



User's Manual AERCOARE Version 1.0

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AERCOARE
Version 1.0

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PREFACE

The work completed under this work assignment is a continuation of an evaluation report prepared by ENVIRON entitled "Evaluation of the COARE–AERMOD Alternative Modeling Approach for Simulation of Shell Exploratory Drilling Sources in the Beaufort and Chukchi Seas" dated December 2010. The Coupled Ocean Atmosphere Response Experiment (COARE) air-sea flux procedure was coded into a meteorological data preprocessor program called AERCOARE. AERCOARE can read overwater measured hourly meteorological data or predicted hourly meteorological data from the Mesoscale Model Interface (MMIF) program. The output from AERCOARE is used by the AERMOD dispersion program in a marine environment. This document is a user's guide on how to run the AERCOARE preprocessor program. The work was funded under a subcontract from the University of North Carolina at Chapel Hill with U.S. Environmental Protection Agency (EPA Prime award EPD07102, Work Assignment 5-17. The EPA Region 10 (R10) Office of Environmental Assessment (OEA) Work Assignment Manager was Ms. Jennifer Crawford and the R10 Technical Lead was Mr. Herman Wong.

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1.0 INTRODUCTION

AERCOARE processes overwater meteorological data for use by the AERMOD air quality dispersion model (hereafter AERMOD) (EPA, 2004a). AERCOARE is the counterpart to AERMET (EPA, 2004b), the overland meteorological preprocessor in the AERMOD modeling system. The combination of AERCOARE and AERMOD may eventually replace the current regulatory approach for offshore projects, the Offshore and Coastal Dispersion (OCD) model (Chang and Hahn, 1997; DiCristofaro and Hanna, 1989) because OCD has not been updated for many years and does not reflect the latest scientific advancements found in AERMOD. AERCOARE applies the Coupled Ocean Atmosphere Response Experiment (COARE) air-sea flux algorithm (Fairall, et. al., 2003) to overwater meteorological measurements to estimate surface energy fluxes and assembles these estimates and other measurements for subsequent dispersion model simulations with AERMOD. As an alternative to overwater measurements, AERCOARE can also use Weather Research Forecast (WRF) model simulations of the marine boundary layer. WRF output files can be processed for AERCOARE by using the Mesoscale Model Interface (MMIF) program (Brashers and Emery, 2012).

The AERMOD-COARE approach was recently approved by the U.S. Environmental Protection Agency (EPA) Region 10 as an alternative model to OCD for application in an Arctic ice-free environment with concurrence from the EPA Model Clearinghouse (EPA, 2011a; EPA, 2011b). In that application, the COARE algorithm was applied to overwater measurements and the results assembled in a spreadsheet. AERCOARE replaces the need for post-processing with a spreadsheet, provides support for missing data, adds options for the treatment of overwater mixing heights, and can consider many different input data formats.

This user's manual documents AERCOARE v1.0 and includes the rationale for the approach, descriptions of the algorithms, the program code, user input, and runtime instructions. The development of AERCOARE was sponsored by the EPA under Contract EP-D-7-102, Work Assignment 4-14 and Work Assignment 5-17.

2.0 RATIONALE

The current EPA guideline model for offshore sources is the OCD model. OCD has not been updated for many years and several of the dispersion model components and procedures are not consistent with AERMOD. The AERMOD modeling system is the U.S. EPA-recommended approach for assessing the near-source (< 50 km) impacts of new or modified sources as part of the New Source Review (NSR) and Prevention of Significant Deterioration (PSD) programs. The modeling system includes an AERMET meteorological processor that processes overland meteorological data for input to AERMOD.

Important routines in OCD that are independent of the onshore/offshore setting are inconsistent with current regulatory practices as embodied within AERMOD, namely:

- OCD does not contain routines for processing either missing data or hours of calm meteorology. Such processing must be performed with a custom post-processing program.
- OCD does not contain the latest regulatory PRIME downwash algorithm (Schulman, L. L. et al, 2000). Many offshore sources are located on ships where downwash effects are important.
- The PVMRM¹ and OLM² methods are not included in OCD. These techniques are crucial for assessing the new 1-hour NO₂ ambient standard.
- The new 24-hour PM_{2.5}, 1-hour NO₂, and 1-hour SO₂ ambient standards are based on the 98th, 98th, and 99th percentile concentrations, respectively. These probabilistic standards and the EPA methods recommended for estimating design concentrations must be obtained by post-processing the hourly OCD output files. Such calculations are included in recent versions of AERMOD.
- OCD does not contain a volume source routine and the area source routine only considers circular areas without allowance for any initial vertical dispersion.
- Although OCD contains routines to simulate the boundary layer over the ocean, the surface energy flux algorithms are outdated and have been replaced within the scientific community by the COARE air-sea flux algorithms.

The current AERMOD modeling system depends on the AERMET meteorological pre-processor. AERMET was developed primarily to simulate meteorological processes driven by the diurnal cycle of solar heating over land. The marine boundary layer behaves in a fundamentally different manner because the ocean does not respond the same to diurnal heating and cooling effects. Improvements that could be made to AERMET-AERMOD for offshore applications include:

¹ Plume Volume Molar Ratio Method, used to limit NO-to-NO₂ conversion based on available ozone.

² Ozone Limiting Method, used to limit NO-to-NO₂ conversion based on available ozone.

- The surface roughness over the ocean varies with wind speed and wave conditions, and is not a constant. The surface roughness for wind speed is also different than for temperature and humidity.
- AERMET uses the solar angle as an indication of the transition between daytime and nighttime boundary layer régimes. Over the ocean, the stability of the boundary layer does not respond as a strong function of solar heating, and especially in coastal waters, is driven more by advection and horizontal differences in sea surface temperature. Unstable conditions can occur during the night and stable conditions during the day.
- AERMET does not explicitly include the effects of moisture in the assumed temperature and wind speed profiles. The Monin-Obukhov length and convective velocity scale estimated by AERMET also do not incorporate moisture effects. The effect of surface moisture fluxes is typically stronger over the ocean than over land.
- The Bowen Ratio method for the latent heat flux in AERMET is overly simplistic. The ratio between the latent and sensible heat is not a constant.
- AERMOD does not contain routines for elevated platform downwash.
- AERMOD cannot simulate shoreline fumigation or dispersion affected by non-homogenous conditions either in space or time

The alternative approach AERCOARE with the COARE air-sea flux method replaces AERMET by providing a meteorological input file that is technically more appropriate for marine applications. Given an appropriate characterization of meteorological conditions over water, the diffusion algorithms within AERMOD should perform in a fashion similar to the results found in the many field studies that lead to it becoming the EPA Guideline model over land (EPA, 2003). When AERCOARE provides the necessary meteorological data, AERMOD can be used to predict overwater concentration impacts in a manner consistent with new source review procedures over land. This allows the PVMRM, calms processing, volume source, and design concentration calculating procedures in AERMOD to be applied to sources located within the marine boundary layer.³

³ Note the current version of AERMOD does not contain routines for platform downwash or shoreline fumigation.

3.0 FORMULATION

A full technical description of the COARE bulk air-sea flux algorithm and the many field programs used in the method's development can be accessed at the TOGA-COARE website and in many different scientific journal articles (Fairall, et. al., 2003; Brunke, et. el. 2003).⁴

AERCOARE uses Version 3.0 of the COARE algorithm that has been updated several times since the initial international TOGA-COARE field program in the western Pacific Ocean from November 1992 to February 1993. The basic algorithm uses air-sea temperature difference, overwater humidity, and wind speed measurements to estimate the sensible heat, latent heat, and momentum fluxes. The original algorithm was based on measurements in the tropics with winds generally less than 10 m/s, but has since been modified and extensively evaluated against measurements in high latitudes with winds up to 20 m/s (Fairall, et. al., 2003). Based on these studies, AERCOARE is expected to be appropriate for marine conditions found at all latitudes including the Arctic. The current version considers both warm-layer diurnal heating and cool-skin effects (Fairall, et. el, 1996) and allows alternative parameterizations of the surface roughness when wave measurements are available.

AERCOARE writes AERMOD-ready "SFC" and "PFL"⁵ input files using output from the COARE flux algorithm and data from the overwater meteorological input file. In some cases the overwater measurements are simply passed through to AERMOD. For example, turbulence measurements of sigma-theta and sigma-w are not used by the COARE method and when provided, these variables are checked against a range of expected limits and written to the SFC File. The surface roughness, energy fluxes, and Monin-Obukhov length stability parameter are assembled from the COARE output. The user can impose limits on several important variables and use a combination of defaults for some of the less important variables contained in the AERMOD-ready SFC File.

AERMOD's dispersion routines can be sensitive to mixing height. Mixing heights are not predicted by the COARE algorithms and the user should generally provide these data in the overwater meteorological input file.⁶ AERCOARE does provide an option for the calculation of mechanical mixing heights using the same method employed by AERMET. This estimate can also be assigned during convective conditions, but the user is cautioned that overwater mixing heights would typically be controlled by a balance between shear stress, convective heating from the surface, air modification caused by spatial changes in sea temperature, cloud interactions, and subsidence. Such effects are better considered with measurements or by a more sophisticated numerical boundary layer model.

⁴ Version 3.0 of the COARE algorithm with journal references and a User's Manual can be accessed at:
ftp://ftp.etl.noaa.gov/users/cfairall/wcrp_wgsf/computer_programs/cor3_0/ and
http://www.coaps.fsu.edu/COARE/flux_algor/

⁵ Currently AERCOARE only processes a single level of wind, turbulence, or temperature data.

⁶ The Mesoscale Model Interface Program (MMIF) can be applied to convert prognostic meteorological model (e.g. MM5 and WRF) output to an AERCOARE-ready overwater meteorological input file including mixing heights.

4.0 CODE STRUCTURE AND COMPILATION

AERCOARE is written in Fortran90, but retains the “Fixed Source Form” common with legacy Fortran codes including the AERMOD modeling system. The important COARE Version 3.0 subroutines were adapted from the program `cor3_0af.f` accessed at the TOGA-COARE website.⁴ The AERCOARE Fortran code is well documented internally with variable descriptions and the history of modifications included as comments.

The AERCOARE code package has two components:

<code>aercoare.f</code>	AERCOARE data handling routines and COARE subroutines
<code>timesubs.f</code>	Group of date/time manipulation routines

Subroutines and functions within `aercoare.f` include:

<code>aercoare</code>	Main driving routine: processes the Control File
<code>coare</code>	Loops through overwater observations, processing with COARE, and processing COARE output for AERMOD
<code>missing_summary</code>	Summarize missing data for Listing File
<code>write_aermod</code>	Writes AERMOD SFC and PFL Files
<code>process_met</code>	Process COARE output for AERMOD including mixing heights, convective velocity scales, and Bowen ratios. Also imposes user supplied limits on several variables
<code>smthzi</code>	Performs mechanical mixing heights smoothing per the method in AERMET when this option is selected
<code>getobs</code>	Process an overwater meteorological file record and checks data prior to input to COARE routines
<code>bulk_flux</code>	Main COARE subroutine. Invokes warm-layer option and initializes bulk-flux input variables, then calls <code>ASL</code>
<code>ASL</code>	After initial guess, iteratively calculates the momentum, latent heat, and sensible heat fluxes from overwater measurements considering different measurement heights. Also applies cool-skin correction and optional surface roughness treatments
<code>delxtime</code>	Calculates the difference between two COARE GMT times to check of intervening periods of missing data
<code>humidity</code>	Calculates the saturation vapor pressure from pressure and temperature
<code>psiu</code>	Wind speed similarity function

<code>psit</code>	Temperature and specific humidity similarity function
<code>gravity</code>	Calculates for gravitational constant as function of latitude
<code>radflx</code>	Adapted from CALMET, this subroutine calculates the longwave downward radiation from relative humidity, cloud cover, and ceiling height
<code>write_sfc_head</code>	Writes the header for the SFC output file
<code>set_missing</code>	Fills initial AERMOD variables with missing value codes
<code>get_control</code>	Processes the Control File and checks for errors
<code>get_variable_defs</code>	Processes the header of the overwater meteorological file
<code>lowercase</code>	Converts a mixed string to lower case
<code>block data</code>	Contains default variable definitions

4.1 Compiling AERCOARE on WINDOWS

The AERCOARE package includes a batch file named `lahey95.bat` that can be used to compile the program on Windows using Lahey/Fujitsu Fortran95 (LF95). AERCOARE has been tested with LF95 Compiler Release 5.70f on Windows 7.

AERCOARE can be compiled by double-clicking `lahey95.bat` in Windows Explorer; or by opening a Command Prompt (DOS box), changing to the appropriate directory, and typing `lahey95.bat` at the prompt.

4.2 Compiling AERCOARE on LINUX/UNIX

The AERCOARE package includes a `Makefile` to facilitate compilation of the program on Linux/Unix platforms. The Makefile will compile AERCOARE source code into an executable program and currently supports the Portland Group F90 compiler (pgf90) and the Gnu Fortran compiler (gfortran). The user may edit the Makefile, un-commenting the `$FC` and `$FFLAGS` variables for the desired compiler, and commenting out the blocks for the other compilers.

AERCOARE is compiled by issuing the command `make` at a shell prompt within the main source directory. It will generate an executable program called `aercoare` that will reside in the source code directory.

5.0 RUNNING AERCOARE

AERCOARE will by default open and read a Control File named "aercoare.inp" that must exist in the current directory if the program is invoked in this fashion. If a single filename is given on the command line, that file is read as the Control File. The Control File contains all of the user configuration options, flags, and paths to the overwater meteorological input file and the output files ready for AERMOD. If two filenames are provided on the command line, the first file will be the Control File and the second file will be an optional output Debug File. The Debug File contains information that can be compared to legacy COARE program output. The filenames including the paths must be less than or equal to 80 characters.

Run AERCOARE by typing its name at the Command Prompt, optionally supplying a Control File filename, and a second Debug File filename. Some examples from the DOS prompt are shown below:

```
aercoare
```

would open the Control File `aercoare.inp` in the current directory. The executable `aercoare.exe` must exist in the same directory or be included in the DOS path.

```
aercoare test\ventcl.inp test\ventcl.dbg
```

would open the Control File `ventcl.inp` in the `test` subdirectory and create a debug file called `ventcl.dbg` in the same subdirectory.

The user can also double-click the AERCOARE executable in the Windows Explorer, though the utility of this method is reduced when the Command Prompt automatically closes after the run has finished, before its contents can be viewed by the user.

Useful information is printed to the standard output (screen) during execution, including the current hour being processed, error messages prior to an abnormal termination, and on successful completion, the number of records processed, number of missing hours and the number of calm hours. These messages are also written in the Listing File using the filename provided in the Control File.

5.1 Control File Format and Options

The AERCOARE Control File has the following syntax:

```
'ventmet.csv'      / 1: filein  - Overwater Input Met file
'ventcl.sfc'       / 2: filesfc - Output AERMOD SFC file
'ventcl.pfl'       / 3: filepfl - Output AERMOD PFL file
'ventcl.out'       / 4: fileout - Output Listing file
34.3              / 5: xlatn  - Latitude (degn)
119.2             / 6: xlonw  - Longitude (degW)
8                / 7: tzone  - Time Zone (5-EST.. 8-PST)
600.             / 8: defzi  - COARE Gust Mix Ht (m)
25.             / 9: zimin  - Mininum Overwater Mix Ht (m)
5.              / 10: dlmin  - Min Abs(L) allowed
.5              / 11: wscalm- Calm Threshold (m/s)
.01            / 12: dvptg  - Default VPTG (degC/m)
20.5           / 13: defzw  - Default Wind Meas. Ht (m)
7.0           / 14: defzt  - Default Temp Meas. Ht (m)
7.0           / 15: defzq  - Default RelH Meas. Ht (m)
0.5           / 16: defdep- Default Sea Temp Depth (m)
1            / 17: mixopt- Mix Ht Option (-2 to 2)
0            / 18: jwarm  - COARE Warm-Layer Option (0-1)
0            / 19: jcool  - COARE Cool-Skin Option (0-1)
0            / 20: jwave  - COARE Wave Option (0-2)
'end',1.,0.,100. / 21: vnam,vscal,vmin,vmax - variable name,scale,min,max
```

The Control File has 20 or more lines and the order of the variables in the file must be as shown in the example above. Variables on each line are read using a Fortran list-directed free-format read (e.g. `read(*,*) variable`). The record ends once the variable is read or when a slash (character `"/"`) is encountered. If the field is blank and a slash is encountered then the preexisting default for the variable will be used. The descriptions following the slash are arbitrary and can be used to provide reminders to the user or provide any other comment. The form of each variable allowed depends on the Fortran compiler, but generally character variables should be contained within quotes, real variables should have a decimal, and integers should not have a decimal. Default variables are based on experience from the model evaluation studies supporting AERCOARE (Richmond and Morris, 2012) and COARE recommended defaults. The following describes each line of the Control File.

Record 1: <code>filein</code>	Name of the overwater meteorological input file including the path. The path should follow the applicable Linux or Windows definitions and the variable can have up to 80 characters. If a path is provided containing a slash, space, or comma, the variable must be contained within quotes. If this file does not exist an error is written to the standard output (screen) and the program is terminated. The default is <code>"aercoare.csv"</code> .
-------------------------------	--

Record 2: <code>filesfc</code>	Name of the resulting SFC File including the path. The path should follow either the Linux or Windows definitions and the variable can have up to 80 characters. If a path is provided containing a slash, space, or comma, variable must be contained within quotes. Any existing file with this name will be overwritten without warning. The default is " <code>aercoare.sfc</code> ".
Record 3: <code>filepfl</code>	Name of the output AERMOD PFL File including the path. The path should follow applicable Linux or Windows definitions and the variable can have up to 80 characters. If a path is provided containing a slash, space, or comma, variable must be contained within quotes. Any existing file with this name will be overwritten without warning. The default is " <code>aercoare.pfl</code> ".
Record 4: <code>fileout</code>	Name of the listing output file including the path. The Listing File echoes the variables of the input Control File and contains information about the overwater meteorological file including the variables and data recovery. The path should follow either the Linux or Windows definitions and the variable can have up to 80 characters. If a path is provided containing a slash, space, or comma, variable must be contained within quotes. The default is " <code>aercoare.out</code> ".
Record 5: <code>xlatn</code>	Latitude of the overwater measurement site in decimal degrees North. If the measurement site location is variable such as from a mixture of several buoys, a drifting buoy or a ship, then hourly positions can be specified in the overwater meteorological file. <code>xlatn</code> is used if hourly data are not provided or are missing in the overwater meteorological file. There is no default.
Record 6: <code>xlonw</code>	Longitude of the overwater measurement site in decimal degrees West (positive for the western hemisphere and negative for the eastern). If the measurement site location is variable, then hourly positions can be specified in the overwater meteorological file. <code>xlonw</code> is used if hourly data are not provided or are missing in the overwater meteorological file. There is no default.
Record 7: <code>timez</code>	Integer time zone from GMT of the meteorological input file and corresponding SFC and PFL Files. Following AERMET conventions a positive time zone corresponds to longitudes west of GMT. For example PST has a time zone of 8 and EST has a time zone of 5. The default is 0 (e.g. times will be in GMT).

Record 8: <code>defzi</code>	Scale height (m) or mixing height to be used for COARE gust calculations. The COARE algorithm contains a small term that accounts for wind gusts associated with large eddies. The eddy size scales with the height of the mixed layer. Primarily during free convection conditions, such gusts add to the momentum flux even as the mean wind velocity approaches zero. A climatological average overwater mixing height can be used. The user can also remove such effects by specifying a low scale height. The COARE recommended default is <code>defzi</code> = 600 m.
Record 9: <code>zimin</code>	Minimum mixing height (m) allowed. A minimum limit allowed for observed and/or calculated overwater mixing heights provided to AERMOD. During light winds friction velocities and associated mechanical mixing heights calculated with the Venketram Method (See below: <code>ABS(mixopt)</code> =1 or 2) become very small. Currently AERMOD internally limits mixing heights to 1 m. AERMOD can be very sensitive to mixing height and the model evaluation studies supporting AERCOARE found better performance could be obtained with the recommended default of <code>zimin</code> = 25 m.
Record 10: <code>dlmin</code>	Minimum absolute value (m) of the Monin-Obukhov length (L) allowed. Stability in the surface layer at a given height is inversely proportional to L and small absolute values can result in unrealistic stability ($L > 0$) or instability ($L < 0$). This variable (<code>dlmin</code>) restricts the output of the COARE algorithm to avoid very unstable and very stable conditions usually not found over the ocean. Currently AERMOD internally limits <code>ABS(L)</code> < 1 m. OCD and CALPUFF further restrict <code>ABS(L)</code> < 5 m. The model evaluation studies supporting AERCOARE found better performance could be obtained with the recommended default of <code>dlmin</code> = 5 m.
Record 11: <code>wscalm</code>	Threshold wind velocity (m/s) used to identify calm periods. Measurement periods with wind speeds less than <code>wscalm</code> are treated as missing and missing value codes for the variables are passed to the SFC and PFL output files. The default is <code>wscalm</code> = 0.5 m/s.
Record 12: <code>dvptg</code>	Default virtual potential temperature gradient (degC/m) in the 200 m layer above the mixed layer height. This variable can also be provided in the overwater meteorological file and <code>dvptg</code> is used when such hourly data are not provided and/or are missing. The default is <code>dvptg</code> = 0.01 degC/m.

Record 13: <code>defzw</code>	Default overwater wind measurement height (m). This variable can also be provided in the overwater meteorological file and <code>defzw</code> is used when such hourly data are not provided and/or are missing. The default is <code>defzw = 3.5 m</code> .
Record 14: <code>defzt</code>	Default overwater air temperature measurement height (m). This variable can also be provided in the overwater meteorological file and <code>defzt</code> is used when such hourly data are not provided and/or are missing. The default is <code>defzt = 3.5 m</code> .
Record 15: <code>defzq</code>	Default overwater relative humidity measurement height (m). This variable can also be provided in the overwater meteorological file and <code>defzq</code> is used when such hourly data are not provided and/or are missing. The default is <code>defzq = 3.5 m</code> .
Record 16: <code>defdep</code>	Default depth of the sea temperature measurement (m). This variable can also be provided in the overwater meteorological file and <code>defdep</code> is used when such hourly data are not provided and/or are missing. The default is <code>defdep = 0.5 m</code> .
Record 17: <code>mixopt</code>	<p>Mixing height option. An integer between -2 and 2, this variable controls the calculation of overwater mixing heights for AERMOD. AERMOD requires estimates for both the convective (z_{ic}) and mechanical (z_{im}) mixing heights. AERCOARE assigns mixing heights according to:</p> <p><code>mixopt = 0</code>: z_{ic} and z_{im} set equal to each other and are based on observations in the overwater meteorological file</p> <p><code>mixopt = 1</code>: z_{ic} is taken from observations in the overwater meteorological file; z_{im} is calculated from the friction velocity using the Venketram Method; and z_{im} is not smoothed.</p> <p><code>mixopt = 2</code>: z_{im} is calculated from the friction velocity using the Venketram Method; $z_{ic} = z_{im}$; and z_{im} is not smoothed.</p> <p><code>mixopt = -1</code>: As <code>mixopt = 1</code>, only z_{im} is smoothed using the same equations employed by AERMET.</p> <p><code>mixopt = -2</code>: As <code>mixopt = 2</code>, only z_{im} is smoothed using the same equations employed by AERMET.</p>

For all the options above, convective mixing heights are only assigned during convective conditions ($L < 0$) and mixing heights are not allowed to be less than z_{imin} . The Venketram Method in AERMET (Venketram, 1980) calculates the mechanical mixing height from the friction velocity (u_s) according to:

$$z_{im} = 2300u_s^{3/2}$$

In AERMET the initial estimate is smoothed based on the previous estimate to allow for residual turbulence from the previous hour. In AERCOARE and AERMET the smoothing is reset during periods of missing or calm data. Note for typical overwater mixing heights the degree of smoothing is negligible. The default is $mixopt = 0$ (observed overwater mixing heights used for z_{ic} and z_{im})

Record 18: `jwarm`

COARE warm-layer option. An integer either 0 or 1, this variable controls the optional COARE warm-layer calculations. The surface buoyancy flux depends on the difference between the air temperature and sea surface temperature (SST). Typically, SST data remotely sensed by a radiometer are not available and sea temperatures are measured at depth with a sensor mounted on a buoy, ship or mast. During the day, the upper few meters of the ocean can be heated and SSTs can be warmer than sea temperatures measured at depth resulting in an overestimate of the heat flux. The amount of heating depends on the amount of radiation input to the sea and the depth of the mixing depends on the wind speed. In the tropics during the COARE cruises, the peak afternoon warming for light winds can be as much as 4 degC over a depth of 0.7 m, decreasing to about 0.2 degC warming over a depth of 19 m under a 10 m wind speed of 7 m/s (Fairall, et. al., 1996).

AERCOARE can correct for warm-layer effects on estimated heat fluxes using the COARE warm-layer effects option. The algorithm predicts larger corrections as the measurement depth increases. The user is cautioned that the algorithm employed depends on a more extensive set of continuous overwater measurement data. Periods of more than four hours of missing data during the day cause the warm-layer effects algorithm to reset and should be used with caution. AERCOARE employs the warm-layer effects options according to:

- `jwarm = 0:` warm-layer effects are not included in the COARE calculations
- `jwarm = 1:` warm-layer effects are included as described by Fairall, et. al., 2003 and Fairall, et. al., 1996. This option requires solar radiation measurements and downward longwave radiation. AERCOARE will estimate downward longwave radiation when not available using ceiling height, cloud cover, and relative humidity based on the `radflx` subroutine from CALMET.

The default is `jwarm = 0`.

Record 19: `jcool`

COARE cool-skin option. An integer either 0 or 1, this variable controls the optional COARE cool-skin calculations. As mentioned above, bulk measurements do not truly measure the temperature of the "surface" of the ocean. Sensible, latent, and longwave radiative fluxes cool the upper fractions of a millimeter of the ocean surface typically by about 0.2 - 0.5 degC (Fairall, et. al., 1996). Such effects can be considered by invoking the COARE cool-skin option.

- `jcool = 0:` cool-skin effects are not included in the COARE calculations
- `jcool = 1:` cool-skin effects are included as described by Fairall, et. al., 2003 and Fairall, et. al., 1996. This option requires solar radiation measurements and downward longwave radiation. AERCOARE will estimate downward longwave radiation when not available using ceiling height, cloud cover, and relative humidity based on the `radflx` subroutine from CALMET.

The default is `jcool = 0`.

Record 20: `jwave`

COARE surface roughness options. An integer either 0, 1, or 2, this variable controls the optional COARE surface roughness calculations. This option only applies to the wind speed surface roughness length. Different parameterizations are used for the humidity and temperature profiles.

The COARE default treatment of the surface roughness length and subsequently momentum transfer does not depend directly on

wave conditions. As these relationships were generally developed for well-developed sea conditions, smaller waves or different shaped waves in coastal waters may result in a different surface roughness. Given wave measurements, COARE can optionally consider two alternative treatments of surface roughness:

- `jwave = 0:` COARE default treatment of surface roughness as a function of the friction velocity
- `jwave = 1:` surface roughness is calculated as a function of friction velocity and wave measurements according to Oost, et. al., 2002
- `jwave = 2:` surface roughness is calculated as a function of wave measurements of significant wave height and period according to Taylor and Yelland, 2001

Options 1 and 2 depend on significant wave height and period measurements in the overwater meteorological file. If wave measurements are not provided or missing for an hour, wave properties are estimated as functions of wind speed by COARE using relationships for a well-developed sea state (Taylor and Yelland, 2001). The COARE authors included such alternative treatments to encourage testing in coastal waters, but have not evaluated the optional treatments against any datasets. The default is `jwave = 0`.

Optional Records: `vnam`, `vsca`, `vmin`, `vmax`

Optional scaling and allowable limits for overwater meteorological variables. AERCOARE assumes overwater observations are provided in a default set of units and each variable is tested against a range of permitted limits. Observations outside the limits are treated as missing, which depending on the variable, may be replaced by a default value or cause the entire calculation to be skipped and missing data codes passed to the AERMOD SFC and PFL Files. The internal default units and limits for the overwater meteorological file are shown in Table 1.

Table 1. Overwater Variable Definitions.

Name (Vnam)	Units	Definition	Scale (Vsca)	Minimum (Vmin)	Max (Vmax)
wspd	m/s	wind speed	1.0	0	50
wdir	deg	wind direction	1.0	0	360
tsea	degC	sea temperature	1.0	-3	50
tair	degC	air temperature	1.0	-30	50
relh	%	air relative humidity	1.0	0	100
pres	mb	air pressure	1.0	900	1100
srad	W/m ²	solar radiation	1.0	0	1500
tsky	1-10	cloud cover	1.0	0	10
ceil	100's ft	ceiling height	1.0	0	1000
rain	mm/hr	rainfall	1.0	0	254
sigt	deg	sigma-theta (standard deviation of the wind direction)	1.0	0	105
sigw	m/s	sigma-w (standard deviation of the vertical wind speed)	1.0	0	5
zwsp	m	wind measurement height	1.0	0	50
ztem	m	air temperature measurement height	1.0	0	50
zrel	m	relative humidity measurement height	1.0	0	50
zdep	m	sea temperature measurement depth	1.0	0	10
hwav	m	significant wave height	1.0	0	60
twav	sec	significant wave period	1.0	0	40
rdow	W/m ²	longwave downward radiation	1.0	0	1000
mixh	m	mixing height	1.0	0	5000
vptg	degC/m	virtual potential temperature gradient above the mixed layer	1.0	0.005	0.10
latn	degN	latitude	1.0	-90	90
lonw	degW	longitude	1.0	-180	180
xtim	sec	COARE GMT time yyyymdyhrmnse.	1.0	1.9e13	3.0e13

These records are optional and only need to be provided to override the defaults shown in Table 1. A character variable and three real numbers are read in for each record unless terminated by a slash. The variables on each optional record are:

<code>vnam:</code>	1-4 character variable name. <code>vnam = 'end'</code> will cause the termination of input from the Control File. Names not contained in Table 1 will be skipped
<code>vsca:</code>	scalar multiplied by the variable in the overwater file's units to convert to the units for the variable in Table 1.
<code>vmin:</code>	variables less than <code>vmin</code> are considered missing
<code>vmax:</code>	variables greater than <code>vmax</code> are considered missing

For example a record containing: `'wspd', .447, 0., 100.` would convert wind speeds in the input file from mph to m/s. Allowed wind speeds would be from 0 to 100 mph

AERCOARE compares each variable in the Control File against a range of allowed limits. Any variable outside these limits results in an error message to the standard output (screen) and to the Listing File followed by termination of the program. The Listing File echoes the variables in the Control File and shows the data limits used to assess missing overwater data.

5.2 Overwater Meteorological File Format

The overwater meteorological file contains the necessary hourly observations to estimate surface fluxes using the COARE algorithm, plus additional variables that are directly passed through to AERMOD. As an alternative to measured data, MMIF can also be applied to create an overwater meteorological file suitable for AERCOARE using simulations from WRF. Table 2 provides a list of the variables that can be included in the overwater meteorological file. The minimum set of overwater observations for the COARE algorithm must include wind speed, air temperature, sea temperature, and relative humidity. Ideally these variables should be obtained from the same exact location. If the warm-layer or cool-skin options are employed then solar radiation data are necessary, combined with downward longwave radiation and/or cloud cover and ceiling heights observations. Wind direction and overwater mixing heights, either measured or estimated, are further required by AERMOD. The overwater meteorological file can also contain locations and measurement heights if these vary from the variables contained in the Control File. Turbulence measurements and many other variables if provided are simply passed through to AERMOD. All variables are checked using the limits listed in Table 1.

Typically, the overwater meteorological file can be assembled in a spreadsheet and exported as a text file or as a comma delimited file (in Excel a "CSV" formatted file). An example of a free formatted text file is shown below:

yr	mo	dy	hr	wspd	wdir	tsea	tair	relh	pres	sigt	mixh
80	9	24	16	4.1	270.	17.25	15.15	72.	1000.	8.0	400.
80	9	24	18	6.2	270.	16.85	14.85	78.	1000.	6.5	400.
80	9	24	19	6.9	270.	16.95	14.85	77.	1000.	6.0	400.
80	9	27	14	6.3	270.	16.75	14.85	80.	1000.	4.7	400.
80	9	27	19	6.1	270.	16.85	15.85	80.	1000.	3.6	400.
80	9	28	18	3.1	270.	16.85	16.85	80.	1000.	4.4	250.
80	9	29	14	3.3	270.	15.44	15.55	76.	1000.	5.0	100.
80	9	29	16	5.1	270.	16.04	16.15	76.	1000.	3.9	100.
80	9	29	18	5.2	270.	15.94	16.05	76.	1000.	5.2	50.
81	1	6	16	4.0	270.	15.55	17.15	60.	1000.	21.5	50.
81	1	6	17	5.1	270.	15.75	17.45	58.	1000.	13.1	50.
81	1	6	18	4.9	270.	15.45	17.25	60.	1000.	9.4	50.
81	1	9	15	4.7	270.	15.35	14.45	87.	1000.	3.4	100.
81	1	9	16	4.6	270.	15.35	14.85	85.	1000.	4.8	100.
81	1	9	18	4.9	270.	15.35	15.05	87.	1000.	3.1	100.
81	1	13	15	5.8	270.	15.55	16.95	65.	1000.	11.6	50.
81	1	13	17	4.2	270.	15.45	15.85	84.	1000.	8.5	50.

The first line of the file is a header record. AERCOARE uses the record to establish the content of the file and the order of the variables on each subsequent record. The variable names in the header must match one of the names in Table 2 and be separated by spaces or a comma. By default, the units of the variables in this input file and the allowed minimum and maximum values are listed in Table 1. The units of the variables can be redefined with options in the Control File. The year (`yr`), month (`mo`), day (`dy`), and hour (`hr`) must be the first four variables on each line. The other variables and columns of data can be in any order.

The records following the header record are read in using a Fortran list-directed free-format read statement where the variables can be delimited by spaces or by a comma. Missing data should be coded in using extreme values outside the limits in Table 1. For example, `-999` might be used as a missing flag for wind speed. A single missing value code can be used for all variables as long as the value is outside the limits in Table 1. Normally the observations would be sequential hourly data, but as shown in the example above, any collection of observations can be included. The `xtim` variable can also be used to pass the minute and seconds of the observation through to COARE, however the SFC and PFL output files will contain the date specified by the `yr`, `mn`, `dy`, and `hr` variables. Note, the warm-layer option (`jwarm=1`) should not be applied for non-sequential data, datasets with large gaps or prolonged periods of missing data.

5.3 Output Files

AERCOARE generates SFC and PFL output files ready for AERMOD. A Listing File and optional Debug File are also created. Examples of the SFC, PFL, and Listing Files for the example input files shown in Section 5.1 and Section 5.2 are provided in Appendix A.

Table 2. Overwater Meteorological File Notes.

Column	Name (Vnam)	Units	Required	Default	Definition
1	yr	4 digits	yes	None	A four digit year
2	mn	1-12 (LST)	yes	None	month of the year
3	dy	1-31 (LST)	yes	None	day of the month
4	hr	1-24 (LST)	yes	None	hour ending convention in LST
*	wspd	m/s	yes	None	wind speed measured at height <i>zwsp</i>
*	wdir	deg	yes	None	wind direction measured at height <i>zwsp</i>
*	tsea	degC	yes	None	sea temperature measured at depth <i>zdep</i>
*	tair	degC	yes	None	air temperature measured at <i>ztem</i>
*	relh	%	yes	None	air relative humidity at <i>zrel</i>
*	pres	mb	no	1013.2	air pressure
*	srad	W/m ²	maybe	None	solar radiation, needed for warm-layer or cool-skin options
*	tsky	1-10	maybe	None	cloud cover, needed for warm-layer or cool-skin options if <i>rdow</i> not provided or missing
*	ceil	100's ft	maybe	None	ceiling height needed for warm-layer or cool-skin options if <i>rdow</i> not provided or missing
*	rain	mm/hr	no	0.0	rainfall
*	sigt	deg	no	None	sigma-theta measured at height <i>zwsp</i>
*	sigw	m/s	no	None	sigma-w at measured height <i>zwsp</i>
*	zwsp	m	no	defzw	wind measurement height
*	ztem	m	no	defzt	air temperature measurement height
*	zrel	m	no	defzq	relative humidity measurement height
*	zdep	m	no	defdep	sea temperature measurement depth
*	hwav	m	no	None	significant wave height, needed for optional surface roughness options. Will be calculated from <i>wspd</i> if not provided
*	twav	sec	no	None	significant wave period needed for optional surface roughness options. Will be calculated from <i>wspd</i> if not provided
*	rdow	W/m ²	maybe	None	longwave downward radiation needed for warm-layer and cool-skin options. Will be estimated from cloud data when missing or not provided
*	mixh	m	no	None	mixing height. Not needed for COARE, but necessary to run AERMOD
*	vptg	degC/m	no	dvptg	virtual potential temperature gradient above the mixed layer
*	latn	degN	no	xlatn	latitude
*	lonw	degW	no	xlonw	longitude
*	xtim	sec	no	None	COARE GMT time (yyyymodyhrmnse). Can be used to provide observations off the hour for comparison to COARE test cases. Normally calculated from <i>yr, mn, dy, hr</i> and <i>tzone</i>

6.0 REFERENCES

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APPENDIX A: OUTPUT FILE EXAMPLES

Example of Listing Output File:

AERCOARE Summary

```
-----
AERCOARE Version           : D12275

Run Date                   : 20120823
Run Time (hour:min:sec)    : 14:21:53.444
Run Time Zone              : -0700
Control/Option file        : ventcl.in
Overwater meteorological file: ventmet.csv
Output SFC file for AERMOD  : ventcl.sfc
Output PFL file for AERMOD  : ventcl.pfl
```

Control File Options

```
-----
Latitude (degN)           : 34.3000
Longitude (degW)          : 119.2000
Time Zone (5-EST.. 8-PST) : 8
COARE Gust Mix Ht (m)     : 600.0
Minimum Overwater Mix Ht (m) : 25.0
Min Abs(L) allowed        : 5.0
Calm Threshold (m/s)      : 0.50
Default VPTG (degC/m)     : 0.010
Default Wind Meas. Ht (m) : 20.50
Default Temp Meas. Ht (m) : 7.00
Default RelH Meas. Ht (m) : 7.00
Default Sea Temp Depth (m) : 0.500
Mix Ht Option (-2 to 2)   : 1
COARE Warm Layer Option (0-1): 0
COARE Cool Skin Option (0-1) : 0
COARE Wave Option (0-2)   : 0
```

Overwater Input File Variables and Limits

n	name	column	scale	min	max
1	wspd	5	1.00	0.00	50.0
2	wdir	6	1.00	0.00	360.
3	tsea	7	1.00	-3.00	50.0
4	tair	8	1.00	-30.0	50.0
5	relh	9	1.00	0.00	100.
6	pres	10	1.00	900.	0.110E+04
11	sigt	11	1.00	0.00	105.
20	mixh	12	1.00	0.00	0.500E+04

Missing Data Summary by Variable (1)

Vname	No. Miss
wspd	0
wdir	0
tsea	0
tair	0

relh	0
pres	0
sigt	0
mixh	0

(1) - does not include whole missing hours caused
by non-sequential data.

AERCOARE processed	17	records	
number of records with insufficient data :			0
number of calm records		:	0

Example of PFL Output File:

80	9	24	16	7.0	0	999.0	999.00	15.15	99.00	99.00
80	9	24	16	20.5	1	270.0	4.10	99.90	8.00	99.00
80	9	24	18	7.0	0	999.0	999.00	14.85	99.00	99.00
80	9	24	18	20.5	1	270.0	6.20	99.90	6.50	99.00
80	9	24	19	7.0	0	999.0	999.00	14.85	99.00	99.00
80	9	24	19	20.5	1	270.0	6.90	99.90	6.00	99.00
80	9	27	14	7.0	0	999.0	999.00	14.85	99.00	99.00
80	9	27	14	20.5	1	270.0	6.30	99.90	4.70	99.00
80	9	27	19	7.0	0	999.0	999.00	15.85	99.00	99.00
80	9	27	19	20.5	1	270.0	6.10	99.90	3.60	99.00
80	9	28	18	7.0	0	999.0	999.00	16.85	99.00	99.00
80	9	28	18	20.5	1	270.0	3.10	99.90	4.40	99.00
80	9	29	14	7.0	0	999.0	999.00	15.55	99.00	99.00
80	9	29	14	20.5	1	270.0	3.30	99.90	5.00	99.00
80	9	29	16	7.0	0	999.0	999.00	16.15	99.00	99.00
80	9	29	16	20.5	1	270.0	5.10	99.90	3.90	99.00
80	9	29	18	7.0	0	999.0	999.00	16.05	99.00	99.00
80	9	29	18	20.5	1	270.0	5.20	99.90	5.20	99.00
81	1	6	16	7.0	0	999.0	999.00	17.15	99.00	99.00
81	1	6	16	20.5	1	270.0	4.00	99.90	21.50	99.00
81	1	6	17	7.0	0	999.0	999.00	17.45	99.00	99.00
81	1	6	17	20.5	1	270.0	5.10	99.90	13.10	99.00
81	1	6	18	7.0	0	999.0	999.00	17.25	99.00	99.00
81	1	6	18	20.5	1	270.0	4.90	99.90	9.40	99.00
81	1	9	15	7.0	0	999.0	999.00	14.45	99.00	99.00
81	1	9	15	20.5	1	270.0	4.70	99.90	3.40	99.00
81	1	9	16	7.0	0	999.0	999.00	14.85	99.00	99.00
81	1	9	16	20.5	1	270.0	4.60	99.90	4.80	99.00
81	1	9	18	7.0	0	999.0	999.00	15.05	99.00	99.00
81	1	9	18	20.5	1	270.0	4.90	99.90	3.10	99.00
81	1	13	15	7.0	0	999.0	999.00	16.95	99.00	99.00
81	1	13	15	20.5	1	270.0	5.80	99.90	11.60	99.00
81	1	13	17	7.0	0	999.0	999.00	15.85	99.00	99.00
81	1	13	17	20.5	1	270.0	4.20	99.90	8.50	99.00

Example of SFC Output File:

34.300N		119.200W		UA_ID:		99999		SF_ID:		99999		OS_ID:		99999		AERCOARE:D12275									
80	9	24	268	16	14.3	0.140	0.605	0.010	400.0	121.0	-12.5	0.000034	0.19	0.06	4.10	270.0	20.5	288.3	7.0	9999	-9.00	72.	1000.	99	NAD-OS
80	9	24	268	18	18.1	0.210	0.647	0.010	400.0	221.1	-34.2	0.000057	0.22	0.06	6.20	270.0	20.5	288.0	7.0	9999	-9.00	78.	1000.	99	NAD-OS
80	9	24	268	19	20.8	0.235	0.677	0.010	400.0	262.3	-41.9	0.000069	0.22	0.06	6.90	270.0	20.5	288.0	7.0	9999	-9.00	77.	1000.	99	NAD-OS
80	9	27	271	14	17.3	0.213	0.635	0.010	400.0	225.6	-37.6	0.000058	0.23	0.06	6.30	270.0	20.5	288.0	7.0	9999	-9.00	80.	1000.	99	NAD-OS
80	9	27	271	19	8.2	0.201	0.620	0.010	400.0	207.2	-57.6	0.000053	0.14	0.06	6.10	270.0	20.5	289.0	7.0	9999	-9.00	80.	1000.	99	NAD-OS
80	9	28	272	18	-0.3	0.097	0.215	0.010	250.0	69.2	-57.2	0.000027	-1.00	0.06	3.10	270.0	20.5	290.0	7.0	9999	-9.00	80.	1000.	99	NAD-OS
80	9	29	273	14	-0.8	0.102	0.146	0.010	100.0	74.7	-84.8	0.000027	-1.00	0.06	3.30	270.0	20.5	288.7	7.0	9999	-9.00	76.	1000.	99	NAD-OS
80	9	29	273	16	-1.2	0.158	0.171	0.010	100.0	145.0	-199.7	0.000038	-1.00	0.06	5.10	270.0	20.5	289.3	7.0	9999	-9.00	76.	1000.	99	NAD-OS
80	9	29	273	18	-1.3	0.162	0.136	0.010	50.0	149.5	-211.0	0.000039	-1.00	0.06	5.20	270.0	20.5	289.2	7.0	9999	-9.00	76.	1000.	99	NAD-OS
81	1	6	6	16	-5.4	0.087	-9.000	-9.000	-999.0	58.9	17.4	0.000027	-1.00	0.06	4.00	270.0	20.5	290.3	7.0	9999	-9.00	60.	1000.	99	NAD-OS
81	1	6	6	17	-8.8	0.125	-9.000	-9.000	-999.0	102.0	32.1	0.000031	-1.00	0.06	5.10	270.0	20.5	290.6	7.0	9999	-9.00	58.	1000.	99	NAD-OS
81	1	6	6	18	-8.2	0.114	-9.000	-9.000	-999.0	88.3	23.8	0.000029	-1.00	0.06	4.90	270.0	20.5	290.4	7.0	9999	-9.00	60.	1000.	99	NAD-OS
81	1	9	9	15	5.9	0.152	0.283	0.010	100.0	136.8	-39.0	0.000037	0.19	0.06	4.70	270.0	20.5	287.6	7.0	9999	-9.00	87.	1000.	99	NAD-OS
81	1	9	9	16	2.9	0.147	0.240	0.010	100.0	129.0	-56.7	0.000035	0.10	0.06	4.60	270.0	20.5	288.0	7.0	9999	-9.00	85.	1000.	99	NAD-OS
81	1	9	9	18	1.6	0.154	0.210	0.010	100.0	139.2	-99.3	0.000037	0.07	0.06	4.90	270.0	20.5	288.2	7.0	9999	-9.00	87.	1000.	99	NAD-OS
81	1	13	13	15	-9.3	0.156	-9.000	-9.000	-999.0	141.2	56.7	0.000038	-1.00	0.06	5.80	270.0	20.5	290.1	7.0	9999	-9.00	65.	1000.	99	NAD-OS
81	1	13	13	17	-2.3	0.118	-9.000	-9.000	-999.0	92.9	121.2	0.000029	-1.00	0.06	4.20	270.0	20.5	289.0	7.0	9999	-9.00	84.	1000.	99	NAD-OS