\theta_0}$  only increases linearly with  $u_*$ , and so the stability, as characterised by  $1/L_{MO}$  or  $u_* / |\omega| L_{MO}$ , decreases as  $u_*$  increases.

When  $U_g$  and  $F_{\theta_0}$  are given, solutions of equations (4a-b) for  $u_*$  are only possible if  $|B_0|/U_g^2$  ( $B_0$  being the surface buoyancy flux  $F_{\theta_0}g/\rho_a c_p T_0^K$ ) is less than some critical value  $(|B_0|/U_g^2)_{crit} = 0.145|\omega|$  (see discussion given by Derbyshire 1990). Physically this implies that there is an upper limit to the amount of heat that the turbulence can transport. This critical value corresponds to a collapsed boundary layer with  $u_* = L_{MO} = h = 0$  and so it is very difficult to estimate  $u_*$  reliably from the geostrophic wind when conditions are close to critical. To ensure a solution for  $u_*$  and avoid this sensitivity, whenever  $u_*$  needs to be calculated from  $U_g$  and  $F_{\theta_0}$  we somewhat arbitrarily alter  $F_{\theta_0}$  if necessary to ensure that  $|B_0|/U_g^2$  is always less than or equal to  $0.8(|B_0|/U_g^2)_{crit}$ . If  $\theta_*$  and  $U_g$  are given (for example if (5b) is being used) the relevant equations (i.e. (4a-b) and (5a)) always have a solution for  $u_*$ .

Similar considerations apply if  $U_s$  and either  $F_{\theta_0}$  or  $\theta_*$  are given. Solutions for  $u_*$  are possible only if  $|B_0|/U_s^3$  or  $|B_*|/U_s^2$  (where  $B_* = \theta_*g/T_0^K$ ) are less than certain critical values - however now the critical values can only be found numerically. To ensure a solution for  $u_*$ , whenever  $u_*$  needs to be calculated from  $U_s$  and  $F_{\theta_0}$  (or  $\theta_*$ ) we alter  $F_{\theta_0}$  (or  $\theta_*$ ) if necessary to ensure that  $|B_0|/U_s^3$  (or  $B_*/U_s^2$ ) is always less than or equal to  $(|B_0|/U_s^3)_{crit}$  (or  $(B_*/U_s^2)_{crit}$ ).

The above scheme for estimating  $F_{\theta_0}$  is based to a large extent on results obtained over midlatitude vegetated surfaces (but not forests) without snow-cover. Estimates of  $F_{\theta_0}$  elsewhere must be regarded as more uncertain.

(f)  $K^+$  and  $F_{\theta_0}$  during the daytime: For  $s > 0$ , the incoming solar radiation in  $W/m^2$ ,  $K^+$ , is assumed to be given by

$$K^+ = (990s - 30)(1 - 0.75(c_L/8)^{3.4})$$

and the net radiation in  $W/m^2$ ,  $Q^*$ , is assumed to be given by

$$Q^* = \frac{(1 - r)K^+ + 5.31 \times 10^{-13} (T_0^K)^6 - 5.67 \times 10^{-8} (T_0^K)^4 + 60(c_L/8)}{1.12}$$

(Holtslag and van Ulden 1983).  $F_{\theta_0}$  (over land) is assumed to be given by

$$F_{\theta_0} = \frac{(1 - \alpha)S + 1}{S + 1} 0.9Q^* - 20\alpha \quad (6)$$

(Holtslag and van Ulden 1983). Here  $S = (\lambda/c_p)dq_s/dT$  evaluated at  $T = T_0^K$ ,  $q_s(T)$  being the saturated specific humidity at temperature  $T$  and  $\lambda$  the specific latent heat of vaporization of water.  $S$  can be approximated by  $\exp(0.055(T_0^K - 279))$  (van Ulden and Holtslag 1985). If the value of  $F_{\theta_0}$  given by (6) is more negative than the night time prediction given in (e) above, then the night time value is assumed instead. Of course in reality  $K^+$  cannot be negative and so, whenever the above formula is used to calculate  $K^+$ , any negative values are replaced by zero when  $K^+$  is output from the module. However, because the Holtslag and van Ulden scheme for  $F_{\theta_0}$  has been developed and tested with the formula as given above, we do not make this modification to  $K^+$  until after calculating  $Q^*$  and  $F_{\theta_0}$ .

As at night time, the above scheme for estimating  $F_{\theta_0}$  is based to a large extent on results obtained over mid-latitude vegetated surfaces (but not forests) without snow-cover. Estimates of  $F_{\theta_0}$  elsewhere must be regarded as more uncertain although some aspects of the effect of snow can be accounted for by adjusting  $r$ .

The above schemes for estimating  $F_{\theta_0}$  are not suitable for use over the sea. When ADMS is used to model dispersion over the sea, a separate scheme is used to calculate the heat fluxes. This is described in (l) below.

(g)  $h$  in stable conditions: The boundary layer depth for  $F_{\theta_0} \leq 0$  is taken to be:

$$h = \frac{0.6u_*}{|\omega|(1 + \sqrt{1 + \alpha})} \quad (7)$$

where

$$\alpha = \frac{2.28u_*}{|\omega|L_{MO}}$$

However, near dawn, the boundary layer depth predictions from (7) can occasionally give unreliable results. This happens when a set of met data has a time associated with it which falls just before the time when the heat flux turns positive. Because the heat flux is negative and small, this can result in a large boundary layer depth that is close to the neutral estimate. The difficulty arises because, at this time of day, the heat flux is changing rapidly but, while the heat flux remains  $\leq 0$ , the model assumes the boundary layer depth adjusts instantly to the surface heat flux. Similar problems can also occur near dusk, but these are less noticeable because the



boundary layer depth at the end of the day (but before the heat flux goes negative) is generally larger.

To avoid the near dawn problem the following approach is adopted. Whenever (i)  $s > 0$  and  $F_{\theta_0} \leq 0$ , and (ii)  $F_{\theta_0} \leq 0$  holds at all previous hours back to and including an hour with  $s \leq 0$ , then the value of  $L_{MO}$  from the previous hour is used to calculate boundary layer depth. To avoid the near dusk problem we adopt the following scheme. If  $F_{\theta_0} \leq 0$  but was  $> 0$  in the previous hour, then  $h$  is limited by the value it would have if the negative value of  $F_{\theta_0}$  were replaced by 0.1. The aim here is to make the predictions less sensitive to where sunrise and sunset fall relative to the hourly met data cycle. Since this prescription for boundary layer depth depends on more than just the current hour's data, much of the data needed will often be unavailable. The extents to which we go to estimate this data, and what we do when they are unavailable, are described in §5.2 below.

(h)  $h$  in unstable conditions: The boundary layer depth for  $F_{\theta_0} > 0$  is assumed to evolve according to

$$\frac{dh}{dt} = \frac{S}{\Delta\theta} \quad (8a)$$

$$\frac{d\Delta\theta}{dt} = \frac{\gamma_\theta S}{\Delta\theta} - \frac{F_{\theta_0}}{\rho_a c_p h} - \frac{S}{h} \quad (8b)$$

$$S = \frac{c_F F_{\theta_0}}{\rho_a c_p} + \frac{A u_*^3 T_0^K}{gh} \quad (8c)$$

(Tennekes 1973; Tennekes and Driedonks 1981; Driedonks 1982). The constants  $c_F$  and  $A$  are assumed to take the values recommended by Driedonks (1982), namely  $c_F = 0.2$  and  $A = 5$ .  $\gamma_\theta$ , the rate of increase of potential temperature with height above the boundary layer, can be calculated from  $N_u^2 = g\gamma_\theta/T_0^K$  (see Gill 1982, p54). We assume the initial conditions  $h = \Delta\theta = 0$  at dawn, where dawn here corresponds to the last time when  $F_{\theta_0}$  changed from  $\leq 0$  to  $> 0$ . Conceptually these initial conditions correspond to a picture in which the growing daytime boundary layer erodes first the stable lapse rate in the stable boundary layer and then the overlying stable air. Of course, if the top of the growing daytime boundary layer is below that of the stable boundary layer, there would still be turbulence in the region between the two tops. We therefore assume  $h$  equals whichever is the larger of the boundary layer depth predicted by (8) and the stable boundary layer depth just before dawn. Since this prescription for boundary layer depth depends on more than just the current hour's data, much of the data needed will often be unavailable. The extents to which we go to estimate this data are described in §5.2 below. If the data required cannot be estimated, the neutral limit of (7),  $h = 0.3u_*/|\omega|$ , is assumed instead. This value is also adopted when the values

of  $F_{\theta_0}$  in the preceding 23 hours (or estimates thereof) are all positive (as could just occur at mid-summer in polar regions). This is in order to prevent  $h$  growing indefinitely.

*Limits on boundary layer height for all stability conditions*

Minimum and maximum values of boundary layer height are imposed to prevent extreme values occurring. In ADMS 6, the minimum and maximum values are 50 m and 4000 m respectively. In ADMS-Urban, ADMS-Roads and ADMS-Airport the minimum value is  $\max(50 \text{ m}, 120 z_0)$ , where  $z_0$  is the roughness at the dispersion site; the maximum is again 4000 m. The inclusion of the  $120 z_0$  factor in the calculation of the minimum boundary layer height for these urban models attempts to account for the increased turbulence due to buildings in urban areas – in urban areas, the boundary layer height is likely to be at least four times the building height, and it is usual to set the roughness length in an urban area to be around 1/30 of a representative building height.

(i)  $\Delta\theta$ : If the value of  $h$  assumed is given by (8) then  $\Delta\theta$  is assumed to be also given by (8). Otherwise  $\Delta\theta$  is assumed to be given by

$$\Delta\theta = \begin{cases} \gamma_{\theta} h c_F / (1 + 2c_F) & \text{if } F_{\theta_0} > 0 \\ 0 & \text{otherwise} \end{cases} \quad (9)$$

The value given by (9) for  $F_{\theta_0} > 0$  is that implied by equations (8) for constant  $F_{\theta_0}$  and  $\gamma_{\theta}$  with  $u_* = 0$  and  $h = \Delta\theta = 0$  initially – the assumption  $u_* = 0$  gives the smallest value of  $\Delta\theta$  for the given value of  $h$ . The value given by (9) is of course not expected to be accurate in general; however any better estimate would require more data than are available here.

*Adjustment to  $\Delta\theta$  in ADMS-Airport, ADMS-Urban and ADMS-Roads*

If the minimum urban boundary layer height restriction of  $120 z_0$  has been applied, then a small temperature inversion is assumed to occur, with the value of  $\Delta\theta$  being set to  $0.1^{\circ}\text{C}$ . The minimum boundary layer height restriction is most likely to occur in stable conditions, where  $\Delta\theta$  would initially have been zero.

(j)  $\sigma_{\theta}$ : This is assumed to be given by  $\sigma_{\theta}^{rad} = 0.065 (7 T_{sample}/U_{10})^{1/2}$  following Moore (1976), where  $U_{10}$  is the 10 m wind speed and  $T_{sample}$  the sampling time in hours.

(k) Moisture variables and latent heat flux: Specific humidity  $q$  (mass of water vapour per unit total mass) is related to mixing ratio  $r_m$  (mass of water vapour per unit mass of dry air) by  $r_m = q/(1 - q)$ . The relative humidity  $r_h$  is related to  $r_m$  by  $r_h = 100 r_m/r_w$  where  $r_w$  is the saturated mixing ratio. The vapour pressure  $e'$  of water vapour in moist air is given by

$$e'/p = r_m/(\varepsilon + r_m)$$

where  $\varepsilon = 0.62197$  is the ratio of the molecular weight of water to that of dry air. In applying this formula the pressure  $p$  is taken from the boundary layer profile of pressure for the relevant height, as described in P09/01. The saturation vapour pressure  $e_w'$  as a function of temperature is assumed to be given by the expression due to Wexler (1976) and reported in P26/01. This is similar to the expressions given by Gill (1982, p605-606).

For  $F_{\theta_0} > 0$ , we adopt the expression for the latent heat flux consistent with the Holtslag and van Ulden (1983) scheme for  $F_{\theta_0}$ , i.e.

$$\lambda E = (F_{\theta_0} + 20\alpha) \frac{\alpha S}{(1 - \alpha)S + 1} + 20\alpha$$

For  $F_{\theta_0} \leq 0$ ,  $\lambda E$  could in reality take either sign and we adopt the value  $\lambda E = 0$ . This implies a discontinuity as  $F_{\theta_0}$  crosses zero, but it's not easy to do better in a simple scheme.

This scheme for  $\lambda E$  is not appropriate for use over the sea – please see (1) below.

(1) Wind profile and heat fluxes over the sea: Over the sea, the roughness length is affected by the shape and size of the waves, which is affected by the wind profile. Hence the roughness length and wind speed are co-dependent. In ADMS, when dispersion over the sea is modelled, any user-specified values of roughness length are ignored, and instead the roughness length is calculated using

$$z_0 = \alpha_m \frac{\nu}{u_*} + \alpha_{ch} \cdot \frac{u_*^2}{g}$$

(Beljaars) where  $\nu$  (m<sup>2</sup>/s) is the kinematic viscosity of air,  $\alpha_m = 0.11$  (Brutsaert) and the default Charnock parameter  $\alpha_{ch} = 0.018$  (although this may be modified by the user). The velocity profiles used are then the same as those used over the land, described in the ADMS Technical Specification. The equations are solved by iteration.

The heat fluxes over the sea are also different from those on land. The temperature of the sea varies only very slowly with incident solar radiation. This is because the sea has a higher specific heat capacity than land, the radiation is absorbed over the first few metres of the depth of the sea rather than just at the surface and there is vertical mixing within the sea which mixes heat away from the surface. Also, a larger proportion of the incident radiation is used in evaporation, as

there is more moisture available. These effects reduce the ratio of the surface sensible heat flux to the latent heat flux, and will tend to cause the stability to be more neutral over the sea than over the land (Garratt). In ADMS, surface roughnesses for sensible heat ( $z_{0H}$ ) and moisture ( $z_{0q}$ ) are defined (Beljaars) as

$$z_{0H} = \alpha_H \frac{\nu}{u_*}$$

$$z_{0q} = \alpha_q \frac{\nu}{u_*}$$

where  $\alpha_H = 0.4$  and  $\alpha_q = 0.62$  (Brutsaert).

Then the sensible heat flux  $F_{\theta_0}$  is given by

$$F_{\theta_0} = \frac{-\rho c_p \kappa^2 (\theta(z) - \theta_0) u(z)}{\left[ \ln \left( \frac{z + z_{0H}}{z_{0H}} \right) - \Psi_H \left( \frac{z + z_{0H}}{L_{MO}} \right) \right] \left[ \ln \left( \frac{z + z_0}{z_0} \right) - \Psi \left( \frac{z + z_0}{L_{MO}} \right) \right]}$$

(Panofsky and Dutton) where  $\rho$  is the density of air ( $\text{kg/m}^3$ ),  $c_p$  is the specific heat capacity of air ( $\text{J/kg/K}$ ),  $\theta$  is potential temperature ( $\text{K}$ ), and  $\theta_0$  is the potential temperature corresponding to the temperature of the sea surface. For stable and neutral conditions,  $\Psi_H = \Psi$ , and for convective conditions  $\Psi_H$  is given by

$$\Psi_H = \ln \left[ \frac{(1 + y)^2}{(1 + y_{surface})^2} \right]$$

where

$$y = \left[ 1 - 16 \left( \frac{z + z_{0H}}{L_{MO}} \right) \right]^{1/2}$$

$$y_{surface} = \left[ 1 - 16 \left( \frac{z_{0H}}{L_{MO}} \right) \right]^{1/2}$$

Similarly, the latent heat flux  $\lambda E$  is given by

$$\lambda E = \frac{-\rho \lambda \kappa^2 (q(z) - q_{sat0}) u(z)}{\left[ \ln \left( \frac{z + z_{0q}}{z_{0q}} \right) - \Psi_q \left( \frac{z + z_{0q}}{L_{MO}} \right) \right] \left[ \ln \left( \frac{z + z_0}{z_0} \right) - \Psi \left( \frac{z + z_0}{L_{MO}} \right) \right]}$$

(Panofsky and Dutton) where  $\lambda$  is the specific latent heat of vaporization of water ( $\text{J/kg}$ ),  $q_{sat0}$  is the

saturation specific humidity at the sea surface, and  $\Psi_q = \Psi_H$ .

It should be noted that whilst the approach for calculating the roughness lengths over the sea, and the parameter values used within this approach, are appropriate in the open sea where the wind has been blowing over the sea for a considerable distance so that there is a long fetch, modifications may be required in other situations. For example, the appropriate value of  $\alpha_{ch}$  will vary, and may be higher near land, where wavelengths are shorter and waves steeper.

(m) Default values: The following default values are assumed when no other information is available:  $N_u = 0.013$ ,  $r_{hu} = 65\%$ ,  $(dr_h/dz)_u = 0$ ,  $r = 0.23$ ,  $\alpha = 1$ ,  $1/L_{M0max} = 1$ . The value of  $N_u$  is based on observations and is slightly larger than the value of 0.011 implied by the U.S. Standard Atmosphere (Gill 1982, p49). The US Standard atmosphere quotes  $r_m = 3.7 \times 10^{-3}$  at a height of 1 km as an average value obtained from radiosondes at 45°N. The temperature and pressure at 1 km in the US Standard Atmosphere are 8.5°C and 899 mb, respectively, so this corresponds to a relative humidity of 47%. However we adopt the slightly larger value of  $r_{hu} = 65\%$  as a compromise reflecting the fact that the humidity above shallow stable boundary layers may be larger due to moisture mixed from the surface during the previous day's convective boundary layer. The default is expressed in terms of relative humidity as this is likely to be more robust than specific humidity. The US Standard Atmosphere gives values of  $r_h$  of 51% and 47% at 2 km and 4 km, respectively, and so we adopt a default of zero for  $(dr_h/dz)_u$ . The default value of  $r$  is typical of short grass and is also an average value for a range of non snow-covered surfaces (Oke (1987, p12); see also Nielsen et al (1981) and Holtslag and van Ulden (1983)). The default value of  $\alpha$  is that found by Holtslag and van Ulden (1983) to be appropriate to grass covered surfaces which are not affected by drought. The default for  $1/L_{M0max}$  is simply intended to prevent extremes of stability where many of the assumptions break down.

In addition we adopt value for temperature of  $T_0^C = 15^\circ\text{C}$  when no other information is available. This is the value in the U.S. Standard Atmosphere (Gill 1982, p49). However  $\Delta T$  and the saturated specific humidity are of course very sensitive to the value of  $T_0^C$ , and so the default value of  $T_0^C$  is not used in estimating  $\Delta T$  or in relating  $q_0$  to  $r_{h0}$ .

When there is no information on cloud amount, we adopt a default value of 5 oktas, but only for the purpose of estimating  $Q^*$  from  $K^+$  and/or estimating  $F_{\theta_0}$  at night. These calculations are relatively insensitive to cloud amount and Galinski and Thomson (1995) presented observational data from Cardington which showed that using default cloud amounts in these situations did not cause a large deterioration in the accuracy of the heat flux estimates.

Finally, if  $P_{corr}$  is missing, a value of 1.0 is assumed.

(n) Corrections for site differences:

If one or more of the *site-representative* flags are not set, then corrections are made for differences between the met site and the dispersion area. It is assumed that the geostrophic wind at the two locations is the same. The variables that are not input but are calculated by the met input module are recalculated for the dispersion area as necessary. However, if the roughness length at the met site differs from that at the dispersion site, and if  $F_{\theta_0}$  or  $L_{MO}$  are input, then we make the following assumptions. If  $F_{\theta_0} > 0$ , we assume  $F_{\theta_0}$  is the same at both sites while, if  $F_{\theta_0} \leq 0$ , we assume  $\theta_*$  is the same at both sites. This enables corrections for roughness changes to be made in a way that is consistent with the assumptions for  $F_{\theta_0}$  made in (e) and (f) above (in the sense that the latter imply that  $F_{\theta_0}$  is independent of roughness in unstable conditions and that  $\theta_*$  is independent of roughness in stable conditions).

## 5.2 Structure of the computation

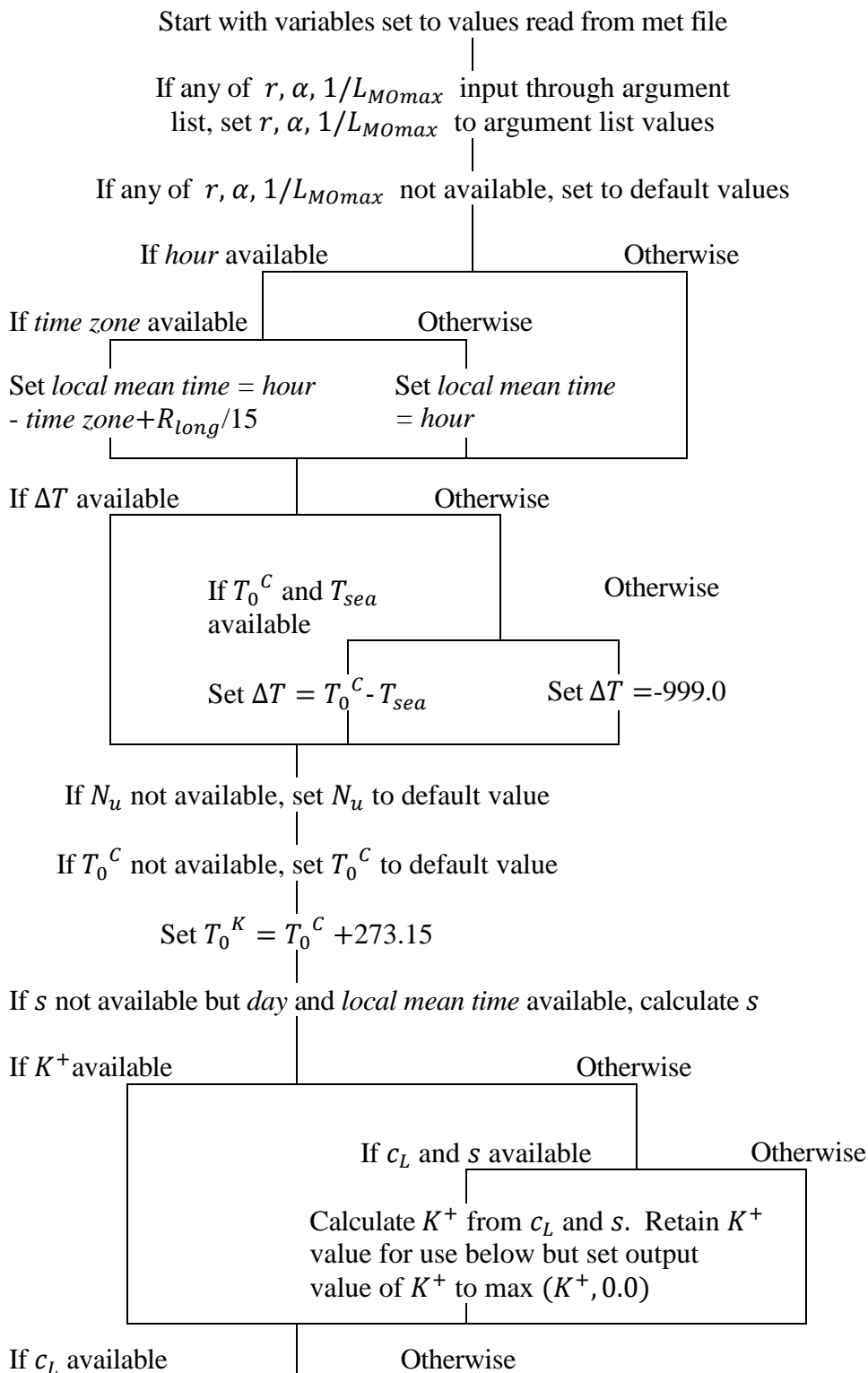
In this section we discuss the computation of the variables in the processed-met structure. (Note that the procedure differs slightly from that described below when ADMS is used to model dispersion over the sea.)

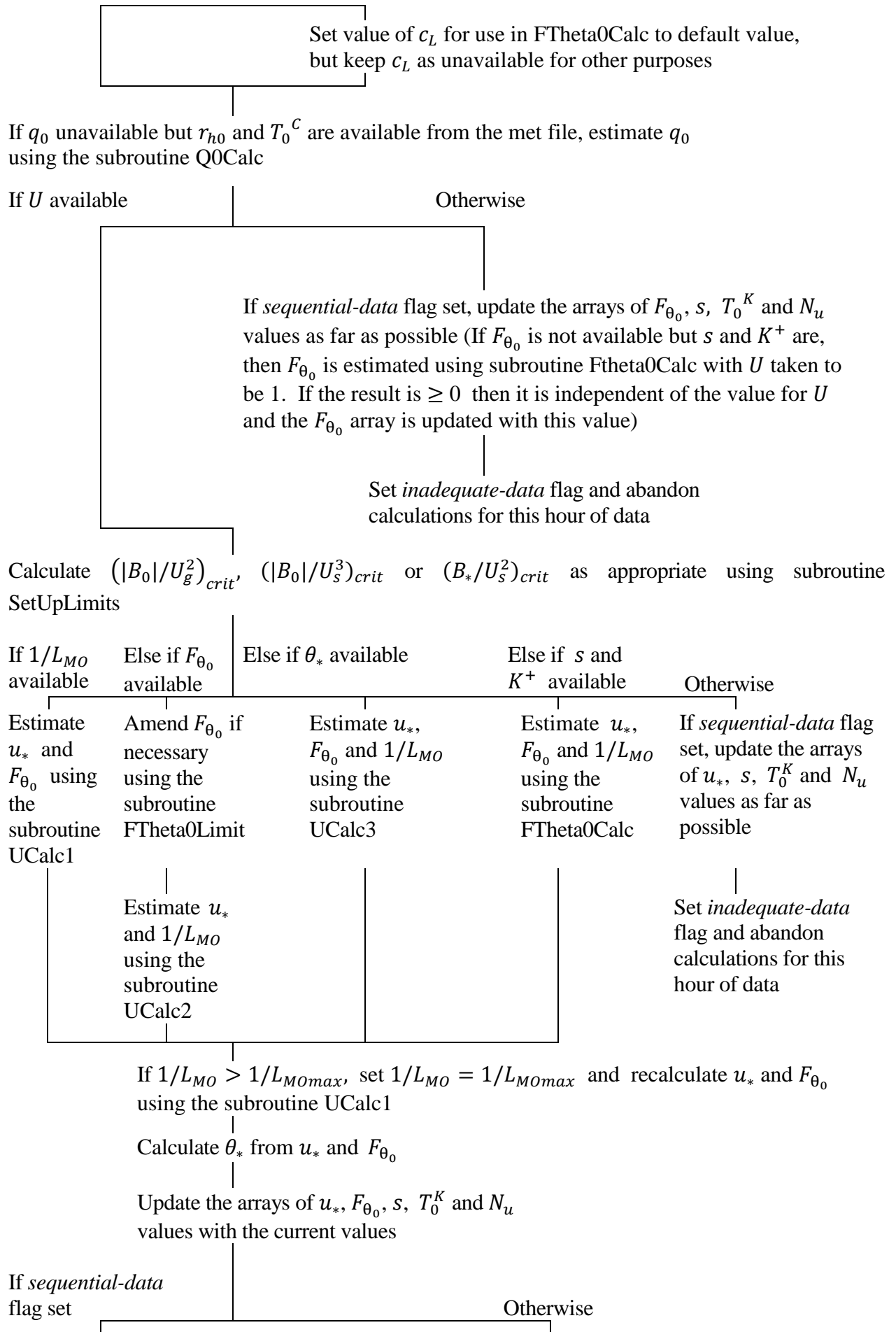
If one or more of the *site-representative* flags are not set then, as noted in 5.1(m) above, the various computations may need to be performed twice. However in the following we discuss only one set of computations and make no distinction between the values at the two sites – which values we are referring to will depend on which of the two sets of computations are being performed. Both computations are identical in structure, the only difference being the inputs to the computations. In the following we refer to input from the met file. If we are considering the met site this means what it says. However, when we are considering the dispersion area, it means an analogous set of data obtained from the met file input by (i) replacing  $(U, \phi)$  by  $(U_g, \phi_g)$  as output from the met site calculation and (ii) if the roughness at the met site differs from that at the dispersion site, and  $F_{\theta_0}$  or  $L_{MO}$  are input in the met file, setting  $F_{\theta_0}$  to the output of the met site calculation if it is  $> 0$  and setting  $\theta_*$  to the output of the met site calculation if  $F_{\theta_0}$  as output from the met site calculation is  $\leq 0$ , while setting all other values of  $F_{\theta_0}$ ,  $L_{MO}$  and  $\theta_*$  to -999.9 to indicate missing data.

The first time the computations are performed, the values of  $|\omega|$  and  $\text{sign}(\omega)$  are calculated by the subroutine CoriolisCalc. Also an array is maintained of the values of  $u_*$ ,  $F_{\theta_0}$ ,  $s$ ,  $T_0^K$  and  $N_u$  which occur during the preceding 24 hours (including the current hour); this is to assist with estimating  $h$  which may depend on data from previous hours. For these arrays -999.0 is used for missing values. These arrays are also used even with non-sequential data, but in this case the values

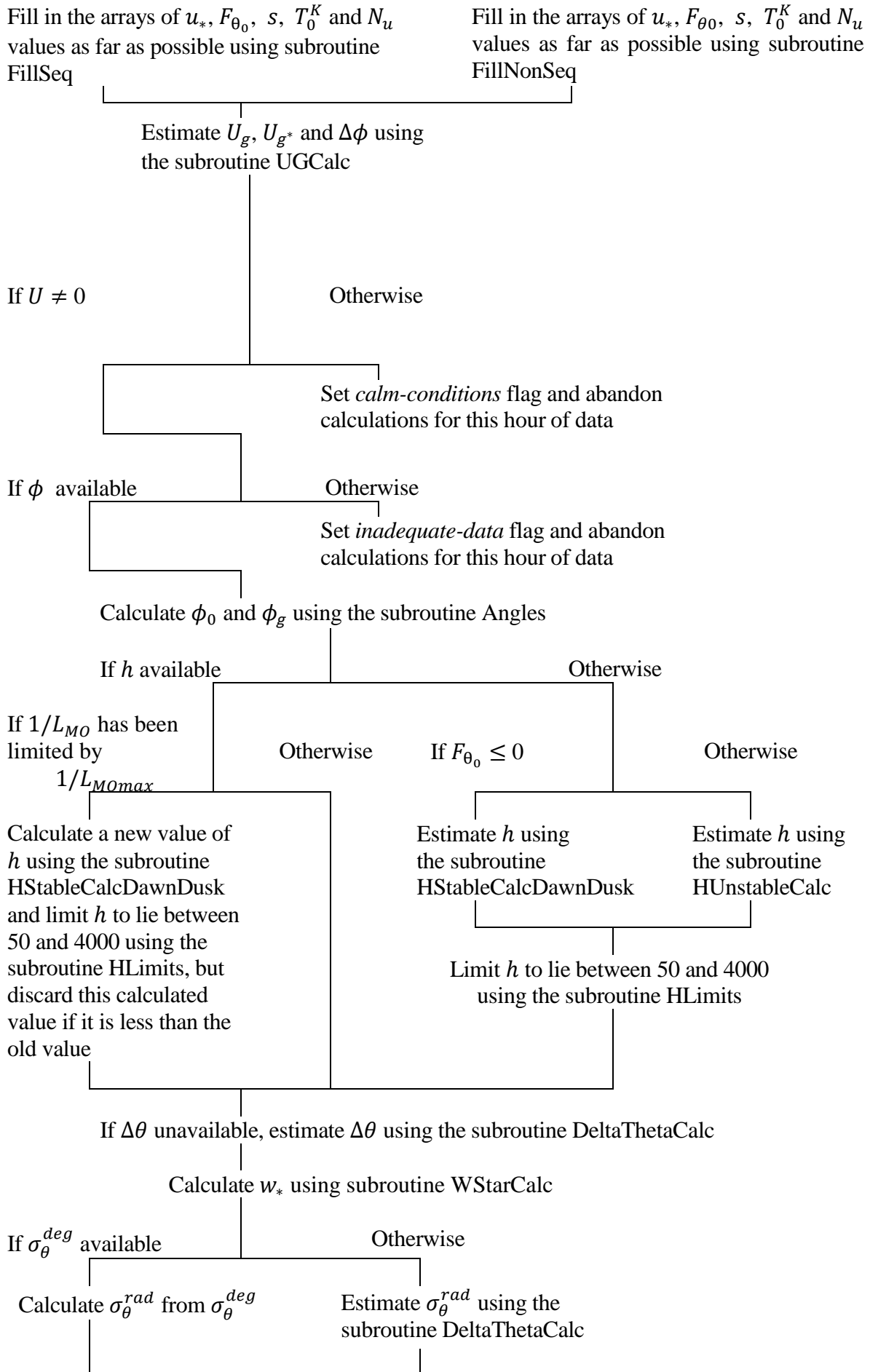
all need to be estimated from the current hour's data. At the start of the computations for each hour of data, the arrays are updated by shifting them by one hour in the case of sequential data and by setting them to -999.0 for non-sequential data. (Of course two sets of history arrays may be needed if one or more of the *site-representative* flags are not set.)

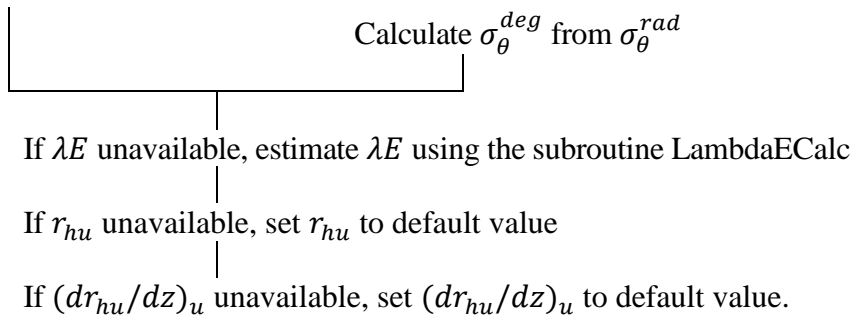
After these preliminaries the subroutine ProcessMet is called. The flow diagram below outlines the structure of the subroutine.











Some details of some of the subroutines used are now described.

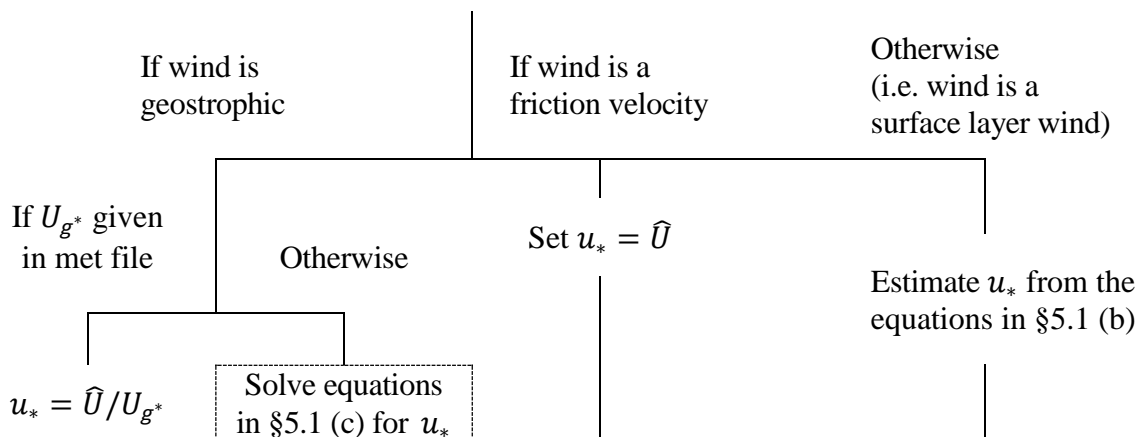
CoriolisCalc: This routine calculates  $|\omega|$  and  $\text{sign}(\omega)$  and, if  $|\omega| < 5 \times 10^{-5}$ , sets  $|\omega|$  equal to  $5 \times 10^{-5}$  and issues a warning.

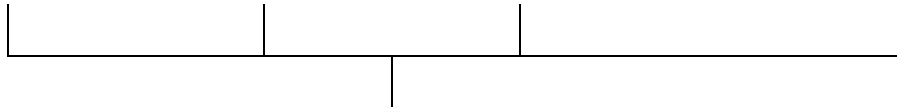
SetupLimits: This routine calculates  $(B_0/U_g^2)_{crit}$ ,  $(B_0/U_s^3)_{crit}$  and  $(B_*/U_s^2)_{crit}$ . In calculating  $(B_0/U_s^3)_{crit}$  and  $(B_*/U_s^2)_{crit}$ , it uses two subroutines UCalc2A and UCalc3A which are slightly modified versions of the subroutines UCalc2 and UCalc3 described below.

FTheta0Limit: This routine amends  $F_{\theta_0}$  if necessary to take account of the critical values described in §5.1 (e). If the input wind speed is geostrophic and an amendment is necessary then a warning is issued.

ThetaStarLimit: This routine amends  $\theta_*$  if necessary to take account of the critical value described in §5.1 (e).

UCalc1: This routine estimates  $u_*$  and  $F_{\theta_0}$  from given values of  $1/L_{MO}$ ,  $T_0^K$ ,  $z_0$ ,  $|\omega|$  and a wind speed  $\hat{U}$  (either a geostrophic wind, surface layer wind or friction velocity, but not necessarily that obtained from the met file) and from  $U_{g^*}$  if this is available from the met file. The following flow diagram outlines the structure of the routine.

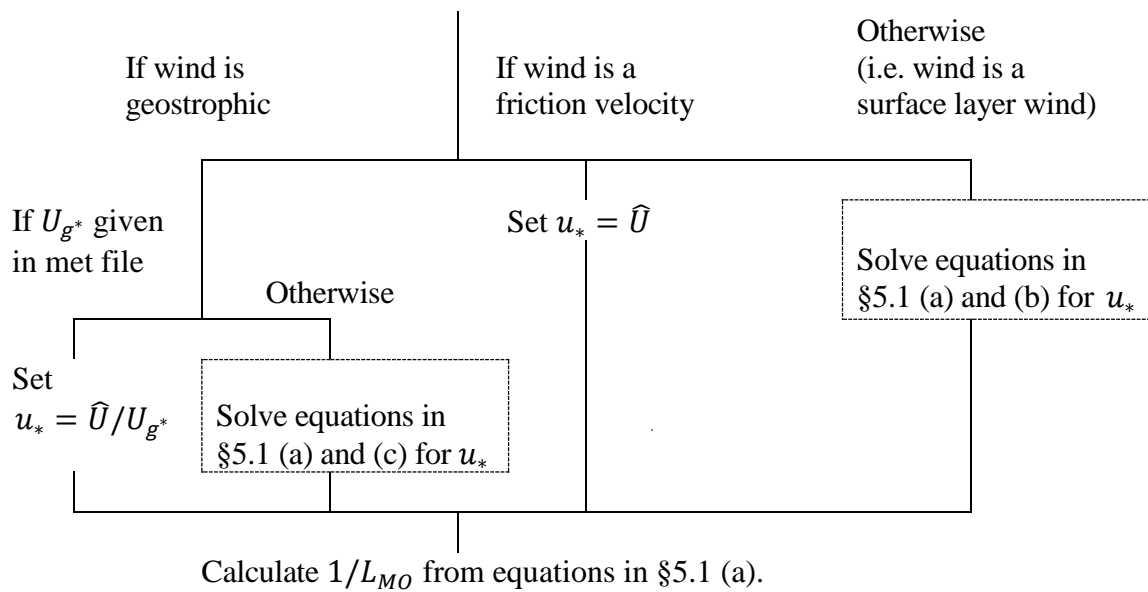




Calculate  $F_{\theta_0}$  from equations in §5.1 (a).

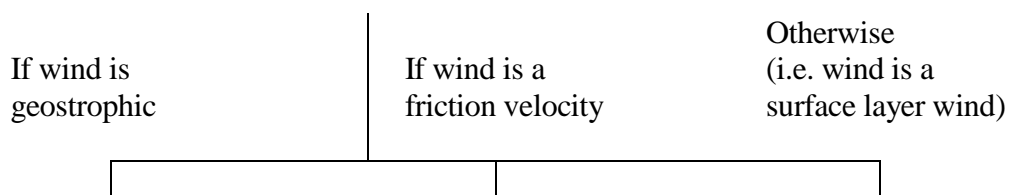
The calculation in dashed lines requires numerical solution. This is done with an iterative technique.

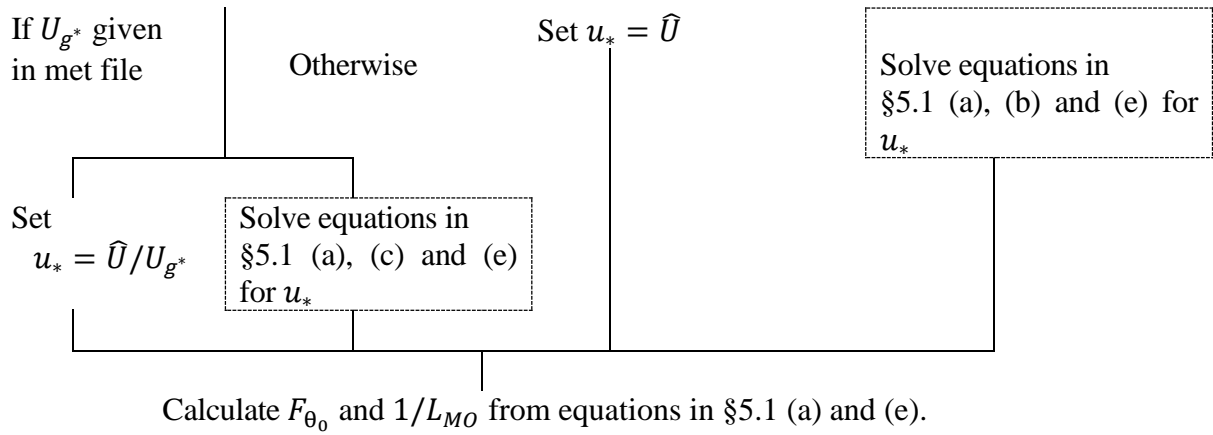
UCalc2: This routine estimates  $u_*$  and  $1/L_{MO}$  from given values of  $F_{\theta_0}$ ,  $T_0^K$ ,  $z_0$ ,  $|\omega|$  and a wind speed  $\hat{U}$  (either a geostrophic wind, surface layer wind or friction velocity, but not necessarily that obtained from the met file) and from  $U_{g^*}$  if this is available from the met file. The following flow diagram outlines the structure of the routine.



The calculations in dashed lines require numerical solution. This is done with an iterative technique. When  $F_{\theta_0} < 0$  and  $\hat{U}$  is a surface layer wind there may be more than one positive solution for  $u_*$ . The solution chosen is the largest value since this gives the correct limit in neutral conditions.

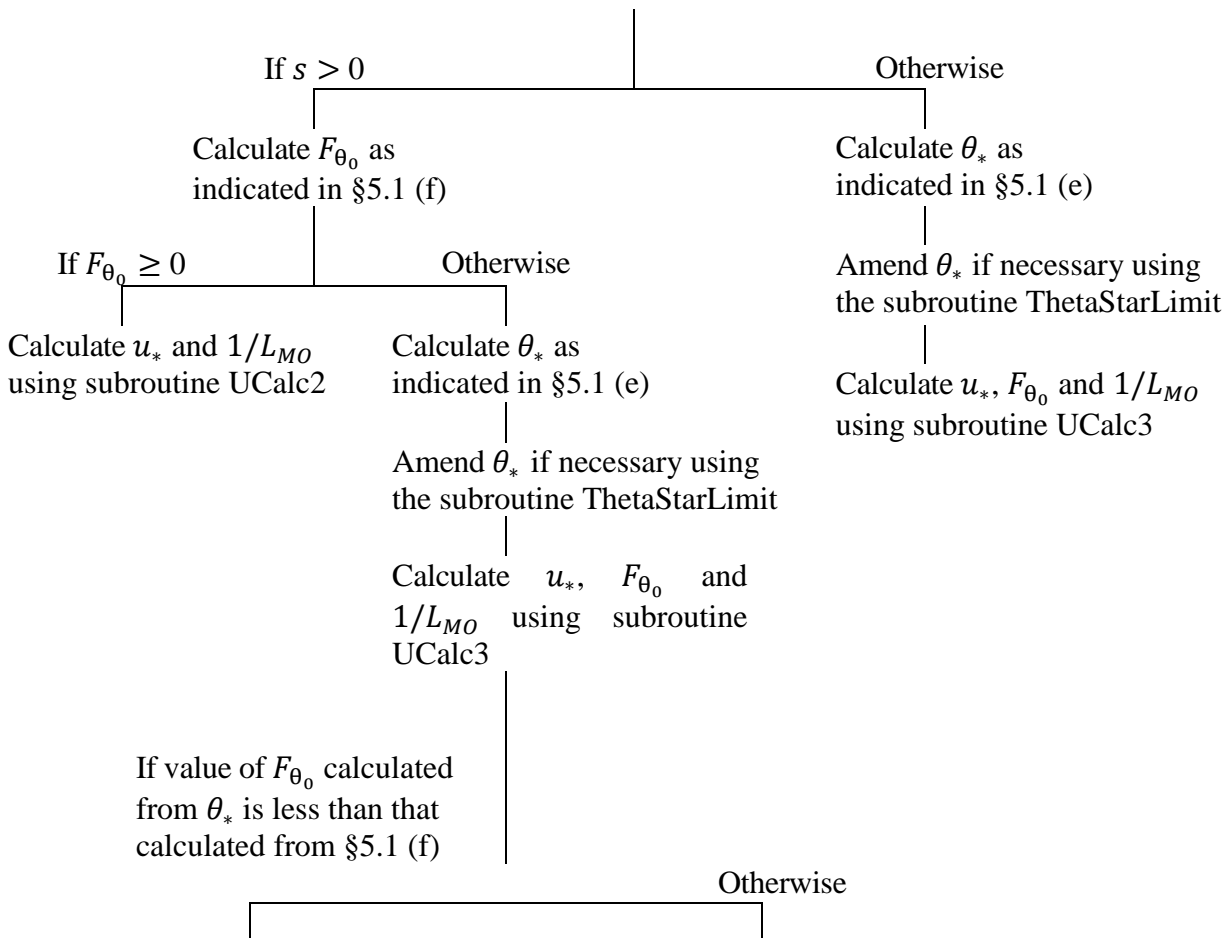
UCalc3: Provided  $\theta_* \geq 0$ , this routine estimates  $u_*$ ,  $F_{\theta_0}$  and  $1/L_{MO}$  from given values of  $\theta_*$ ,  $T_0^K$ ,  $z_0$ ,  $|\omega|$  and a wind speed  $\hat{U}$  (either a geostrophic wind, surface layer wind or friction velocity, but not necessarily that obtained from the met file) and from  $U_{g^*}$  if this is available from the met file. The following flow diagram outlines the structure of the routine.





The calculations in dashed lines require numerical solution. This is done with an iterative technique. When  $\hat{U}$  is a surface layer wind there may be more than one positive solution for  $u_*$ . The solution chosen is the largest value since this gives the correct limit in the approach to neutral conditions.

FTheta0Calc: This routine estimates  $u_*$ ,  $F_{\theta_0}$  and  $1/L_{MO}$  from given values of  $T_0^K$ ,  $s$ ,  $c_L$ ,  $K^+$ ,  $r$ ,  $\alpha$ ,  $z_0$ ,  $|\omega|$ ,  $(B_*/U_s^2)_{crit}$ , and a wind speed  $\hat{U}$  (either a geostrophic wind, surface layer wind or friction velocity) and from  $U_{g^*}$  if this is available from the met file. The following flow diagram outlines the structure of the routine.

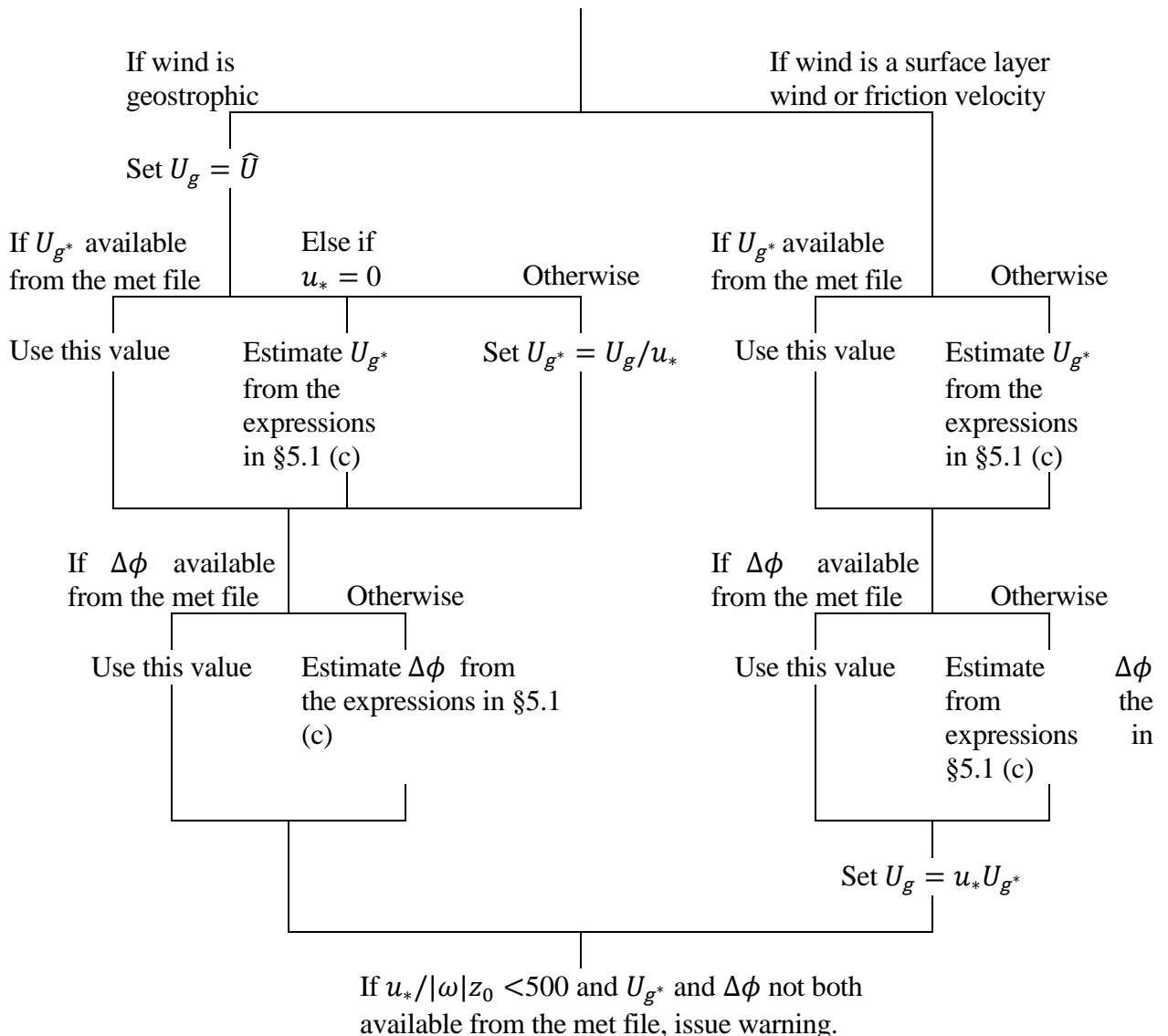


Adopt value of  $F_{\theta_0}$   
calculated from §5.1 (f)

Adopt values of  $u_*$ ,  $F_{\theta_0}$   
and  $1/L_{MO}$  calculated in  
UCalc3

Calculate  $u_*$  and  $1/L_{MO}$   
using subroutine UCalc2.

UGCalc: This routine estimates  $U_g$ ,  $U_{g^*}$  and  $\Delta\theta$  from  $u_*$ ,  $1/L_{MO}$ ,  $z_0$ ,  $|\omega|$ ,  $\text{sign}(\omega)$  and a wind speed  $\hat{U}$  (either a geostrophic wind, surface layer wind or friction velocity) and from  $U_{g^*}$  and  $\Delta\theta$  if these are available from the met file. The following flow diagram outlines the structure of the routine.



Note that if  $U_{g^*}$  is not available from the met file but  $\Delta\phi$  is,  $U_{g^*}$  is estimated without reference to  $\Delta\phi$ . However if  $U_{g^*}$  is available but  $\Delta\phi$  isn't,  $\Delta\phi$  is estimated from  $u_*$  which, if the wind from the met file is geostrophic, depends on  $U_{g^*}$ .

Angles: This routine calculates  $\phi_0$  and  $\phi_g$  from  $\Delta\phi$  and a wind direction  $\phi$  (either a geostrophic wind, surface layer wind or friction velocity, but not necessarily that obtained from the met file).

HStableCalcDawnDusk: This routine estimates  $h$  from  $|\omega|$  and from the arrays of  $u_*$ ,  $F_{\theta_0}$ ,  $s$ ,  $N_u$  and  $T_0^K$  values whenever  $F_{\theta_0} \leq 0$ , as described in §5.1 (h). First the value of  $h$  with ‘near dawn’ corrections is calculated using the routine HStableDawn. Then, if  $F_{\theta_0}$  in the previous hour is  $> 0$ , the ‘near dusk’ correction is applied by (i) recalculating  $h$  with  $F_{\theta_0}$  in the current hour set to 0.1 using the routine HUnstableCalc, and (ii) taking  $h$  to be the smaller of the two values. Note a separate routine is used for HStableDawn to avoid the possibility of recursion.

HStableCalcDawn: This routine estimates  $h$  from  $|\omega|$  and from the arrays of  $u_*$ ,  $F_{\theta_0}$ ,  $s$  and  $T_0^K$  values whenever  $F_{\theta_0} \leq 0$ , as described in §5.1 (h) but without the ‘near dusk’ correction. Because it is called from the routine HUnstableCalc as well as from HStableCalcDawnDusk, this routine is designed to be able to calculate  $h$  for any of the previous hours in the arrays of past values as well as for the current hour. The hour for which  $h$  is required is passed through the argument list. First it establishes whether the near dawn correction is needed. It is needed unless (i)  $s$  for the hour in question is unknown, or (ii)  $s$  for the hour in question is  $\leq 0$ , or (iii) the hour in question is the earliest time in the arrays of values, or (iv)  $u_*$ ,  $F_{\theta_0}$ , or  $T_0^K$  for the hour preceding the hour in question is unknown, or (v) when going back in time from the current hour an occasion is found with  $F_{\theta_0}$ , or  $s$  unknown or with  $F_{\theta_0} > 0$ , up to and including the first time encountered with  $s \leq 0$ . Then, using the routine UCalc2,  $1/L_{MO}$  is calculated for the hour in question if no near dawn correction is needed and for the preceding hour if a correction is needed. Finally, using the routine HStableCalc,  $h$  is calculated from  $u_*$  for the hour in question, from the value of  $1/L_{MO}$  just calculated, and from  $|\omega|$ .

HStableCalc: This routine estimates  $h$  from  $u_*$ ,  $1/L_{MO}$  and  $|\omega|$  using equation (7). By putting  $1/L_{MO} = 0$  this routine can be used to return the neutral limit of (7), namely  $h = 0.3u_*/|\omega|$ .

HUnstableCalc: This routine estimates  $h$  from  $|\omega|$  and the arrays of  $u_*$ ,  $F_{\theta_0}$ ,  $s$ ,  $N_u$  and  $T_0^K$  values whenever  $F_{\theta_0} > 0$ , as described in §5.1 (h). If it has proved impossible to fill in the arrays of  $u_*$ ,  $F_{\theta_0}$ ,  $N_u$  and  $T_0^K$  values using subroutines FillSeq or FillNonSeq, or if, after filling in, there is no  $F_{\theta_0}$  value in the  $F_{\theta_0}$ -array which is  $\leq 0$ ,  $h$  is set to the neutral value  $0.3u_*/|\omega|$  and a warning is issued. Otherwise the boundary layer depth  $h_s$  corresponding to the last hour with  $F_{\theta_0} \leq 0$  is calculated using HStableCalcDawn. Then (8) is solved using subroutine BLGrowth to obtain values of  $h$  and  $\Delta\theta$  corresponding to the mid point of the current hour. In doing this, values of  $u_*$ ,  $F_{\theta_0}$ ,  $N_u$

and  $T_0^K$  are taken from the arrays of these quantities and are assumed to remain constant in each hour, while  $h$  and  $\Delta\theta$  are assumed to be zero at the end of the last hour with  $F_{\theta_0} \leq 0$ . Finally  $h$  is set equal to the maximum of the value of  $h$  obtained from BLGrowth and  $h_s$ .

The routine also returns the estimate of  $\Delta\theta$  obtained from BLGrowth whenever the value of  $h$  returned is also obtained from that subroutine. Otherwise  $\Delta\theta$  is returned as missing (-999.0).

BLGrowth: This routine solves the equations (8) for  $h$  and  $\Delta\theta$ . The routine takes as input (i) initial conditions for  $h$  and  $\Delta\theta$ , (ii) the length of the period between the time corresponding to the initial conditions and the time at which output is required, and (iii) values of  $u_*$ ,  $F_{\theta_0}$ ,  $N_u$  and  $T_0^K$  which are assumed to remain constant during the period referred to in (ii). The equations are solved using the analytic solution for  $t$  as a function of  $h$  described by Thomson (1992) which is inverted using a bisection technique. Several variables are held in double precision and, if the input value of  $F_{\theta_0}$  is less than 1, the value 1 is adopted instead; this is to avoid difficulties due to the presence of large nearly balancing terms in the expression for  $t$  when  $F_{\theta_0}$  is small.

HLimits: This routine limits  $h$  to the range 50 to 4000. If  $h$  would otherwise lie outside this range a warning is issued.

DeltaThetaCalc: This routine estimates  $\Delta\theta$  from  $F_{\theta_0}$ ,  $h$ ,  $N_u$ ,  $T_0^K$  and the value of  $\Delta\theta$  estimated using HUnstableCalc (if any), as described in §5.1(i).

WStarCalc: This routine calculates  $w_*$  from  $u_*$ ,  $1/L_{MO}$  and  $h$  as described in §5.1 (a).

FillSeq and FillNonSeq: These routines attempt to fill in the missing data in the arrays of  $u_*$ ,  $F_{\theta_0}$ ,  $s$ ,  $N_u$ , and  $T_0^K$  values, working back from the current hour until (i) an hour for which  $F_{\theta_0}$  can't be filled is reached, or (ii) an hour with  $F_{\theta_0} \leq 0$  for which  $s$  can't be filled or for which  $s \leq 0$  is found, or (iii) the beginning of the arrays are reached. FillSeq is used when the input data are sequential and FillNonSeq is used otherwise. FillSeq will be described first. The missing values of  $u_*$  are filled in by linear interpolation where possible using the routine Interpolation. Where this is not possible  $u_*$  is set to the first available subsequent value. The missing values of  $N_u$  and  $T_0^K$  are filled in by using the default values (linear interpolation is not used for  $N_u$  and  $T_0^K$  so as to make the results the same as if adequate data had been given for the preceding hours but with  $N_u$  or  $T_0^K$  missing – in this situation the default values would have been adopted). Then the missing values of  $s$  are estimated where possible using *hour* and *day*, using the fact that *hour* decreases by 1 as we look back through each past hour. Finally the missing values of  $F_{\theta_0}$  are addressed. First we attempt to estimate  $F_{\theta_0}$  by linear interpolation using the routine Interpolation. Interpolations for  $F_{\theta_0}$  are not

made if the gap is longer than two hours. If values of  $F_{\theta_0}$  are still missing but  $s$  is available for the same hour (in the history arrays) and  $c_L$  is available from the met file, then  $K^+$  is calculated from  $c_L$  and  $s$  using the equation in §5.1 (f) and  $F_{\theta_0}$  is calculated with subroutine FTheta0Calc by making use of the arrays of  $u_*$ ,  $s$  and  $T_0^K$  values on the assumption that  $c_L$ ,  $r$  and  $\alpha$  are unchanged in the preceding hours. The routine FillNonSeq is very similar to FillSeq although there are two differences. Firstly there are a number of the steps in FillSeq which would have no effect and are therefore omitted. Also  $N_u$  and  $T_0^K$  are filled in by adopting the current values instead of the defaults.

## **Appendix – Example met file**

\*\*\*\*\*

This is a demonstration met file designed to illustrate the format required for such files.

Only the information following the keywords 'VARIABLES:' and 'DATA:' is read by the model. This enables extra information which is not read by the model to be included in the met file - for example information on the measurement site or comments such as these describing the format of the file.

The met data are presented as a sequence of records, each record giving the data for a particular hour. In each record, a number of met variables (e.g. wind speed, surface sensible heat flux etc.) are given. The same variables must be given for each hour, although if some values are unknown this can be indicated by -999.0 as described below. The information following the keyword 'VARIABLES:' describes how many variables are given for each hour and what the variables are, while the met data itself follows the keyword 'DATA:'.

In the information after the keyword 'VARIABLES:', various keywords are used to indicate which met variables are given for each hour's data and the order in which they are given. The number of possible input variables is quite large in order to support a range of applications and to allow for a variety of data sources - however the number of variables used in any one application is likely to be a small fraction of those possible. The variables fall into 4 categories, true met variables, site characteristics, time variables and frequency information. Several of the variables have aliases, i.e. alternative keywords. These are either expanded definitions which are more self-explanatory or are present for compatibility with past versions. The keywords are not case sensitive. The meaning of the keywords is as follows:

### 1) Met variables:

#### WIND SPEED

Alias (supported for past compatibility only): U

Definition: Wind speed at measurement height (friction velocity if measurement height = 0; geostrophic wind if measurement height = 1000.0).

#### UG/USTAR

Alias: GEOSTROPHIC WIND SPEED/FRICTION VELOCITY

Alias (supported for past compatibility only): UGSTAR

Definition: Geostrophic wind speed/friction velocity.



WIND DIRN

Alias: WIND DIRECTION (DEGREES)

Alias (supported for past compatibility only): PHI

Definition: Wind direction (angle wind is coming from in degrees clockwise from north) at measurement height (surface wind direction if measurement height = 0; geostrophic wind direction if measurement height = 1000.0).

DIRN CHANGE

Alias: GEOSTROPHIC MINUS SURFACE WIND DIRECTION (DEGREES)

Alias (supported for past compatibility only): DELTAPHI

Definition: Geostrophic wind direction minus surface wind direction (degrees).

HEAT FLUX

Alias: SENSIBLE HEAT FLUX

Alias (supported for past compatibility only): FTHETA0

Definition: Surface sensible heat flux.

1/LMO

Alias: 1/MONIN-OBUKHOV LENGTH

Alias (supported for past compatibility only): RECIPLMO

Definition: 1/Monin-Obukhov length.

BL DEPTH

Alias: BOUNDARY LAYER DEPTH

Alias (supported for past compatibility only): H

Definition: Boundary layer depth.

CLOUD

Alias: CLOUD AMOUNT (OKTAS)

Alias (supported for past compatibility only): CL

Definition: Cloud amount (oktas).

SOLAR RAD

Alias: INCOMING SOLAR RADIATION

Definition: Incoming solar radiation.

TEMPERATURE

Alias: TEMPERATURE (C)

Alias (supported for past compatibility only): T0C

Definition: Near surface temperature (degrees C).

N ABOVE BL

Alias: BUOYANCY FREQUENCY ABOVE BOUNDARY LAYER

Alias (supported for past compatibility only): NU

Definition: Buoyancy frequency above the boundary layer.

DELTA THETA

Alias: TEMPERATURE JUMP ACROSS BOUNDARY LAYER TOP

Alias (supported for past compatibility only): DELTATHETA

Definition: Temperature jump across the boundary layer top.

PRECIP

Alias: PRECIPITATION RATE (MM/HOUR)

Alias (supported for past compatibility only): P

Definition: Precipitation rate (mm/hour).

SEA TEMP

Alias: SEA SURFACE TEMPERATURE (C)

Alias (supported for past compatibility only): TSEA

Definition: Sea surface temperature (degrees C).

DELTA T

Alias: TEMPERATURE OVER LAND MINUS SEA SURFACE TEMPERATURE

Alias (supported for past compatibility only): DELTAT

Definition: Near surface temperature over land minus sea surface temperature.

SIGMA THETA

Alias: SIGMA THETA (DEGREES)

Alias (supported for past compatibility only): SIGMATHETA

Definition: Standard deviation of changes in mean wind direction (in degrees).

S HUMIDITY

Alias: SPECIFIC HUMIDITY

Definition: Near surface specific humidity.

R HUMIDITY

Alias: RELATIVE HUMIDITY (PERCENT)

Alias (supported for past compatibility only): RHUM

Definition: Near surface relative humidity (percent).

RH ABOVE BL

Alias: RELATIVE HUMIDITY ABOVE BOUNDARY LAYER (PERCENT)

Definition: Relative humidity just above the boundary layer (percent).

DRH/DZ

Alias: D(RELATIVE HUMIDITY)/DZ ABOVE BOUNDARY LAYER (PERCENT/M)

Definition: d(Relative humidity)/dz above the boundary layer (percent/m).

LAT HT FLUX

Alias: LATENT HEAT FLUX

Definition: Surface latent heat flux.

2) Site variables:

WIND HEIGHT

Alias: WIND MEASUREMENT HEIGHT

Definition: Height of wind measurement at met site (1,000.0 is used to indicate geostrophic wind, 0.0 to indicate friction velocity).

Z0 (D)

Alias: ROUGHNESS LENGTH (DISPERSION AREA)

Definition: Surface roughness at dispersion site.

ALBEDO (D)

Alias: ALBEDO (DISPERSION AREA)

Definition: Surface albedo at dispersion site.

ALPHA (D)

Alias: MODIFIED PRIESTLEY-TAYLOR PARAMETER (DISPERSION AREA)

Alias (supported for past compatibility only): ALPHA

Definition: Modified Priestley-Taylor parameter at dispersion site (as defined in Holtslag and van Ulden, 1983, J. Clim. Appl. Met., vol 22, 517-529).

Z0 (M)

Alias: ROUGHNESS LENGTH (MET SITE)

Definition: Surface roughness at met site.

ALBEDO (M)

Alias: ALBEDO (MET SITE)

Alias (supported for past compatibility only): R

Definition: Surface albedo at met site.

ALPHA (M)

Alias: MODIFIED PRIESTLEY-TAYLOR PARAMETER (MET SITE)

Alias (supported for past compatibility only): ALPHA

Definition: Modified Priestley-Taylor parameter at met site (as defined in Holtslag and van Ulden, 1983, J. Clim. Appl. Met., vol 22, 517-529).

3) Time variables:

HOURL

Alias (supported for past compatibility only): THOUR

Definition: Hour of day (local time, i.e. GMT + longitude in degrees (east positive)/15).

DAY

Alias (supported for past compatibility only): TDAY

Definition: Day of year (1st Jan = 1).

YEAR

Definition: Year.

4) Frequency variables:

FREQUENCY

Alias (supported for past compatibility only): FR

Definition: Frequency with which a given set of met conditions occurs (arbitrary units, e.g. percentage of occasions or number of hours per year).

MONTHS ww TO xx, HOURS yy TO zz

Definition: Detailed frequency information giving the frequency with which a given set of met conditions occurs for certain months of the year or times of day. (arbitrary units, e.g. percentage of occasions or number of hours per year - must be same for each such variable).

Input requirements and usual inputs: ....

The frequency variables must, if they are mentioned in the header, be present for every set of met data (i.e. -999.0 will cause a fatal error).

The met data itself which follows the keyword 'DATA:' must be formatted as appropriate for a FORTRAN 'list-directed read' (a comma separated list is the easiest way to achieve this). Each variable must be a real (as opposed to an integer - i.e. it must contain a '.') and missing data can be indicated by -999.0 or, assuming a comma separated list is used, by omitting the variable (the comma must however still be present). Missing data or invalid data (e.g. negative boundary layer depth) may cause error messages to be generated.

Units are SI units except where stated in the variable definitions above.

All keywords must start in the first column.

In this example file, an invalid variable name 'PRESSURE' has been included. This will generate a warning message and the data for this variable will be ignored. This file also includes some examples of missing and invalid data.

VARIABLES:

6  
U  
PRESSURE  
FTHETA0  
PHI  
H  
P

Comments can also be added to the met file between the 'VARIABLES:' part of the file and the 'DATA:' part, as illustrated by this comment.

DATA:

10.0, 1013.2, 100.0, 30.0, 1000.0, 2.0  
5.0, 1013.2, 300.0, 150.0, 1500.0, 0.0  
7.5, 950.1, 0.0, 240.0, 500.0, 3.0  
7.5, 950.1, 0.0, , 500.0, 3.0  
7.5, 950.1, 0.0, 240.0, 500.0, -999.0  
7.5, 950.1, 0.0, 240.0, -500.0, 3.0  
15.5, 1020.1, -20.0, 240.0, 500.0, 3.0

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