

# SOHFEA Sulfide-Oxygen-Heat-Flux Eddy Analysis Software Package Version 2.0

## DRAFT User Manual

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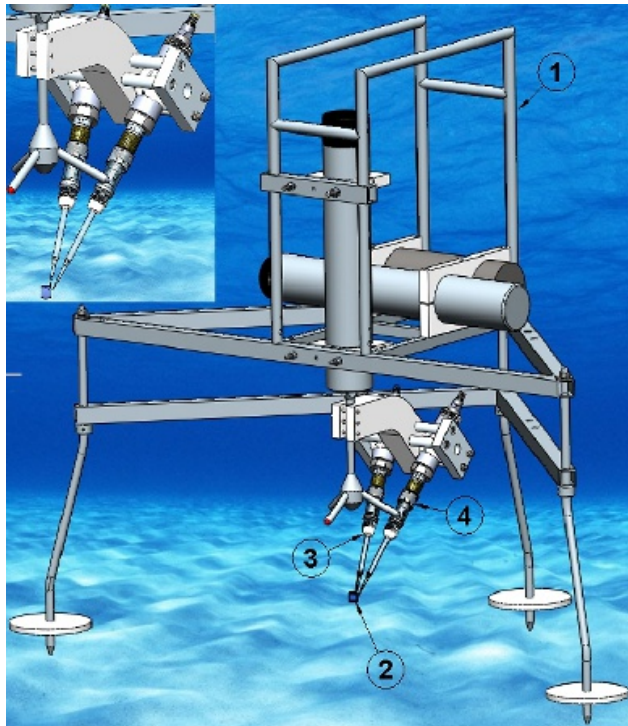
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*Figure from McGinnis et al. 2011 (R. Schwarz, GEOMAR)*

# Synopsis

The aquatic eddy correlation technique is an exciting new technology for measuring benthic fluxes that is rapidly gaining in popularity. This increasing popularity fortunately comes with advancing equipment specifications, especially battery and memory capacity.

With the birth of the aquatic eddy technique over a decade ago, deployments were typically limited to less than about 24 hours. However, with today's eddy instrumentation, deploy lengths can theoretically be in excess of 30 days with sampling rates of 64 Hz. This has led to much longer and larger data sets; dramatically increasing data handling requirements.

The sheer volume of data produced by the eddy correlation can be intimidating, especially for newcomers to the field. While most deployments these days seem to be between 3-5 days long, this still produces over 16 million lines of data that must be processed for quality control and data analyses in an efficient and expedient manner.

The purpose of the SOHFEA software package is to provide the eddy correlation community with a fast and efficient means to both preprocessing, averaging and analyzing their eddy flux data. SOHFEA is designed for both rapid "field-processing" of data for a first look on data quality and fluxes as well as for final processing for publication-level results.

SOHFEA is written in Fortran 90 and uses a Fortran digital compiler to ensure fast program execution times (minutes for a 5-day long data set). SOHFEA is free to the academic and scientific community and can be downloaded at <http://dfmcginnis.com/SOHFEA/>.

This instruction manual assumes an introductory knowledge of the eddy correlation technique; however some key references are provided. The manual is geared towards (but not limited to) the GEOMAR eddy configuration (McGinnis et al. 2011) and the recommended eddy data collection settings: continuous mode (as opposed to burst) at 64 Hz. In my opinion, these settings provide optimum flexibility for extracting high quality data.

Please send any comments, feedback, suggestions or bug-reports to [dfmcginnis@yahoo.com](mailto:dfmcginnis@yahoo.com) – I would be happy to hear from you.

## Acknowledgements

I would like to express my thanks to Karl Attard and Kasper Hancke (University of Southern Denmark) and Andreas Lorke (Uni. Landau – Koblenz) for providing excellent feedback on SOHFEA and the manual and website.

# Software Package Overview

**SOHFEA Ver. 2.0 consists of three processing categories**

- **Preprocessing routings containing 3 programs**
- **Eddy flux program, SOHFEA**
- **Postprocessing and ancillary routines**

## 1. Preprocessing

The preprocessing routine contains three programs to be run sequentially. These three programs are run separately so the user has the opportunity to inspect the output after each step to ensure the results are meeting expectations or to adjust filtering/output parameters. If the user wishes, these programs can be run sequentially by creating a BATCH program (downloadable on the website).

The programs consist of:

**Step1\_filter.exe** – this program averages the data down, while flagging and removing low-quality (user-defined) data.

**Step2\_despike.exe** – the next program replaces data flagged in Step1 and despikes the velocity and O<sub>2</sub> data.

**Step3\_rotate.exe** – the final preprocessing program performs a simple double-rotation of the data to minimize the average vertical velocity and converts the ADV velocity data from instrument coordinates to earth coordinates.

**To run the programs: Simply place your data in the same folder with the programs, fill out the configuration file, and then execute the programs sequentially.**

## 2. SOHFEA

**SOHFEA.exe** (and **SOHFEAHeat.exe**) extracts and outputs the eddy fluxes. In addition, the program computes the average measured parameters and several other variables of interest.

**SOHFEA.exe** is used for standard O<sub>2</sub> or H<sub>2</sub>S fluxes (and in principle other constituents).

**SOHFEAHeat.exe** extracts heat fluxes and is uses the same configuration file.

All software is programmed with Digital Fortran 90 and compiled with global optimizations. The software is designed for Windows XP, but should operate on any Windows based system. It has not been tested for other operating systems.

# Getting Started: Preprocessing & Extracting Fluxes

The SOHFEA preprocessing is designed to read the Nortek Vector ADV ASCII output file. The program can be modified to accommodate other input formats – please contact me. An input conversion program is available to convert UNISENSE Eddy data.

All routines use the same input file **ConfigSOHFEA.dat** (see below). The program relevant input blocks are separated by a row of numbers (1234567890123456789x12345678901234567890). The first 20 spaces are the line input description (up until the ‘x’). The next 20 spaces are for the input parameters. The line comments begin after the ‘!’.

```

1 SOHFEA Software Package V2.0 - March 23,2013. !This software is provided "as is" without express or implied warranty of any kind. Copyright (C) 2013 Daniel McGinnis
2 1234567890123456789x12345678901234567890 BLOCK1!Input field starts on space 21 (after 'x') and should not exceed 40 (after last '0'). NO TABS IN INPUT FIELDS!
3 Input File Example64Hz.dat !Begin input fields for Step1_filter.exe. Vector ascii data file
4 Output File DO Out8Hz.Dat !Specify output file name (input file name for Step2_despike)
5 Output File BS OutBS8Hz.Dat !Backscatter output
6 Frequency 64 !Frequency of measured data
7 Averaging points 8 !Number of data points to average (1 = no average)
6 Calibration Amp1 (DOuM = Counts x a + b)
9 a: 0.01579449 !Slope of calibration curve
10 b: -100.88932334 !Intercept
11 Calibration Amp2 (DOuM = Counts x a + b)
12 a: 1
13 b: 0
14 Start Time (Hours) 0 !The program calculates deployment time starting from 0 in hours. You can specify a different starting value.
15 SNR Threshold 5 !Threshold for removing bad data (default = 5)
16 Beam Correlation 70 !Threshold for removing bad data (default = 70)
17 1234567890123456789x12345678901234567890 BLOCK2!Begin input for Step2
18 Despiking Routines !Step2_despike.exe field
19 Output Despike Despike8Out.Dat !Despike output file name (input file name = file name on line 3)
20 Despike Start time 1. !Timerange to despike (note - all data are saved)
21 Despike End time 20. !Endtime to despike (must be specified)
22 O2 detrend win.(s) 300 !Length of running mean to be considered for O2 despiking
23 O2 StDev. Multi. 2 !Factor of O2 standard deviation to remove as spikes
24 Vel. Acceleration 0.3 !Acceleration factor for despiking vertical velocity (default = 0.3 m/s2)
25 Despike Iterations 100 !Number of iterations for velocity despiking
26 Interp. Warning(s) 1 !Writes warning output when interpolation is greater than the time specified.
27 1234567890123456789x12345678901234567890 BLOCK3!Begin input for Step3
28 Coordinate Rotation !Step3_rotate.exe
29 Output Rotation Rotation8Out.Dat !Output for rotation program
30 Heading 0. !Heading to convert to earth coordinates (heading from *.sen Vector file)
31 1234567890123456789x12345678901234567890 BLOCK4!Begin input for SOHFEA
32 Output File Out_60s.Dat
33 Frequency 8 !Frequency after downsampling
34 Start Time(0=EOF) 0 !Specify start time of analysis. A 0 here implies start of file.
35 End Time (0=EOF) 0 !Specify end time of analysis. A 0 here implies the end of file
36 Window Size (sec) 60 !Window or bin for flux extraction
37 Amp1 or Amp2 1 !Channel 1 or Channel 2
38 Use rotated Z 1 !1 specifies to use the rotated velocity data, 0 is unrotated.
39 Running Mean (sec) 30 !Running mean
40 1234567890123456789x12345678901234567890

```

Figure 1. Example input for SOHFEA

**RULES:** The program reads input from the 24<sup>th</sup> space until the 44<sup>th</sup> space (after the ‘x’ until the end of the numbering). Please do not include any ‘TABS’ in this field, only spaces. It is suggested that input be started on the line 1 after the ‘x’. User comments may be added anywhere to the left of the numbered field (44<sup>th</sup> space). Each block between the number lines is for each consecutive processing program. The output file names from one block are the input file names for the next program block.

**Step1\_filter.exe – Block 1:** Performs the following functions:

1. Averages the input data
2. Applies calibration coefficients (only linear function)
3. Filters: Removes data flagged as bad before average is performed. Data are flagged based on user specified signal-to-noise ratio (SNR; default = 5) and beam correlation (BC; default = 70) – Lines 15 & 16, respectively. If all points removed for a bin average, that bin is assigned a -99. The -99 will be replaced in the next step.

4. Outputs time in hours: Line 14 ‘Start Time (Hours)’ allows the user to specify a start time other than 0. This is useful when synchronizing the output with more than 1 eddy or other instruments.

Input: ASCII data file from Vector

Output: Averaged data file (user specified name)

Averaged backscatter (BS) data file with individual beam and average BS.

| TIME (HOURS) | X (CM/S)   | Y (CM/S)   | Z (CM/S)   | O21 (uM)   | O22 (uM) | VIOL | PRESSURE |
|--------------|------------|------------|------------|------------|----------|------|----------|
| 1.18986111   | -0.386667  | 3.720000   | 0.816667   | 335.802666 | 0.000000 | 5    | 73.704   |
| 1.18989583   | -0.451667  | 5.120000   | 1.330000   | 336.04353  | 0.000000 | 2    | 73.818   |
| 1.18993056   | -0.534286  | 5.532857   | 1.667143   | 335.54008  | 0.000000 | 1    | 73.761   |
| 1.18996528   | -99.000000 | -99.000000 | -99.000000 | 335.53810  | 0.000000 | 8    | 73.790   |
| 1.19000000   | -99.000000 | -99.000000 | -99.000000 | 335.29526  | 0.000000 | 8    | 73.761   |
| 1.19003472   | 2.376667   | 5.170000   | 0.996667   | 335.64274  | 0.000000 | 5    | 73.790   |
| 1.19006944   | -5.010000  | 4.700000   | 0.860000   | 335.65261  | 0.000000 | 6    | 73.704   |
| 1.19010417   | -99.000000 | -99.000000 | -99.000000 | 336.12250  | 0.000000 | 8    | 73.790   |
| 1.19013889   | -1.150000  | 6.620000   | 1.870000   | 335.57364  | 0.000000 | 6    | 73.847   |
| 1.19017361   | -0.558000  | 3.750000   | 0.718000   | 335.63682  | 0.000000 | 3    | 73.732   |
| 1.19020833   | 0.543333   | 2.901667   | 0.496667   | 335.82635  | 0.000000 | 2    | 73.847   |

Figure 2. Example output files Step 1. Left – averaged output. VIOL represents the number of instances in an averaging bin that data exceed the threshold BC or SNR criteria. If all the points are discarded (e.g. VIOL = 8) then the velocity values are assigned a -99. The PRESSURE is pressure in dbar. Right – Time (hr), X, Y, Z, and average BS values (dB).

**Step2\_despik.exe – Block 2:** Performs the following functions:

1. Replaces -99 assigned in Step 1 and outputs warning (WARNING\_LOG.DAT) if -99's are greater than a consecutive time span indicated by 'Interp. Warning' (Line 26).
2. Despik time range: User specifies start and end time for despiking algorithms (both velocity and O2) – Lines 20 and 21. It is important that periods of very noisy data are excluded (e.g. when the instrument is being deployed or operated out of water). Extremely noisy data (above the levels commonly measured) may interfere with the despiking algorithms.
3. Despik O2: The user has option of despiking O2 data (use extreme caution) by specifying an O2 running mean length in seconds (Line 22 – O2 detrend win.) and a standard deviation multiple (Line 23 – O2 StDev. Multi). Any data point that falls outside the standard deviation times the multiple will be removed and replaced by the running mean at that point.
3. Despik velocity: Spike removal for X, Y, and Z velocity based on vertical acceleration threshold (default for  $V_z = 0.3 \text{ m s}^{-2}$ , line 24). Removed spikes are replaced by linear interpolation of neighboring data, thus it is necessary to solve iteratively over data set. Default iterations are set to 100 (line 25). See Goring and Nikora, 2002 for more information.

| TIME (HOURS) | X (CM/S)  | Y (CM/S) | Z (CM/S) | O21 (uM)   | O22 (uM) | O21MEAN   | O22MEAN  |
|--------------|-----------|----------|----------|------------|----------|-----------|----------|
| 1.18986111   | -0.386667 | 3.720000 | 0.816667 | 335.802666 | 0.000000 | 336.02802 | 0.000000 |
| 1.18989583   | -0.451667 | 5.120000 | 1.330000 | 336.04353  | 0.000000 | 336.02734 | 0.000000 |
| 1.18993056   | -0.534286 | 5.532857 | 1.667143 | 335.54008  | 0.000000 | 336.02682 | 0.000000 |
| 1.18996528   | 0.426032  | 5.411905 | 1.443651 | 335.53810  | 0.000000 | 336.02624 | 0.000000 |
| 1.19000000   | 1.406349  | 5.290952 | 1.220159 | 335.29526  | 0.000000 | 336.02541 | 0.000000 |
| 1.19003472   | 2.376667  | 5.170000 | 0.996667 | 335.64274  | 0.000000 | 336.02481 | 0.000000 |
| 1.19006944   | -0.351528 | 4.700000 | 0.860000 | 335.65261  | 0.000000 | 336.02427 | 0.000000 |
| 1.19010417   | -3.079722 | 5.660138 | 1.365073 | 336.12250  | 0.000000 | 336.02363 | 0.000000 |
| 1.19013889   | -1.150000 | 6.620000 | 1.870000 | 335.57364  | 0.000000 | 336.02279 | 0.000000 |
| 1.19017361   | -0.558000 | 3.750000 | 0.718000 | 335.63682  | 0.000000 | 336.02209 | 0.000000 |
| 1.19020833   | 0.543333  | 2.901667 | 0.496667 | 335.82635  | 0.000000 | 336.02173 | 0.000000 |
| 1.19024306   | 1.642500  | 3.375000 | 0.745000 | 335.40780  | 0.000000 | 336.02103 | 0.000000 |
| 1.19027778   | 0.450000  | 2.515000 | 0.720000 | 335.85991  | 0.000000 | 336.02040 | 0.000000 |

| STARTTIME (HR) | LENGTH (S) |
|----------------|------------|
| 1.45323        | 1.3        |
| 1.45368        | 2.5        |
| 1.45525        | 1.1        |
| 1.45691        | 1.5        |
| 1.46608        | 1.3        |
| 1.46743        | 1.3        |
| 1.46781        | 4.8        |
| 1.46934        | 4.5        |
| 1.48212        | 1.3        |
| 1.48271        | 1.5        |
| 1.48524        | 1.3        |
| 1.49073        | 3.1        |

Figure 3. Example output files Step 2. Left – Output after spikes/-99 values replaced. Two right columns are the running mean for the O2 despiking. Right – warning if more than X consecutive seconds of data are replaced (X = 1 second in this example, see Line 26 in ConfigSOHFEA.dat example).

Input: Output file from Block 1 (input file name it taken from Line 4).  
 Output: Despiked file (user specified name Line 19)  
 WARNING\_LOG.DAT – warning of more than X consecutive seconds of data are replaced (X is specified on line 26).

**Step3\_rotate.exe – Block 3:** Performs the following functions:

1. Double Rotation: Simple double rotation to minimize the mean vertical velocity.
2. Earth Coordinates: User can enter the ADV compass heading from the \*.sen file (Line 30) to rotate the data from instrument coordinates to earth coordinates.

Input: Output file from Block 2 (input file name it taken from Line 19).  
 Output: Rotated file (user specified name Line 29)

| TIME (HOURS) | X (CM/S)  | Y (CM/S) | Z (CM/S) | ZROT (uM) | O21 (uM)  | O2I (uM) |
|--------------|-----------|----------|----------|-----------|-----------|----------|
| 1.18986111   | -0.396667 | 3.720000 | 0.816667 | 1.027025  | 335.80266 | 0.00000  |
| 1.18989583   | -0.451667 | 5.120000 | 1.330000 | 1.538554  | 336.04353 | 0.00000  |
| 1.18993056   | -0.534286 | 5.532857 | 1.667143 | 1.874511  | 335.54008 | 0.00000  |
| 1.18996528   | 0.436032  | 5.411905 | 1.443651 | 1.651005  | 335.53010 | 0.00000  |
| 1.19000000   | 1.406349  | 5.290952 | 1.220159 | 1.429099  | 335.29526 | 0.00000  |
| 1.19003472   | 2.376667  | 5.170000 | 0.996667 | 1.206392  | 335.64274 | 0.00000  |
| 1.19006944   | -0.351528 | 4.700000 | 0.860000 | 1.070206  | 335.65261 | 0.00000  |
| 1.19010417   | -3.079722 | 5.660138 | 1.365073 | 1.573503  | 336.12250 | 0.00000  |
| 1.19013889   | -1.150000 | 6.620000 | 1.870000 | 2.076655  | 335.57364 | 0.00000  |
| 1.19017361   | -0.558000 | 3.750000 | 0.718000 | 0.928705  | 335.63682 | 0.00000  |
| 1.19020833   | 0.543333  | 2.901667 | 0.496667 | 0.708150  | 335.82635 | 0.00000  |
| 1.19024306   | 1.642500  | 3.375000 | 0.745000 | 0.955610  | 335.40780 | 0.00000  |
| 1.19027778   | 0.450000  | 2.515000 | 0.720000 | 0.930698  | 335.85991 | 0.00000  |

Figure 4. Example output files Step 3. ZROT is the vertical velocity after a simple double rotation.

**Step4: SOHFEA.exe – Block 4:** SOHFEA.exe is now executed to extract fluxes. SOHFEA.exe will work with both O2 and H2S data (and other constituents in the same range). The extracted fluxes in this case use the vertical velocity with the simple double rotation from Block 3. If other rotations are desired, the user must implement this as an independent step and produce a file with readable format (simply comma or space delimited with no more than 1 header at the top of the file – see Figure 4). See Lorke et al. 2012; Wilczak et al. 2001 for more information on coordinate rotation.

Configuration information:

1. Output file: The user specifies the output file name (Line 32)
2. Frequency of the data in the file (Line 33 – I left this option in so users can run SOHFEA without going through the first 3 steps).
3. The start and end times: (Lines 34 & 35) are specified for SOHFEA to solve (0 defaults at start/end of file, respectively).
4. Flux window size: (Line 36) is the time length of the flux window.
5. Channel: (line 37) is either analog output 1 or 2 from the Vector
6. Rotated vertical velocity, z: (Line 38) selecting 1 here will specify using the rotated z velocity, 0 will use the unrotated z velocity for solving the fluxes.
7. Running mean length: (line 39) Time window (seconds) for running mean, can not exceed the value from the flux window (Line 36).

Input: Output file from Block 3 (input file name it taken from Line 29).  
 Output: Flux output file (user specified name Line 32)

cumflux.out & cumfluxSHIFT.out – see example below  
 Cospectra.out – see example below

Figure 5. Example output SOHFEA.dat. See Table SOHFEA for description.

Table SOHFEA

|         |                                      |                                                                                                                                                         |
|---------|--------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------|
| Time    | hours                                |                                                                                                                                                         |
| X-VEL   | cm s <sup>-1</sup>                   | X or East velocity                                                                                                                                      |
| Y-VEL   | cm s <sup>-1</sup>                   | Y or North velocity                                                                                                                                     |
| Z-VEL   | cm s <sup>-1</sup>                   | Vertical velocity                                                                                                                                       |
| Z-STD   | cm s <sup>-1</sup>                   | Standard deviation of vertical velocity                                                                                                                 |
| MAG     | cm s <sup>-1</sup>                   | Velocity magnitude (only X and Y)                                                                                                                       |
| MAG-STD | cm s <sup>-1</sup>                   | Standard deviation of velocity magnitude                                                                                                                |
| DIR     | degrees                              | Current direction                                                                                                                                       |
| O2      | umol L <sup>-1</sup>                 | Mean oxygen concentration over eddy window (60 seconds in this case)                                                                                    |
| O2-STD  | umol L <sup>-1</sup>                 | Standard deviation of vertical velocity                                                                                                                 |
| FLUX-L  | mmol m <sup>-2</sup> d <sup>-1</sup> | Flux with linear detrending <sup>+</sup>                                                                                                                |
| FLUX-R  | mmol m <sup>-2</sup> d <sup>-1</sup> | Flux with running mean detrending <sup>+</sup>                                                                                                          |
| LINMIN  | mmol m <sup>-2</sup> d <sup>-1</sup> | Linear detrending, time shift. The program shifts to O2 data back in time (maximum -2 seconds) and seeks the minimum flux (maximum respiration/uptake)* |
| RUNMIN  | mmol m <sup>-2</sup> d <sup>-1</sup> | Same as LINMIN, but with running mean detrending                                                                                                        |
| LINMAX  | mmol m <sup>-2</sup> d <sup>-1</sup> | Same as LINMIN, but seeks maximum flux (in the case of O2 production)                                                                                   |
| RUNMAX  | mmol m <sup>-2</sup> d <sup>-1</sup> | Same as LINMAX, but with running mean detrending                                                                                                        |
| SLMIN   | seconds                              | Time shift corresponding to LINMIN                                                                                                                      |
| SRMIN   | seconds                              | Time shift corresponding to RUNMIN                                                                                                                      |
| SLMAX   | seconds                              | Time shift corresponding to LINMAX                                                                                                                      |
| SRMAX   | seconds                              | Time shift corresponding to RUNMAX                                                                                                                      |

<sup>+</sup> See Moncrieff et al. 2004 for details on detrending methods.

\* See McGinnis et al. 2008 for more details regarding time shift.

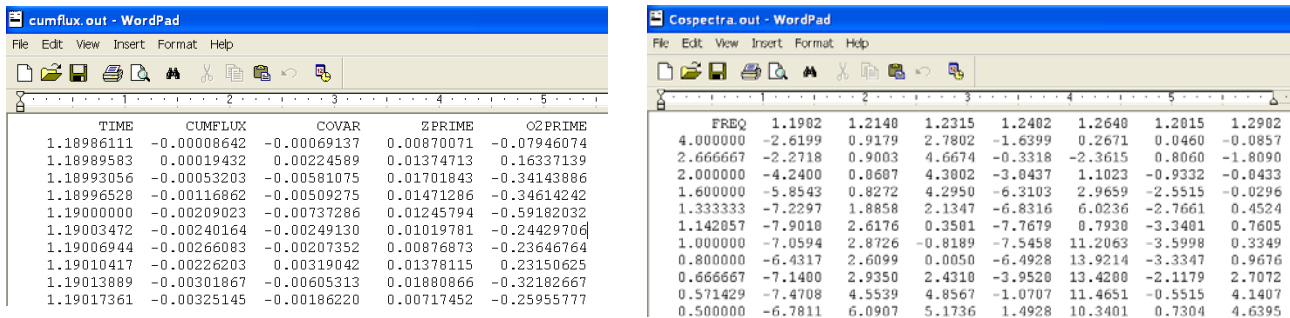


Figure 6. Example output files SOHFEA.exe. Left **cumflux.out** – CUMFLUX is the cumulative flux over the entire data series in  $\text{mmol m}^{-2}$ , which is the time integrated flux. COVAR is the covariance  $z'C'$ , which is the product of the last two columns. **cumfluxSHIFT.out** is the same but with the data shifted seeking the most negative (minimum) value over a particular window. Right **Cospectra.out** – this file provides an estimate for the cumulative cospectra (unshifted data) after the method from McGinnis et al. 2008. The left most column FREQ is the frequency in Hz. The very top row is the mean time of the window (hours), and below that in column 2 – onward are the fluxes associated with a that time and integrated to that frequency (starting at high frequency and going lower – See McGinnis et al. 2008 for more detail).

## CITATIONS

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