



New infrared absorption cross sections of difluoromethane (HFC-32) for atmospheric remote sensing

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ABSTRACT

Difluoromethane (CH_2F_2 ; HFC-32), a hydrofluorocarbon (HFC) used as a refrigerant in air conditioning and heat pump systems, is currently being phased out under the terms of the Montreal Protocol (Kigali Amendment). In order to monitor its concentration profiles using infrared-sounding instruments, for example the Atmospheric Chemistry Experiment – Fourier transform spectrometer (ACE-FTS), accurate laboratory spectroscopic data are required. This work describes new high-resolution infrared absorption cross sections of difluoromethane / dry synthetic air over the spectral range $850\text{--}1335\text{ cm}^{-1}$, derived from spectra recorded using a high-resolution Fourier transform spectrometer (Bruker IFS 125HR) and a 26-cm-pathlength cell. Spectra were recorded at resolutions between 0.009 and 0.03 cm^{-1} (calculated as $0.9/\text{MOPD}$; MOPD = maximum optical path difference) over a range of temperatures and pressures ($7\text{--}760\text{ Torr}$ and $188\text{--}297\text{ K}$). The new absorption cross sections in this work improve upon those currently available in HITRAN for remote sensing.

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1. Introduction

The discovery that chlorofluorocarbon (CFC) refrigerants were destroying stratospheric ozone led to the signing of the 1987 Montreal Protocol. Designed to protect the Earth's ozone layer, whose destruction was catalysed by chlorine atoms reaching the stratosphere, the Protocol mandated the phasing out of CFC production. At least initially, hydrochlorofluorocarbons (HCFCs) were adopted as 'transitional' CFC replacements because of their shorter atmospheric lifetimes on account of their more efficient reaction with OH in the troposphere. However, the race was on to find replacement refrigerants that did not deplete stratospheric ozone. Ultimately, this led to the manufacture and use of a class of molecules known as hydrofluorocarbons (HFCs). Like CFCs and HCFCs, HFCs are potent greenhouse gases, many times more powerful than carbon dioxide. Although the ozone depletion potentials of HFCs are defined to be zero, somewhat ironically they will produce a very small indirect effect on ozone destruction through the increases in tropospheric and stratospheric temperatures, notably by enhancing ozone-destroying catalytic cycles and modifying atmospheric circu-

lation [1]. Historically, HFCs were not regulated by the Montreal Protocol, however this changed in 2016 with the Kigali amendment, which provides a roadmap for their phase out. Monitoring HFCs now takes on a greater importance.

The use of HFC-32 is primarily as a refrigerant in air conditioning and heat pump systems. It also exists in a variety of refrigerant blends: Tables 2–4 in [2] lists 21. In 2016, HFC-32 was the fifth most abundant HFC with a global mean surface mole fraction of 11.9 ppt ; it increased during 2012–2016 by an average of 1.6 ppt yr^{-1} for HFC-32, faster than the average growth rate for the preceding four years. HFC-32 has a 100-year global warming potential of 705 [2], and a total atmospheric lifetime of 5.4 years [2]. It is removed from the atmosphere by reaction with OH, resulting in the formation of carbonyl fluoride (COF_2) [3].

In addition to regular in situ monitoring at the surface, HFC-32 has recently been measured from orbit by the ACE-FTS (Atmospheric Chemistry Experiment – Fourier transform spectrometer) [4], which has been recording atmospheric limb spectra for over fifteen years with near-global coverage. The ACE-FTS is the only satellite instrument currently able to measure HFCs, including the more abundant HFC-134a [5] and HFC-23 [6]. With a very congested infrared spectrum, making it difficult to generate line parameters, it is more convenient to use absorption cross sections

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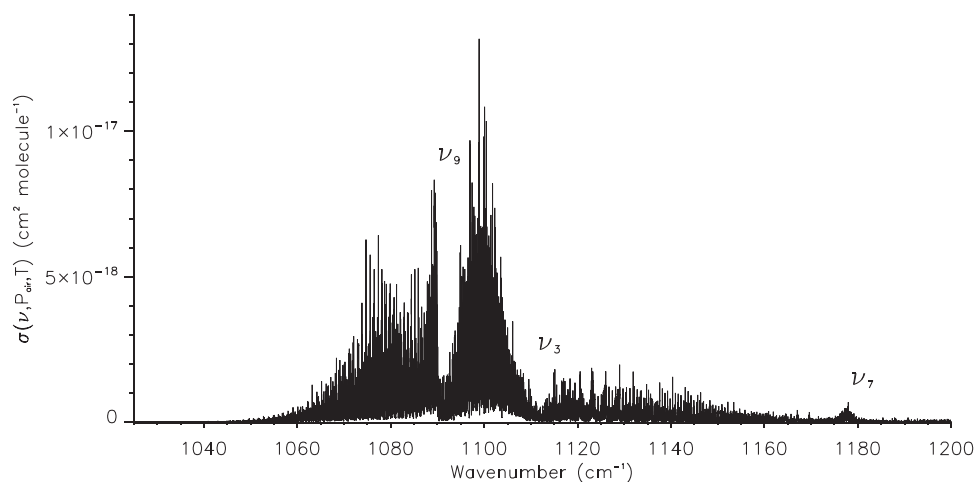


Fig. 1. The absorption cross section of difluoromethane / dry synthetic air at 188.9 K and 24.96 Torr (this work), with fundamental bands labelled.

of air-broadened HFC-32 over a range of atmospherically relevant temperatures and pressures in retrieval schemes. This work describes a new such dataset, which is utilised in a companion paper within this HITRAN special issue to obtain the first measurements of HFC-32 from orbit [7].

2. Infrared spectroscopy of difluoromethane

Carbon has two stable isotopes found in nature, fluorine only one, so there are two stable isotopologues of difluoromethane (not considering deuterated forms), $^{12}\text{CH}_2\text{F}_2$ and $^{13}\text{CH}_2\text{F}_2$, with approximate abundances of 99 and 1%, respectively. Both forms possess C_{2v} symmetry and have nine vibrational modes. The 850–1335 cm^{-1} spectral range covered in the present work includes four fundamental band systems: $\nu_3 \sim 1111.5 \text{ cm}^{-1}$, $\nu_5 \sim 1255.8 \text{ cm}^{-1}$, $\nu_7 \sim 1178.6 \text{ cm}^{-1}$, and $\nu_9 \sim 1090.1 \text{ cm}^{-1}$ (wavenumbers are for $^{12}\text{CH}_2\text{F}_2$ [8]). Of these, ν_3 and ν_9 give rise to the strongest absorptions, with ν_7 having medium intensity; strictly, ν_5 is infrared inactive but becomes weakly allowed through Coriolis interactions. As difluoromethane is an asymmetric rotor, its infrared spectrum contains highly complex, congested rotational structure. Fig. 1 is a plot of the new absorption cross section at 188.9 K and 24.96 Torr, with fundamental bands labelled. Details on the measurement conditions and derivation of this cross section are given in Section 3.

Absorption cross sections of difluoromethane were first included in HITRAN 2000 [9] for 17 different conditions over two wavenumber ranges (995–1236 and 1385–1475 cm^{-1}) for both pure (at 203, 212, 222, 243, 253, 264, 287, and 297 K) and air-broadened samples (203, 251, and 297 K at pressures of 5, 20, and 100 kPa air); henceforth referred to as the Smith dataset [10], all cross sections were derived from spectra recorded by Fourier transform infrared spectroscopy at 0.03 cm^{-1} spectral resolution. Previously, these have been the only cross sections available for remote sensing, although three 760-Torr- N_2 -broadened difluoromethane spectra (at 278, 298, and 323 K) from the Pacific Northwest National Laboratory (PNNL) IR database [11] were added to the HITRAN 2016 compilation [12]. A number of weaknesses have been identified in the Smith dataset, namely the poor pressure and temperature coverage, the poor wavenumber calibration, and the poor spectral resolution of the low-pressure measurements. The motivation for this work has been to provide the community with improved absorption cross sections, which will provide a more accurate basis for retrievals for HFC-32.

3. New absorption cross sections of air-broadened difluoromethane

3.1. Experimental

The measurements were performed at the Rutherford Appleton Laboratory (RAL) in the High Resolution Spectroscopy Facility (HRSF), formerly known as the Molecular Spectroscopy Facility (MSF). The experimental setup and the experimental procedures have been described previously for related measurements [e.g. 12–14]. FTS instrumental parameters used for the measurements, sample details, and the cell configuration are summarised in Table 1. The sample pressures and temperatures for each air-broadened spectrum, along with their experimental uncertainties and associated spectral resolutions, are listed in Table 2.

3.2. Generation of absorption cross sections

The procedure used to generate absorption cross sections from measured spectra has been reported previously [e.g. 13–15], so the full details are not provided here. The wavenumber scale was calibrated using the positions of isolated N_2O absorption lines in the range 1140 to 1320 cm^{-1} from NIST heterodyne wavenumber calibration tables [16]. The absorption cross sections, $\sigma(\nu, P_{\text{air}}, T)$, with units of $\text{cm}^2 \text{ molecule}^{-1}$, at wavenumber ν (cm^{-1}), temperature T (K) and synthetic air pressure P_{air} , were normalised according to

$$\int_{850 \text{ cm}^{-1}}^{1335 \text{ cm}^{-1}} \sigma(\nu, P_{\text{air}}, T) d\nu = 5.9594 \times 10^{-17} \text{ cm molecule}^{-1}, \quad (1)$$

where the value on the right hand side is the average integrated band intensity over the spectral range 850–1335 cm^{-1} for three 760-Torr- N_2 -broadened difluoromethane spectra (at 278, 298, and 323 K) from the Pacific Northwest National Laboratory (PNNL) IR database [11]. This intensity calibration procedure counters problems with difluoromethane adsorption in the vacuum line and on the cell walls, under the assumption that the integrated intensity over each band system is independent of temperature. The reader is referred to Ref. [13] for a more complete explanation of the underlying assumption, and references cited within Refs. [14] and [15] for details on previous successful uses of this approach.

Table 1

FTS parameters, sample conditions, and cell configuration for all measurements.

Spectrometer	Bruker Optics IFS 125HR
Mid-IR source	Globar
Detector	Mercury cadmium telluride (MCT) D313 ^a
Beam splitter	Potassium bromide (KBr)
Optical filter	~700–1350 cm ⁻¹ bandpass
Spectral resolution	0.009 to 0.03 cm ⁻¹
Aperture size	3.15 mm
Apodisation function	Boxcar
Phase correction	Mertz
HFC-32 (Fluorochem Ltd)	99.6% purity, natural-abundance isotopic mixture
Air zero (BOC Gases)	total hydrocarbons < 3 ppm, H ₂ O < 2 ppm, CO ₂ < 1 ppm, CO < 1 ppm; used 'as is'
Cell pathlength	26 cm
Cell windows	Potassium bromide (KBr) (wedged)
Pressure gauges	3 MKS-690A Baratron (1, 10 & 1000 Torr) ($\pm 0.05\%$ specified accuracy)
Refrigeration	Julabo F95-SL Ultra-Low Refrigerated Circulator (with ethanol)
Thermometry	4 PRTs, Labfacility IEC 751 Class A
Wavenumber calibration	N ₂ O

^a Due to the non-linear response of MCT detectors to the detected radiation, all interferograms were Fourier transformed using Bruker's OPUS software with a non-linearity correction applied.

Table 2

Summary of the sample conditions for all measurements.

Temperature (K)	Initial CH ₂ F ₂ Pressure (Torr) ^a	Total Pressure (Torr)	Spectral resolution (cm ⁻¹) ^b
188.9 ± 0.3	0.131	24.96 ± 0.04	0.0090
188.6 ± 0.3	0.194	49.99 ± 0.08	0.0100
188.1 ± 0.3	0.283	100.1 ± 0.1	0.0150
188.0 ± 0.3	0.366	199.9 ± 0.3	0.0225
202.7 ± 0.3	0.153	24.98 ± 0.09	0.0090
202.7 ± 0.3	0.221	50.04 ± 0.05	0.0100
202.7 ± 0.3	0.303	99.96 ± 0.08	0.0150
202.7 ± 0.3	0.414	200.7 ± 0.1	0.0225
202.7 ± 0.3	0.450	300.1 ± 0.5	0.0300
217.1 ± 0.2	0.165	25.15 ± 0.08	0.0090
217.1 ± 0.2	0.244	51.34 ± 0.04	0.0100
217.1 ± 0.2	0.348	101.0 ± 0.1	0.0150
217.1 ± 0.2	0.446	202.1 ± 0.5	0.0225
217.1 ± 0.2	0.523	359.8 ± 0.2	0.0300
232.9 ± 0.2	0.189	25.37 ± 0.02	0.0090
232.9 ± 0.2	0.241	50.02 ± 0.02	0.0100
232.9 ± 0.2	0.423	100.4 ± 0.1	0.0150
232.9 ± 0.2	0.522	203.5 ± 0.1	0.0225
232.9 ± 0.2	0.590	400.0 ± 0.1	0.0300
252.8 ± 0.2	0.191	24.70 ± 0.02	0.0090
252.8 ± 0.2	0.245	50.77 ± 0.02	0.0100
252.8 ± 0.2	0.523	200.0 ± 0.1	0.0225
252.8 ± 0.2	0.683	403.5 ± 0.1	0.0300
252.8 ± 0.2	0.764	600.2 ± 0.1	0.0300
273.8 ± 0.2	0.306	7.645 ± 0.006	0.0100
273.8 ± 0.2	0.692	203.6 ± 0.3	0.0225
273.8 ± 0.2	0.852	360.7 ± 0.1	0.0300
273.7 ± 0.2	0.821	760.4 ± 0.2	0.0300
296.6 ± 0.1	0.847	362.4 ± 0.1	0.0300
296.7 ± 0.1	1.007	760.3 ± 0.2	0.0300

^a MKS-690A Baratron readings are specified accurate to $\pm 0.05\%$.

^b Using the Bruker definition of 0.9/MOPD.

3.3. Absorption cross section uncertainties

The uncertainty of the wavenumber scale is comparable to the uncertainty of the N₂O lines used in the calibration, which according to the NIST heterodyne wavenumber calibration tables [16] is between 0.00005 cm⁻¹ and 0.00008 cm⁻¹.

The signal-to-noise ratios (SNRs) for the measured transmittance spectra range from 2400 to 4600 (rms); these were calculated using Bruker's OPUS software at ~980 cm⁻¹ where the transmittance is close to 1, and indicate that the contribution from noise to the uncertainty in the cross section intensities is below 0.1%. In fact, systematic errors dominate this intensity uncertainty. As shown in Table 2, the maximum systematic errors in the sample temperatures (μ_T) and total pressures (μ_P) are 0.2% and 0.4%,

respectively. The photometric uncertainty (μ_{phot}), associated with the detection of radiation by the MCT detector and systematic error arising from the use of Bruker's non-linearity correction for MCT detectors, is estimated to be ~2%. The pathlength error (μ_{path}) is estimated to be lower than 0.1%. According to the relevant meta-data files, the systematic error in the PNNL difluoromethane spectra used for the intensity calibration is estimated to be less than 3% (2σ); this incorporates errors in the partial pressures and cell pathlength, so these do not have to be considered further. Equating the error, μ_{PNNL} , with the 1σ value, i.e. 1.5%, and assuming that the systematic errors for all the quantities are uncorrelated, the systematic error, $\mu_{\text{systematic}}$, can be expressed as:

$$\mu_{\text{systematic}}^2 = \mu_{\text{PNNL}}^2 + \mu_T^2 + \mu_P^2 + \mu_{\text{phot}}^2. \quad (2)$$

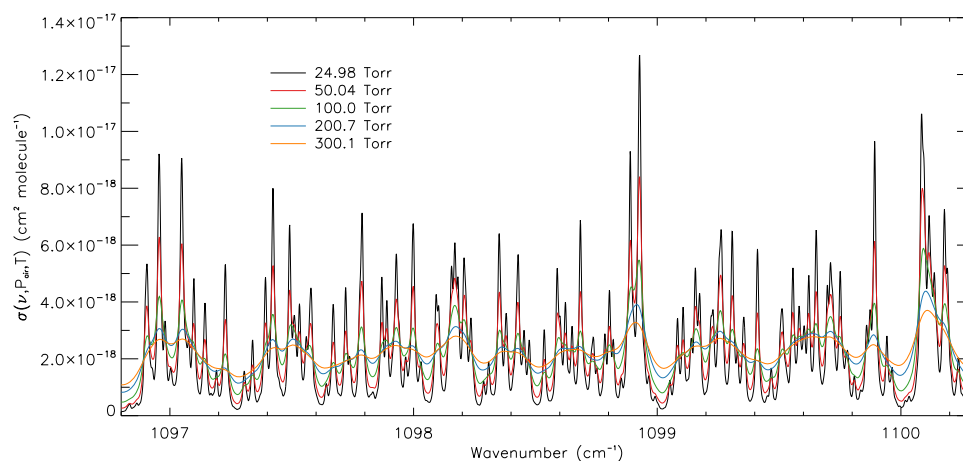


Fig. 2. The absorption cross sections of difluoromethane / dry synthetic air over the spectral region 1096.8–1100.3 cm^{-1} at a temperature of ~ 202.7 K and a range of pressures.

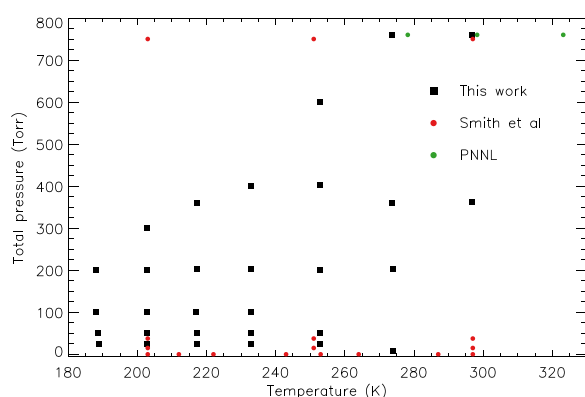


Fig. 3. A graphical representation of the PT coverage for the three difluoromethane cross section datasets.

Eq. (2) gives a systematic error of $\sim 3\%$ (1σ) for the new HFC-32 absorption cross section dataset.

4. Discussion

This work extends the range of pressure and temperature combinations for the absorption cross sections of air-broadened difluoromethane, providing a more suitable range for remote sensing than hitherto available.

A selection of the air-broadened absorption cross sections is presented in Fig. 2 for five pressures (24.98–300.1 Torr) at 202.7 K.

Overall, the pressure – temperature (PT) coverage of the air-broadened cross sections has been extended from only three temperatures to seven (188–297 K), and now covers a more appropriate range of pressures. The PT coverage can be visualised in Fig. 3, in which the temperature for each cross section is plotted against the corresponding total pressure. Overall, this new cross-section dataset contains 30 different combinations of pressure and temperature (see Table 2).

The choice of spectral resolution is an important one in ensuring that features are adequately resolved; under-resolved bands in absorption cross sections can contribute to systematic errors in retrievals when utilised in remote sensing. All the Smith measurements were taken at 0.03 cm^{-1} spectral resolution. For those at 0.0 (i.e. pure sample) and 37.5 Torr, this is too low and the spectra are under-resolved; Norton-Beer strong apodisation has also been applied to the measured spectra, which has the effect of degrading the resolution even further. Fig. 4 provides a comparison of a new cross section at 202.7 K and 50.04 Torr with two Smith cross sections at a similar temperature but lower pressures; it is evident that the Smith cross sections are under-resolved due to the lower spectral resolution chosen.

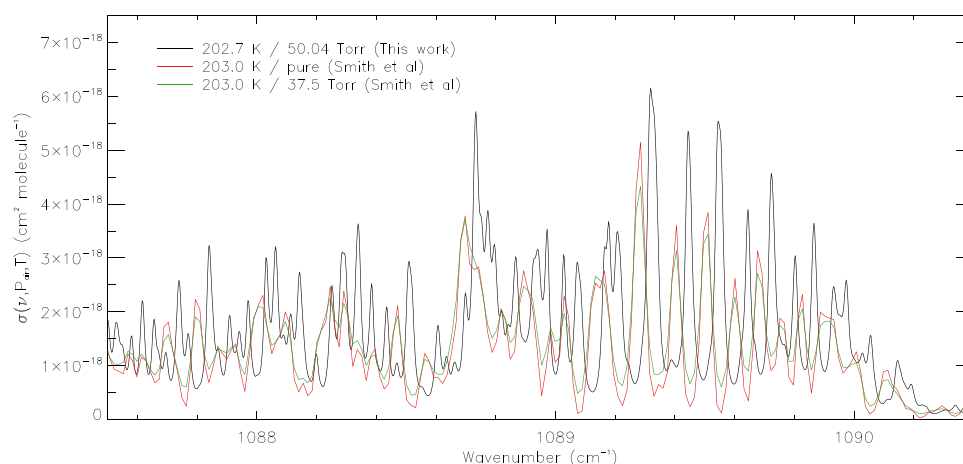


Fig. 4. The absorption cross section of difluoromethane / dry synthetic air over the spectral range 1087.5–1090.4 cm^{-1} at a temperature of 202.7 K and 50.04 Torr; overplotted are two Smith cross sections for pure and air-broadened (37.5 Torr total) difluoromethane, both at 203.0 K.

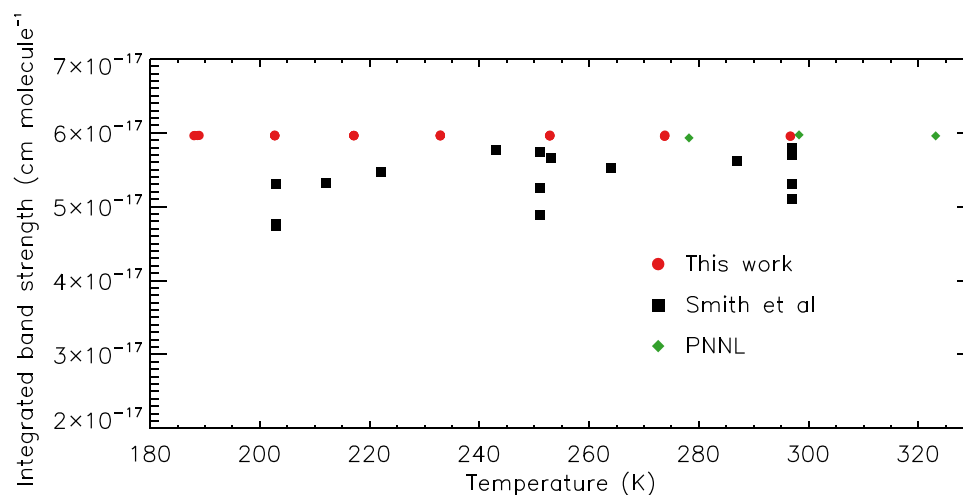


Fig. 5. Integrated band intensity versus temperature for three difluoromethane cross section datasets (Smith, PNNL, present work) calculated over the wavenumber range 995–1236 cm^{-1} .

Furthermore, the wavenumber scale of the Smith cross sections is not calibrated. With an absolute accuracy in the wavenumber scale of between 0.00005 cm^{-1} and 0.00008 cm^{-1} for the new cross sections, it is clear that the Smith measurements are significantly shifted too low by $\sim 0.04 \text{ cm}^{-1}$ (a calibration factor of ~ 1.00004). This can also be observed in Fig. 4.

Integrated band intensities have been calculated over the wavenumber range 995–1236 cm^{-1} for the Smith, PNNL, and new cross sections; these are plotted against temperature in Fig. 5. Scatter in the Smith integrated band intensities approaches 20%, likely due to errors in these measurements associated with the sample concentrations. The integrated band intensities for the new cross sections agree well with those for PNNL, however this is to be expected due to the normalisation procedure.

The new HFC-32 absorption cross section dataset will be made available to the community via the HITRAN [12] and GEISA [17] databases, but in the meantime is available electronically from the author.

5. Conclusions

New high-resolution IR absorption cross sections for air-broadened difluoromethane (HFC-32) have been determined over the spectral range 850–1335 cm^{-1} , with an estimated systematic uncertainty of $\sim 3\%$ (1σ). Spectra were recorded at resolutions between 0.009 and 0.03 cm^{-1} (calculated as 0.9/MOPD) over a range of temperatures and pressures (7.6–760 Torr and 188–297 K). This new cross-section dataset greatly expands the number of PT combinations available for air-broadened HFC-32 absorption cross sections, and additionally improves upon the Smith dataset [10] in terms of wavenumber calibration, and the spectral resolution of the low-pressure measurements.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Jeremy J. Harrison: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Writing - original draft,

Writing - review & editing, Visualization, Supervision, Project administration.

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