Comparing methods of identifying non-stationary, non-linear processes from stream temperature time series data

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Abstract

The determination of flow state remains an important challenge in non-perennial river catchments. Previous studies interpreted stream channel temperature time series data using the moving standard deviation method to identify the timing and duration of flow. However, the performance of this technique requires the user to specify multiple subjective constraints. We implemented six variations of time-frequency analysis from three categories: (1) Fourier transform methods, (2) wavelet transform methods, and (3) Empirical Mode Decomposition methods. We evaluated and compared their ability to discern periods of flow from synthetic and field data of stream temperature time series data. Overall, all methods performed reasonably well, with performance of 63–99 % success in matching flow and no-flow periods. Greater variability in performance was observed when evaluating field data. Differences between methods include the ease of implementation and evaluation of results, computational needs, and ability to handle discontinuous data. We suggest five primary areas for future research to improve the general understanding of these time-frequency analysis techniques.

1	Comparing methods of identifying non-stationary, non-linear processes from stream
2	temperature time series data
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13	Key Points:
14 15	• Ephemeral streamflow events were successfully identified from stream temperature time series data using seven time series analysis methods
16 17	• Compared reductions in the amplitude of the diurnal temperature signal of stream water compared using seven time series analysis approaches
18 19 20	• For the specific case study assessed, the continuous wavelet transform was found to be the most efficacious and most parsimonious method

21 Abstract

The determination of flow state remains an important challenge in non-perennial river 22 catchments. Previous studies interpreted stream channel temperature time series data using the 23 24 moving standard deviation method to identify the timing and duration of flow. However, the performance of this technique requires the user to specify multiple subjective constraints. We 25 implemented six variations of time-frequency analysis from three categories: (1) Fourier 26 transform methods, (2) wavelet transform methods, and (3) Empirical Mode Decomposition 27 methods. We evaluated and compared their ability to discern periods of flow from synthetic and 28 29 field data of stream temperature time series data. Overall, all methods performed reasonably well, with performance of 63–99 % success in matching flow and no-flow periods. Greater 30 variability in performance was observed when evaluating field data. Differences between 31 methods include the ease of implementation and evaluation of results, computational needs, and 32 ability to handle discontinuous data. We suggest five primary areas for future research to 33 improve the general understanding of these time-frequency analysis techniques. 34

Plain Language Summary More than half of the world's rivers have no surface flow for some 35 36 part of the year. In these rivers, measuring which parts of the catchment surface water network 37 are flowing remains a key challenge to a full understanding of habitat connectivity, groundwater recharge, and other key ecosystem services. Temperature measurements have been used to 38 identify flow state (i.e. periods of flow or no-flow) in rivers in previous studies, in which the 39 moving standard deviation of time series data was typically calculated, and conditions applied to 40 41 the results to identify periods of flow. In this study, we tested six variations of time-frequency transforms for identifying stream flows from temperature time series data. We found that all of 42 these transforms worked well, with subtle differences in their performance, assumptions, and 43 ease of use. The main advantage of these transforms over the moving standard deviation analysis 44 is the avoidance of subjective criteria when determining flow states. 45

46 **1. Introduction**

47 Non-perennial river networks constitute over half of total river length worldwide (Datry
48 et al., 2014). However, knowledge of the spatial and temporal variability of non-perennial flows
49 is often limited (Costigan et al, 2017) and stream gauging networks are typically biased toward
50 perennial rivers (De Girolamo et al., 2015; Eng et al., 2016). Even where gauges on non-

perennial rivers exist, often insufficient data are available to identify spatial variations in flows within a catchment. However, since the duration and volume of surface flows control both the availability and quality of water for flora and fauna along stream reaches (Datry et al., 2016), as well as the potential for groundwater recharge (Morin et al., 2009; Shanafield et al., 2012; Tooth, 2000), identifying and quantifying non-perennial flow patterns is critical.

The need for low-cost technologies that can be widely deployed has spurred several 56 efforts to develop methods of streamflow detection and quantification beyond the traditional 57 gauging station. The availability of inexpensive, easily programmable devices has led to the 58 59 development of several types of streamflow monitoring devices, including electrical resistance sensors (Fritz and Johnson, 2006; Adams et al., 2006; Blasch et al., 2002; Goulsbra et al., 2009; 60 Jaeger and Olden, 2011; Peirce and Lindsay, 2013; Jensen et al., 2019), float switch state loggers 61 (Epting et al., 2018; Assendelft and van Meerveld, 2019), and temperature sensors (Blasch et al., 62 2004; Assendelft and van Meerveld, 2019). Combinations of sensors have been developed to 63 provide more accurate determination of flow presence in certain settings, such as in headwater 64 65 streams (Assendelft and van Meerveld, 2019) or where ice forms in a channel (Chapin et al., 2014). The use of temperature sensors on (or in) a streambed has received a great deal of 66 attention, because temperature remains one of the easiest physical states to monitor. A variety of 67 small, readily deployable, and relatively inexpensive loggers are now available. These loggers 68 can often be secured to streambeds that sustain frequent scouring (Rodríguez-Burgueño et al., 69 2017), which is common in non-perennial rivers. Unlike flow meters, pressure transducers, or 70 float sensors, they typically do not contain moving parts or openings that can become clogged 71 with sediment. While a multitude of studies have used temperature time series pairs to calculate 72 vertical flux rates in the shallow streambed of perennial streams (e.g. Rau et al., 2017), relatively 73 fewer studies explored the use of paired temperature loggers to quantify vertical fluxes below 74 non-perennial rivers. Even fewer studies used loggers on the streambed surface to identify 75 surface flows. 76

In one of the earliest uses of temperature data to identify the presence or absence of streamflow, Constantz et al. (2001) used longitudinal changes in streambed temperature compared to a "benchmark" sensor (e.g. a sensor at stream gauge or other location where the presence of streamflow is known) to qualitatively evaluate the frequency and duration of downstream flows. The authors suggested installing sensors 0.15 m into the streambed to

minimize atmospheric noise, which had confounded their analysis. Used this approach of 82 burying temperature sensors, Gungle (2005) detected periods of streamflow within a catchment 83 by identifying a critical temperature drop that signaled the onset of streamflow. Rau et al. (2017) 84 also examined longitudinal changes in temperature but concluded that temperature measurements 85 alone were insufficient to detect streamflow. They further developed the amplitude ratio method 86 87 commonly used to estimate vertical streambed fluxes (i.e. comparing temperatures measured at the surface and buried in the streambed) to also detect the presence of unsaturated conditions, in 88 89 order to understand streamflow permanence.

Blasch et al. (2004) addressed the problem of "noise" measured by in-stream temperature 90 devices by applying a moving standard deviation technique to the time series data. This method 91 highlighted variations due to infiltration while removing long-term fluctuations. This technique 92 was further improved by van Assendelft and van Meerveld (2019) who included additional 93 94 criteria in their temperature measurement analyses. These were derived from visual inspection of temperature and flow data patterns from several monitoring stations in their study catchment. 95 96 The authors found that periods of zero flow greater than three hours' duration could be identified from temperature time series, although precise estimation of timing of changes between flowing 97 and no-flow conditions was not possible. 98

99 To date, quantitative temperature time series methods to identify the presence of surface 100 flows have typically used conventional time series modeling methods, such as the Fourier 101 transform (e.g. Rau et al., 2017). While such methods are well-established, their accuracy is 102 limited by assumptions of linearity and stationarity (Jothiprakashet al., 2009). Here, we explore 103 alternative analysis methods that avoid these assumptions. Several time-frequency (TF) transforms have evolved for the analysis of non-stationary time series data (Thakur et al., 2013; 104 Dadu and Deka, 2016). TF transforms have previously been used within the hydrologic literature 105 examining intermittent streamflow. Wavelets, for example, have been shown to be more useful 106 than classical Fourier transforms for identifying long-term patterns of intermittency in rivers 107 (Labat et al. 2005a,b). They have also been used within the pre-processing of flow and rainfall 108 data to remove deterministic components in the data such as trends, variance, and daily or 109 seasonal cycles before streamflow forecasting methods such as artificial neural networks were 110 applied (Abdollahi et al., 2017; Maier and Dandy, 2000). To our knowledge, TF transforms have 111 112 not been applied to streambed temperature time series data for flow state prediction.

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In the present study we take advantage of time series data of stream stage, which indicates flow within the stream channel, and the temperature measured at the surface of the streambed. In a non-perennial river, this time series of temperature data would reflect local air temperatures during periods of no-flow and the temperature of the well-mixed stream discharge during periods of flow (Figure 1). Air and surface water temperatures both oscillate over seasonal and diurnal cycles (i.e. one cycle per year and one cycle per day, respectively). For investigations of flow presence, the diurnal cycle provides the most useful information.

120 A variety of methods is available to extract amplitude and phase information from 121 temperature time series over a range of frequencies. These methods are continuously evolving, with various modifications offering advantages in certain applications. We selected six methods 122 for comparison from three categories: (1) Fourier transform methods, including the short-time 123 Fourier transform; (2) wavelet transform methods including the continuous wavelet transform 124 125 (CWT) and synchrosqueezed CWT; and (3) empirical mode decomposition (EMD) methods, including the EMD with Hilbert-Huang transform, the Complete Ensemble Empirical Mode 126 127 Decomposition with Adaptive Noise, and the Nonlinear Mode Decomposition. The theoretical basis of each method is briefly described in Section 2. The performance, advantages, and 128 disadvantages of each method are described in Section 3. Additionally, the moving standard 129 deviation (MSD) technique used in previous studies was computed for comparison. The basis for 130 comparisons was defined in terms of the ability to identify flow presence. Three examples were 131 used for comparison purposes: two synthetic cases featuring either low or high amplitude signal 132 noise, and one field data example. 133



Figure 1. (a) Conceptual model of the relationship between the temperature recorded by a sensor
installed on the streambed surface and the observed streamflow. When the stream is not flowing
(b), the sensor records daily air temperature oscillations, but rapidly equilibrates with the
temperature of the water during periods of flow (c).

140 **2. Theory**

Seven methods were compared: (1) short-time Fourier transform (STFT); (2) continuous
wavelet transform (CWT); (3) synchrosqueezed CWT; (4) empirical mode decomposition with
Hilbert-Huang transform; (5) complete ensemble empirical mode decomposition with adaptive
noise (CEEMDAN); (6) nonlinear mode decomposition (NMD); and (7) moving standard
deviation (MSD).

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2.1. Short-time Fourier transform

The short-time Fourier transform (STFT; also known as the sliding window Fourier transform, or windowed Fourier transform) involves calculating the discrete Fourier transform (DFT) of a given time series over a given subset (i.e. window) size and advancing the window position by a uniform time increment through the duration of the original time series (Jacobsen and Lyons, 2003). In this manner, amplitude and phase results are calculated continuously through time, and are calculated over the windowed, rather than total, time series duration.

However, when applying the STFT, non-stationary processes that occur over timescales 153 that are smaller than the window size are difficult to detect. In addition, the resolution of DFT 154 results is inversely proportional to input dataset length. For this reason, a distinct trade-off occurs 155 between window size and the resolution required in Fourier transform results in order to 156 accurately quantify energies at specific frequencies. For example, larger window sizes will 157 enable greater separation between component frequencies, but the amplitude and phase values 158 calculated at these frequencies will be quantified over a larger timeframe. In particular, if abrupt 159 changes in frequency amplitudes and/or phases occur then these will be difficult to detect, due to 160 the "smearing" effect of the STFT. 161

The limitations of the STFT have been recognised for decades (e.g. Rudi et al., 2010). 162 For this reason, published applications of the STFT in hydrology and related fields are scarce. 163 Instead, following their development in the 1990s, wavelet transforms were incorporated into 164 165 STFT approaches. For example, Kunkel and Pierce (2009) combined wavelet basis functions and the STFT approach to identify the timing of peak snowmelt events at 28 gauged sites in Idaho, 166 167 USA over a 12-month period. The efficacy of the method was assessed through comparisons to measured snowmelt fluxes. Using the STFT, peak snowmelt dates were estimated to within ±4 168 days accuracy during approximately 95 % of the study period, and to within ± 7 days accuracy 169 during the entire study period. In the present study, the STFT was provided as a basis for 170 171 comparisons with other methods, as it is conceptually the simplest of the time-frequency methods and highlights the advantages of newer, alternative methods. The STFT was 172 implemented using the Python Numpy library (van der Walt et al. 2011). To minimize spectral 173 leakage, Hanning window filtering was applied prior to calculation of the discrete Fourier 174 transform. 175

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2.2. Continuous wavelet transform

Wavelet transforms provide an alternative to Fourier transforms, which are based on trigonometric basis functions. Unlike Fourier analysis, which uses a single sinusoidal basis function type, a range of basis functions may be used in wavelet analyses. Unlike spectral analyses, wavelet-based methods detect the distribution of periodic variabilities over a given time span, rather than the average periodicities present (Andreo et al., 2006). Wavelet transforms are widely used in a range of fields, including image analysis and compression, as well as a variety of signal processing applications. The use of wavelet transforms was first introduced to

184 Earth sciences by Grosmann and Morlet (1984); specifically, for the interpretation of seismic

signals. Applications of wavelet transforms for time series analysis in hydrology were reviewed

186 by Sang (2013) and Rhif (2019).

187 The theoretical development of wavelet transforms was described by Daubechies (1992)
188 and Daubechies et al. (2000). Wavelet basis functions (*w*) are described as (Daubechies, 1990):

$$w(t,a,b) = \int_{-\infty}^{+\infty} \frac{1}{\sqrt{a}} \psi\left(\frac{\overline{t-b}}{a}\right) dt$$
 Equation 1

where *a* is a scaling parameter and *b* is a time shift parameter, for which values of 2 and 1 are commonly specified respectively (Daubechies, 1992; Sang, 2013). The continuous wavelet transform (CWT) is used to convolute a specified wavelet type (*w*) with a time series of interest [x(t)]; i.e. (Percival and Walden, 2006):

$$W(t,a,b) = \int_{-\infty}^{+\infty} x(t) \frac{1}{\sqrt{a}} \psi\left(\frac{\overline{t-b}}{a}\right) dt = \int_{-\infty}^{+\infty} x(t) w(t,a,b) dt \qquad \text{Equation } 2$$

Applications of the CWT to hydrological time series analysis include Labat et al. (2000a, 193 2000b), Andreo et al. (2006), and Niu and Sivakumar (2013). Labat et al. (2000a) used Fourier 194 and convolution-based methods to quantify the correlation between karstic spring discharge and 195 precipitation at study sites located in the Pyrenees Mountains, France. It was found that 196 convolution models could not adequately simulate precipitation-discharge dynamics, and that 197 Fourier methods were unable to characterize spring discharge rates. In particular, the methods 198 were unable to characterize non-stationary processes and dynamics. In a companion paper (Labat 199 et al., 2000b) the authors instead used both the continuous and discrete wavelet transform (DWT) 200 201 to characterize both data types. Morlet and Haar wavelets were used for CWT and DWT analyses respectively. Time-dependent correlations were subsequently quantified via cross 202 203 correlation analyses. Wavelet transforms enabled discrimination between rapid responses associated with horizontal karstic flow and slow responses associated with the vertical 204 205 infiltration of recharge. Andreo et al. (2006) used the CWT to characterize karstic spring discharge, precipitation and air temperature time series data from the Iberian Peninsula, Spain. 206 207 Annual periodicities of precipitation and temperature were found to remain constant over more

than 100 years. Shorter periodicities of 0.5, 2.5 and 5.0 years were also observed, which were

209 consistent with observations from other areas of Europe. Niu and Sivakumar (2013)

210 characterized daily streamflow data recorded near Wuzhou on the West River, a tributary of the

211 Pearl River in southern China. Significant contributions to spring discharge from were identified

at two timescales: 6–30 days (representing short-term processes) and one year (representing

213 long-term processes). The latter were hypothesized to result from climatic drivers such as the

Indian Ocean Dipole and the El Nino-Southern Oscillation. The authors applied the CWT to the entire dataset and did not use its unique properties to assess whether contributing processes were non-stationary. In the present study, the CWT featuring the Morlet wavelet type with parameters a=2 and b=1 was implemented using the Wavelet Toolbox for MATLAB (Misiti et al., 1996).

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2.3. Synchrosqueezed CWT

The process of "synchrosqueezing" refers to improving the separation between dominant frequencies in a spectrum. This is achieved via a change in the basis used for the CWT, from parameters that specify scale and shift (i.e. *a* and *b*) to parameters that specify shift and instantaneous frequency (i.e. *b* and ω). The instantaneous frequency associated with any given pair of parameters (*a*, *b*) is calculated as (Daubechies et al., 2011):

$$\omega(a,b) = \frac{-i}{W} \frac{\partial W}{\partial b}$$
 Equation 3

224 The synchrosqueezed transform based on the instantaneous frequency ω is then given as 225 the following indefinite integral with respect to the scale parameter, *a*:

$$T(\omega,b) = \int_{-\infty}^{+\infty} W(t,a,b) \ a^{-3/2} \ \delta[\omega(a,b) - \omega] \ da \qquad \text{Equation 4}$$

The theoretical development of the synchrosqueezed CWT (SCWT) was described by Daubechies and Maes (1996) and Daubechies et al. (2011). Use of the SCWT in Earth sciences has been limited, including applications in hydrology (Coleborn et al. 2013), paleoclimatology (Thakur et al., 2013), seismology (Hererra et al., 2014) and oceanography (Bian et al., 2018).

Coleborn et al. (2013) characterized water drip rates at 12 locations in Glory Hole Cave,
 a karst cave located in Yarrangobilly Caves National Park in southeastern Australia. Correlations
 between transformed drip rate data and SCWT-transformed barometric pressure, air temperature

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and evapotranspiration data recorded at ground surface were used to identify casual mechanisms.

234 Daily and sub-daily oscillations featuring variable temporal and spatial signatures were

235 identified. The authors identified a single hypothesis that was consistent with all available data

and hydrologic theory: that daily fluctuations in drip rate were driven by variations in tree water

use. From this it was inferred that overlying tree roots were of sufficient length to access

238 groundwater present in Glory Hole Cave.

Thakur et al. (2013) characterized paleoclimatic variations during the mid-Pleistocene 239 transition (i.e. 1.8 Mya to 1.2 kya). Application of the SCWT to both solar radiation and delta-240 oxygen-18 data improved estimation of the relative contributions of three variables of the Earth's 241 orbit to paleoclimate variations: precession (axial wobble), obliquity (axial tilt) and eccentricity 242 (orbital divergence from a perfect circle). Herrera et al. (2014) characterized seismic trace data 243 from a sedimentary basin in Canada containing Cretaceous age meandering channels. In 244 245 comparison to results obtained from the CWT, the use of synchrosqueezing improved identification of multiple reflectors at arrival times ranging up to one second. Bian et al. (2018) 246 characterized ocean wave turbulence and Reynolds stress. The SCWT was found to out-perform 247 three other methods (i.e., coherence, co-spectra, and ensemble empirical mode decomposition), 248 due in part to the ability to calculate time series of the instantaneous Reynolds stress. In the 249 present study, the SCWT was implemented using the Synchrosqueezing Toolbox for MATLAB 250 251 (Brevdo and Wu, 2011).

252

2.4. Empirical mode decomposition with Huang-Hilbert transform

Huang et al. (1998) derived an empirical method of decomposing time series data into a 253 linear sum of cubic spline basis functions, known as intrinsic mode functions (IMFs). IMFs are 254 calculated through an iterative procedure known as sifting, in which they are successively 255 subtracted from the dataset until a zero-valued residual is obtained. The mean frequency of each 256 257 IMF decreases during each iteration, which is characterized using a power law relation (Massei 258 and Fournier, 2012). The Hilbert transform can be applied to each mode in order to calculate instantaneous frequencies, amplitudes and phases. The Hilbert transform, y(t), of a given 259 function *x*(*t*) is defined as (Huang et al., 1998): 260

$$y(t) = \frac{1}{\pi} PV \int_{-\infty}^{+\infty} \frac{x(\tau)}{t - \tau} d\tau$$
 Equation 5

where PV is the Cauchy principle value, which is used to avoid solutions of the integral that are equal to \pm infinity, by converting them to a real value such as zero. The sum of the original time series and the Hilbert-transformed function is a complex-valued analytic function; i.e.:

$$z(t) = x(t) + i y(t)$$
 Equation 6

Following Euler's identity, this relation can also be expressed in the form:

$$z(t) = \alpha(t) e^{i\theta(t)}$$
 Equation 7

which contains parameters that describe the instantaneous amplitude (α) and instantaneous phase (θ) at time *t*. These are distinct from the non-instantaneous amplitude and phase parameters used in traditional Fourier analyses that are calculated over the full length of a given time series. Conveniently, instantaneous amplitude and phase values can be calculated as functions of *x*(*t*) and *y*(*t*); i.e.:

$$\alpha(t) = \sqrt{x(t)^2 + y(t)^2}$$
Equation 8
$$\theta(t) = \arctan\left[\frac{y(t)}{x(t)}\right]$$
Equation 9

270 This combination of methods is known as the empirical mode decomposition-Hilbert Huang transform (EMD-HHT, or often simply referred to as EMD). Applications of the EMD-271 272 HHT in geophysical, atmospheric and climate, and oceanographic studies were reviewed by Huang and Zu (2008). Applications of the EMD-HHT in hydrology include Huang et al. (2009a), 273 Rudi et al. (2010), and Massei and Fournier (2012). Huang et al. (2009) decomposed daily flow 274 data recorded over more than 20 years in two rivers in northern France of contrasting sizes: the 275 Seine River (large) and the Wimereaux River (small). Correlations were identified between low 276 frequency (i.e. large period) modes in both rivers. It was hypothesized that both rivers were 277 influenced by the maritime climate of northern France. Power relations between successive 278 modes were used to assess flow intermittency. A power law relationship identified from the 279 Seine River dataset indicated that dominant flow drivers were associated with processes 280 281 occurring over 5–60 days, which correspond to synoptic and inter-seasonal scales. A similar

relationship was not observed in the Wimereaux River dataset, which indicated greater
 intermittency and greater sensitivity to local scale precipitation events.

Rudi et al. (2010) characterized runoff in the Upper Ruhr, Kall and Erkenskur rivers, all 284 of which are located in the Ruhr River catchment of western Germany. Due to the proximity of 285 the gauging stations used in this study (all of which were located within a 10km^2 area), 286 differences between estimated IMFs were limited. Results produced using the EMD-HHT were 287 compared to those based on the STFT and CWT. The EMD-HHT was found to be superior to the 288 289 STFT in two respects. First, EMD-HHT results were more localized, whereas STFT featured 290 considerable "smearing" of energies due to spectral leakage. Second, while EMD-HHT results provided information at periods ranging from one to 256 days, STFT results did not contain 291 information for periods less than 16 days. Massei and Fournier (2012) compared daily flow in 292 the Seine River, France to the North Atlantic Oscillation. EMD-HHT results identified consistent 293 294 timescales of variability; specifically, at inter-annual scales. The EMD-HHT method was capable of accounting for non-stationary processes in Seine River flow gauge data. In particular, for the 295 296 first three estimated IMFs (i.e. representing the highest frequency basis functions), mean instantaneous amplitude values increased consistently after 1985. In the present study, the EMD-297 HHT was implemented using the PyEMD package for Python (Laszuk, 2020). 298

299

2.5. Complete ensemble empirical mode decomposition with adaptive noise

Since publication of the EMD-HHT approach, various improvements have been developed in order to increase the spectral separation between IMFs and to reduce the number of iterations required during the sifting procedure. Wu and Zhang (2009) derived the ensemble EMD method by including a Gaussian noise term when using ensemble averaging to estimate IMFs. The complete ensemble empirical mode decomposition with adaptive noise (CEEMDAN) method derived by Torres et al. (2011) enabled the sharing of noise parameter data between ensemble members.

Applications of the CEEMDAN method in hydrology include Antico et al. (2014), Adarsh and Reddy (2016), Reddy and Adarsh (2016), and Liu et al. (2018). Antico et al. (2014) used the CEEMDAN method to decompose and analyze the monthly mean discharge of the Parana River, South America. The authors identified dominant flow components at two distinct timescales: (1) annual and intra-annual oscillations that reflected seasonal precipitation; and (2) inter-annual to inter-decadal variability. The latter was linked to three large scale climatic

313 patterns: the El Nino Southern Oscillation, the North Atlantic Oscillation, and the Interdecadal

314 Pacific Oscillation. In addition, non-stationary increases in river discharge fluxes were identified,

315 which were attributed to anthropogenic climatic and land use changes. The CEEMDAN method

- 316 was found to be superior to ensemble EMD for achieving frequency separation between intrinsic
- 317 mode functions.

Reddy and Adarsh (2016) used the CEEMDAN approach to characterize monthly 318 319 precipitation data from four meteorological subdivisions in India (i.e. Assam and Meghalaya, 320 Kerala, Orissa, and Telangana) recorded over 142 years (i.e. 1871–2013). The CEEMDAN method was also used to characterize four large-scale climatic indices (i.e., the Atlantic 321 Multidecadal Oscillation [AMO], the El Nino Southern Oscillation [ENSO], the Equatorial 322 Indian Ocean Oscillation, and the Quasi-Biennial Oscillation [QBO]) and one solar index (i.e., 323 324 the sunspot cycle). Analyses were undertaken on a seasonal basis: i.e., pre- and post-monsoon, monsoon, and winter. Qualitative comparisons indicated similarities to selected indices, which 325 326 were quantified via cross-correlation analyses. In particular, the periodicity of individual IMFs was associated with specific indices. IMFs 1, 2 and 5 featured periodicities of 2-5, 5-7, >60 327 years respectively. These were associated with the QBO, ENSO and AMO indices respectively. 328 IMFs 3 and 4 featured periodicities of 11 and 20-24 years, which were associated with the 329 330 sunspot cycle and tidal forcing, respectively. Liu et al. (2018) used the CEEMDAN approach to characterize monthly precipitation in 12 sub-regions of Harbin, the capital of Heilongjiang 331 Province in north-eastern China over a 49-year period (i.e. 1964–2013). The method was 332 combined with the wavelet packet transform (Torresani, 1992) and multifractal detrended 333 fluctuation analysis (Kantelhardt et al., 2002). Sub-regions featuring relatively low variability, 334 and therefore greater predictability, were identified. Spatial variations in precipitation variability 335 were compared to topographic, climatic, oceanographic and anthropogenic drivers. In the present 336 study, the CEEMDAN approach was implemented using the PyEMD package for Python 337 (Laszuk, 2020). 338

339

2.6. Nonlinear mode decomposition

The Nonlinear Mode Decomposition (NMD) method (Iatsenko 2015a; Iatsenko 2015b)
 combined aspects of existing Fourier, wavelet and EMD approaches. Either Fourier or wavelet

transforms can be used to generate a time-frequency representation of a given time series. The 342 fundamental harmonic can be extracted from this representation and subsequently decomposed 343 into a linear sum of frequency components. The parametric result, known as a nonlinear mode 344 (NM) (and equivalent to an intrinsic mode function in EMD analysis), is then subtracted from the 345 "raw" signal and the process is repeated until a pre-defined stopping criterion is met, resulting in 346 the generation of a finite set of NMs. To date, the NMD approach has not been applied in 347 hydrology. Published applications include for signal processing of underwater acoustic and 348 electrocardiogram signals (Xin et al. 2016). In the present study, the NMD approach was 349 implemented using the Nonlinear Mode Decomposition Toolbox for MATLAB (Iatsenko et al., 350 2015a). 351

352

2.7. Moving standard deviation

The moving standard deviation (MSD) method was first applied to temperature time series data to identify periods of streamflow by Blasch et al. (2004), and later modified by Assendelft and van Meerveld (2019). Here, the simplest version of this method was employed, in which the standard deviation of time series data, $\sigma(t)$, is calculated over a specified window size as:

$$\sigma(t) = \sqrt{\frac{1}{n-1} \sum_{i=t}^{n+t-1} [x_i - \bar{x}(t)]^2} \quad \text{for } t = 1, \dots, T \quad \text{Equation 10}$$

where *n* is the number of measurements within the interval specified by the chosen window, $\bar{x}(t)$ is the average of the temperatures within the window, *i* is the sampling interval, *t* is the reference time, and *T* is the total number of measurements. As the window is moved successively forward in time across the time series, the moving standard deviation serves to magnify short-term (e.g. daily) variations in the thermal record, while minimizing larger-scale variability. For this application, a 0.5-day window size was chosen, with the reference time *t* centered within that window.

3. Methods

3.1. Synthetic example

366	An idealized synthetic temperature time series was used to demonstrate how the seven
367	signal processing methods can be used to ascertain the presence or absence of stream flow. A
368	flow signal with a 30 min sampling interval (i.e. 48 samples per day) was generated that
369	comprised, in order of events: sub-daily (0.4 d), daily (1.0 d), and three multi-day flow events (3
370	\times 4.0 d), with magnitudes of 1.0, 1.0, 3.0, 2.0, and 0.6 m ³ /d (the units for flow in this example
371	are arbitrary and only used to represent a differing magnitude). The first four signals are additive
372	in nature, whereas the flow signal was used to dampen the sum of the other signals. A Wiener
373	filter was used to dampen the signal amplitude in order to represent the presence of flow. The
374	degree of dampening was related to the magnitude of flow, with larger flows indicated by
375	stronger dampening.
376	Four components of real annual temperature signals that are typically observed at the
377	surface of a streambed were added to the flow signal. These were:
378	1. A decadal-scale climate variation was represented using linear increasing trend (0.01 $^{\circ}C/d$).
379	2. A seasonal variation due to tilt of the Earth was represented using a sinusoid with an
380	amplitude of 30 °C, a period of 1 year, and an offset of 25 °C.
381	3. A daily variation due to rotation of the earth was represented using a sinusoid with an
382	amplitude of 10 °C and a period of 1 d.
383	4. Signal noise representing local sub-daily variations in temperature (e.g. due to shading or
384	wind) was represented using a continuous uniform distribution. For the low noise case,
385	bounds of $[-0.5, +0.5]$ °C were specified. For a high noise case, bounds of $[-4, +4]$ °C. The
386	range of the latter case (i.e. 8 $^{\circ}$ C) was chosen to ensure that the amplitude of fluctuations due
387	to noise were of the same order of magnitude as "true" daily signals.
388	For each of the TF transform methods tested, it is possible to take a physically
389	meaningful portion of one of the outputs and identify a threshold value that delineates between
390	times of flow and no-flow. This threshold (x) was identified by minimizing an objective function

f(x), which was defined as:

$$f(x) = 1 - [0.5 FM(x) + 0.5 NFM(x)]$$
 Equation 11

where FM(x) and NFM(x) represent the fractions of flow and no-flow periods that were 392 correctly identified when using threshold value x. Because a binary classification of the 393 394 condition of flow or no-flow is used with the threshold, the output of the matching of flow (FM) and no-flow (NFM) results in a step function of matching whereby changes to the threshold 395 might result in no change in the accuracy of the flow matching. This type of objective function 396 can pose problems for gradient-based optimization approaches that rely on a numerically derived 397 gradient due to the gradient becoming zero at non-optimal threshold values. Therefore, a 398 stochastic differential evolution optimization approach (Storn and Price, 1997) was used, which 399 was implemented using the Scipy package for Python (Virtanen et al., 2020). In the transform 400 approaches applied, characteristic signals (seasonal and diurnal) should appear. The magnitude 401 of the transform at diurnal frequency should in theory contain information on the magnitude of 402 flow events. 403



Figure 2. Synthetic temperature (T) time series for synthetic example. Input component signals included: (a) climatic variation; (b) annual seasonal variation; (c) diurnal fluctuation; (d) zeromean white noise; and (e) flow period duration. (f) Resulting year-long temperature signal and (g) detailed view of days 256 to 268, showing attenuation of temperature fluctuations due to presence of stream water over sensor during ephemeral flow event.

410 **3.2. Field example**

In order to compare the efficacy of the seven methods when applied to a real-world 411 dataset, stream flow and streambed temperature data were obtained from a gauging station 412 located on Pedlar Creek near Kangarilla, South Australia (Station A5030503, Department of 413 Environment and Water, Government of South Australia). Pedlar Creek drains an ephemeral and 414 intermittent stream network located in a coastal, Mediterranean climate catchment in the 415 Willunga Basin, located 25 km south of the city of Adelaide, South Australia. The creek 416 typically flows from late June to mid-August (Figure 3), with annual streamflow in the range of 417 10^4 – 10^6 m³ yr⁻¹ (Shanafield et al., 2020) and standard deviation of 0.22. For this study, ~5 years 418 of data from the period 2013 to 2018 were selected. The sampling interval used to analyze the 419 data was 0.02 d (30 min). 420



Figure 3. (a) Stream bed temperature and stream flow observations recorded on Pedlar Creek (Station A5030503) located near Kangarilla, South Australia, 2013–2018. (b) A subset of the same observations, shown for the period May–December 2016, which contains a series of flow events that demonstrate dampening of temperature signal amplitudes in the presence of flow.

426 **4. Results**

427 **4.1. Synthetic example**

Time-frequency transform analyses (Figure 4) focused on the 1 cycle per day (cpd) (i.e. 428 diurnal) signal, as this is typically the dominant frequency (i.e. features the highest signal-to-429 430 noise ratio) observed in stream temperature observations (Stonestrom and Constantz, 2003). Each of the transforms showed a clear decrease in signal energy at the 1 cpd frequency during 431 flow events. Reductions in energy at the 1 cpd frequency resulted in increases in energy at lower 432 frequencies, which reduced the intensity of the amplitude spectra, which also signified flow 433 434 events. Dampening of the temperature signal was observed, with the exception of the EMD spectra which indicated an increase in energy during flow events. Furthermore, larger magnitude 435 flow events (and hence, greater attenuation of the temperature signal) enabled better 436 discrimination of changes in flow for each of the methods. The onset of all synthetic flow events 437 was evident in all transformed temperature signals to various degrees. In the high noise case, 438 discrimination was less clear, particularly for shorter, low magnitude flow events. 439 440



Figure 4. Amplitude and instantaneous amplitude results (with all values normalised to a [0,1] range) derived from six time-frequency transform methods for low and high noise synthetic temperature time series datasets. Flow events (light grey vertical bars) are presented to highlight reductions in signal energy at these times. Note that results from the moving standard deviation technique are not presented as this is not a time-frequency transform method.

To identify flow events, specific frequencies and modes were extracted (Figure 5). For the STFT, CWT, and SCWT methods, time series at the 1 cpd frequency were extracted. For the model decomposition methods, a single mode was selected for each method, based on visual inspection. For the MSD method, only one output signal was generated, which was used to identify flow events. Identification of flow and no-flow conditions using each method was based on the differential evolution-obtained optimal threshold.

Most time-frequency approaches and the MSD method identified flow and no-flow 453 periods in the low noise case exactly, with flow matching of 100 % achieved. In contrast, the 454 455 EMD and CEEMDAN methods featured relatively lower flow matching values of 90.37 % and 92.70 % respectively. No-flow matching performance ranged from 95.18 % to 98.33 % across all 456 time-frequency transform methods, compared to a value of 99.07 % for the MSD method. 457 Misclassified flow and no flow periods were generally clustered around flow events, especially 458 459 for the time-frequency approaches. False negatives were observed both immediately before and after flow events, in response to a sharp shifts in the amplitude or instantaneous amplitude of the 460 461 temperature signal. CEEMDAN method results also featured both false positives and negatives scattered throughout the time series due to extremely noisy instantaneous amplitude values. 462

Results from the high noise case were more varied. While the STFT, SCWT, and MSD 463 methods achieved 100 % flow matching, flow delineation using EMD was compromised by the 464 noisy transformed signal (FM = 87.42 %). Large variability in instantaneous amplitude from 465 these methods resulted in flow delineation that was unrelated to known flow events, i.e. it was 466 467 not just a case of not identifying initiation or cessation of a flow event correctly but rather misidentifying periods as flowing when no flow event occurred. The CWT, CEEMDAN and 468 NMD methods performed equally well, with flow matching of 96.89 % achieved in each case. 469 The proportion of no-flow periods successfully identified ranged from 98.29 % to 99.50 % for 470 each of the TF methods tested, with the exception of the SCWT method (77.29 %). As with the 471 low noise case, flow mismatches occurred directly prior to and after flow events, in response to 472 abrupt shifts in instantaneous amplitude values. Despite achieving the best overall matching of 473 flow and no-flow periods, the STFT and MSD approaches identified a considerable number of 474 false positives. 475



477

Figure 5. Optimal signal extracted from each of the seven methods tested (purple line) and
corresponding optimized threshold frequency for delineating between flow and no-flow periods
(red dashed line). Listed flow matching (FM) and no-flow matching (NFM) values summarise
the proportion of flow and no-flow periods successfully identified, respectively.

482 **4.2. Field Example**

Application of time-frequency transform methods to the Kangarilla temperature signal 483 dataset identified clear patterns for flow and no-flow periods around 1 cpd (Figure 6). 484 Reductions in signal energy were proportional to the magnitudes of flow events. The CWT and 485 NMD approaches performed relatively well, with flow matching greater than 99 % achieved 486 (Figure 7). The EMD method performed relatively poorly, with flow matching of 88.01 % 487 achieved. Flow matching for the remaining methods ranged from 90.44 % to 95.33 %. The 488 489 matching of no-flow periods was markedly lower across all methods. No-flow matching ranged 490 from 84.31 % to 89.44 %, with the exception of the SCWT method (63.66 %). The apparent noise present in the transformed temperature signal derived from the STFT, SCWT, EMD, 491 CEEMDAN and MSD methods created a large number of incorrect classifications of flow. These 492 occurred during no-flow periods that were not associated with any actual flow events, as well as 493 494 at the end of both flow and no-flow periods. Overall, accurate classification of flow and no-flow periods for the field example dataset were achieved using the CWT and NMD methods. All 495 496 intermittent flows were correctly predicted, but ephemeral flows less than one day were not. 497



Kangarilla temperature transforms

498

Figure 6. (a) Stream bed temperature and stream flow observations recorded on Pedlar Creek

(Station A5030503) located near Kangarilla, South Australia, 2013–2018. Stream temperature
 and flow measurements from Pedlar Creek, South Australia. (b-g) Amplitude and instantaneous

amplitude results (with all values normalised to a [0,1] range) derived using six time-frequency

⁵⁰³ transform methods.



Figure 7. Identification of flow and no-flow periods from transformed Kangarilla streambed
 temperature time series dataset. Listed flow matching (FM) and no-flow matching (NFM) values
 summarize the proportion of flow and no-flow periods successfully identified, respectively.

510 **5. Discussion**

The aim of the present study was to identify time-frequency method(s) that are suitable for classifying stream flow states from streambed temperature time series data. The comparative merits of each method are now discussed. Take-home messages from the synthetic and realworld case studies are distilled. Suggestions for future research directions in terms of identifying flow presence using these methods are proposed.

516

5.1. Comparison of methods

517 Differences between the performance of the time-frequency methods tested in this study 518 were found to be minimal, with all methods successfully identifying events greater than 1 day in 519 duration. However, as in previous studies, evaluation of these methods was not achieved by 520 simply comparing the success rate of successful flow or no-flow matching. Instead, it is 521 important to consider several aspects of the method.

The main advantage of time-frequency methods over moving standard deviation 522 approaches is the potential to develop a more objective, non-site-specific analysis that can be 523 applied at multiple locations. For example, Assendelft and van Meerveld (2019) found that 524 applications of simple moving standard deviation methods to stream temperature data did not 525 adequately identify flow states during periodic flow events. The authors added several subjective 526 criteria to their analysis in order to improve their results. In comparison, in this study we have 527 simply applied a default approach across all methods. We expect that, as with the moving 528 standard deviation approach, fine tuning of the methodology (e.g. experimentation with input 529 parameters such as mother wavelet type or wave number, or improved means of determining 530 531 threshold values) would further improve flow and no-flow matching capabilities.

The efficacy of time-frequency methods was found to be equal to or better than the moving standard deviation approach, without the need for subjective post-processing of results, and while offering the advantage of applicability at a catchment scale. Advantages of TF methods include their ease of use and in the minimal requirement for assumptions. For example, the STFT is widely used in hydrologic applications but requires the assumption that processes of interest are stationary within a specified window size. Processes such as the onset and cessation

of streamflow are by definition non-stationary. Identification of discrete changes in states using
the STFT can be difficult and depends upon the length and sampling frequency of an observed
dataset.

In comparison, the CWT method avoids the need for compromises between sampling 541 resolution and measurement duration. The CWT is a more parsimonious approach than other 542 time-frequency methods, is able to accommodate missing values in input datasets, is relatively 543 intuitive in its theory, and mis-identified fewer flow events in comparison to STFT and MSD 544 545 methods. The CWT can easily be implemented in MATLAB, R, Python, or other high-level 546 languages, and periods of flow are relatively easy to identify from visual inspection of CWT outputs (e.g. Figures 3 and 5). Smearing effects may be present in CWT results but can be 547 reduced through weighting of the CWT phase shift parameter. The synchrosqueezed CWT 548 (which is currently only available in MATLAB), performed on par with CWT, but was not found 549 to provide any additional benefits to the CWT for the test cases presented. 550

Mode decomposition methods were found to be less well-suited to the case studies 551 presented, with generally slightly lower flow and no-flow matching accuracies and longer 552 553 computing times. When identifying streamflow, the 1 cpd (i.e. diurnal) frequency was known to 554 be the focus *a priori*, whereas mode methods contain energy from multiple frequencies. There is no physical basis for selecting a given mode. Mode decomposition methods are unable to 555 accommodate missing values in input datasets, and streambed temperature measurements 556 typically contain numerous data gaps, due to field conditions and equipment issues. However, 557 558 the EMD method did identify long period seasonal variations, so this method may be useful for detrending of data prior to analysis. The CEEMDAN approach did not provide any advantage 559 over the traditional EMD approach, and although the NMD method did perform well for flow 560 matching, it was the most computationally cumbersome method tested. 561

562

5.2. Insights from applications to a real-world temperature dataset

The synthetic examples identified two metrics that best identified the onset and duration of flow events. The first was the ratio of temperature variance to noise strength. The second was the strength of a "flow" signal whereby it is necessary to see enough dampening of the temperature time series in order to clearly classify when it is flowing and not flowing correctly. Field data invariably includes a strong "noise" signal, due to climatic forcing, variation in shading, micro-climates within the stream channel, and a variety of other factors. Moreover, the application of TF methods to real-world temperature time series data can be confounded by various aspects that were not represented in the synthetic examples provided in the present study.

571 These real-world factors were apparent in our field example, highlighting subtle differences between the results of the various methods. The Kangarilla field example showed 572 that cessation of flow is typically more difficult to predict than the onset of flow. This may be 573 due to pooling, which occurs in many intermittent rivers. Greater variation in amplitude values 574 575 over time may be observed in real-world datasets, a trend which was clear with larger variance in 576 temperature in the summer then in the winter. Also, temperature drops often accompany rainfall events. These lower the streambed temperature and thereby affect interpretation, allowing mis-577 classification of flow just prior to the onset of flow in the stream. 578

The interpretation of streamflow from streambed temperature time series data assumes the existence of a discernible diurnal temperature variation. Previous studies demonstrated that daily temperature variation in surface in shallow streams can be quite low, especially during spring and autumn (Anibas et al., 2009; Shanafield et al., 2017). This will preclude the application of such methods in some environments, such as low altitude, humid areas.

584 **5.3. Future research directions**

585 Applications of non-traditional time series analysis methods (i.e. other than Fourier and wavelet methods) in hydrology are currently limited. Published applications are generally 586 587 restricted to direct observations of precipitation rates and discharge fluxes. Comparisons to exogenous datasets typically involved large-scale drivers such as climate indices. In comparison, 588 589 in the present study, a range of traditional and non-traditional time series analysis methods were used to decompose a proxy measured variable (streambed surface temperature) in order to 590 estimate a primary variable (stream flow), for physical processes occurring at sub-metre and sub-591 daily to daily to scales. The primary variable, stream flow, was also measured and provided the 592 593 metric for method comparisons. This work provides a first step towards developing a method that can be automated to estimate streamflow state in non-perennial stream catchments without 594 the need for either elaborate, expensive sensors or bespoke analysis routines. 595

596 Further research can greatly improve the methods presented in this study, including the 597 following:

Rather than simply estimating flow state (as was the subject of this study), stream stage
 height could be estimated from the magnitude of signal dampening during flow events. This
 approach may be most appropriate for intermittent streams, for which the onset and duration
 of flow can be relatively well-known. We hypothesize that the ratio of air temperature
 variance to dampened streambed temperature variance could be used to distinguish between
 the two, as this ratio is dependent on the exposure of the sensor as well as the depth of flow.
 In the present study, the 1 cpd (diurnal) frequency was known *a priori* to be the key

605 frequency of interest. Additional investigations are required to determine whether other 606 frequencies yield useful information for understanding stream functioning or flow states.

A temperature sampling frequency of 30 minutes was used in the present study. Future
 investigations should consider the impact of sampling frequency on ability to predict both
 start, continuation and end of flow events of varying timing and magnitude.

In the current application, the identification of flow state was limited to the daily scale, which 610 4. 611 is disadvantageous when compared to previous results of the moving standard deviation method. However, wavelet parameterisation may allow the identification of sub-daily (i.e. < 612 613 1 cpd) frequencies. For example, the frequency of the mother wavelet used in the CWT method is a function of the wave number specified, which in turn affects the amplitude of the 614 615 output signal. The use of wave numbers lower than five should be investigated for their usefulness in identifying sub-daily flow events. Similarly, nested wavelet transforms, as used 616 617 in the CEEMDAN approach, may assist the identification of transitions between flow states. However, the CEEMDAN method will remain subject to compromises between output 618 resolution and smoothing. 619

5. As with the moving standard deviation method, the specification of a subjective, nonphysical (and often site-specific) threshold value to delineate between flow and no-flow
periods is unavoidable with time-frequency analysis techniques. Additional research is
required to determine: whether a single threshold can be used to determine flow state for
multiple sensors within a catchment; how the selection of the threshold can be numerically

optimized; or whether the threshold varies as a function of time (e.g. seasonally due tovariation in the amplitude of daily temperature oscillations).

627 6. Conclusions

This work builds on several attempts to interpret stream flow states from streambed 628 629 temperature time series data. Most previous research compared the amplitudes of air and surface water temperatures. Although such approaches have achieved limited success, it has been 630 proposed that air and surface temperature data alone are not sufficient for deducing the presence 631 of stream flows. Here, we examined the efficacy of non-stationary methods of temperature time 632 633 series analysis. While all methods were able to identify flow events at a daily scale, the CWT method was identified as the most efficacious and most parsimonious. Benefits included the 634 ability to handle discontinuous datasets, ease of implementation and analysis, high performance, 635 and objectivity. Nevertheless, the implementation of CWT approaches presents ample 636 opportunities for improvement. In particular, more objective means of selecting flow/no-flow 637 threshold values are possible; for example, using automated optimization. Further 638 experimentation with algorithm inputs (such as wavelet wave number and convolution of output 639 frequencies) is likely to improve interpretation capabilities and extend the applicability of this 640 method across spatial (e.g. automation at a catchment scale) and temporal domains (e.g. 641 identification of sub-daily events). 642

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