A reporting format for leaf-level gas exchange data and metadata

Authors

Kim S. Ely[1], Alistair Rogers[1], Deborah A. Agarwal[2], Elizabeth A. Ainsworth[3], Loren Albert[4], Ashehad Ali[5], Jeremiah Anderson[1], Michael J. Aspinwall[6], Chandra Bellasio[7], Carl Bernacchi[3], Steve Bonnage[8], Thomas N. Buckley[9], James Bunce[10], Angela C. Burnett[1], Florian A. Busch[11], Amanda Cavanagh[12], Lucas A. Cernusak[13], Robert Crystal-Ornelas[14], Joan Damerow[14], Kenneth J. Davidson[1], Martin G. De Kauwe[15], Michael C. Dietze[16], Tomas F. Domingues[17], Mirindi Eric Dusenge[18], David S. Ellsworth[19], John R Evans[20], Paul P.G. Gauthier[21], Bruno O. Gimenez[22], Elizabeth P. Gordon[23], Christopher M. Gough[24], Aud H. Halbritter[25], David T. Hanson[26], Mary Heskel[27], J. Aaron Hogan[28], Jason R. Hupp[23], Kolby Jardine[29], Jens Kattge[30], Trevor Keenan[14,31], Johannes Kromdijk[32], Dushan P. Kumarathunge[33], Julien Lamour[1], Andrew D.B. Leakey[34], David S. LeBauer[35], Qianyu Li[1], Marjorie R. Lundgren[36], Nate McDowell[37], Katherine Meacham-Hensold[38], Belinda E. Medlyn[19], David J.P. Moore[39], Robinson Negrón-Juárez[2], Ülo Niinemets[40], Colin P. Osborne[41], Alexandria L. Pivovaroff[42], Hendrik Poorter[43], Sasha C. Reed[44], Youngryel Ryu[45], Alvaro Sanz-Saez[46], Stephanie C. Schmiege[47], Shawn P. Serbin[1], Thomas D. Sharkey[48], Martijn Slot[22], Nicholas G. Smith[49], Balasaheb V. Sonawane[50], Paul F. South[51], Daisy C. Souza[52], Joseph Ronald Stinziano[53], Ellen Stuart-Haëntjens[54], Samuel H. Taylor[36], Mauricio D. Tejera[55], Johan Uddling[18], Vigdis Vandvik[25], Charuleka Varadharajan[14], Anthony P. Walker[56], Berkley J Walker[48,57], Jeffrey M. Warren[56], Danielle A. Way[58], Brett T. Wolfe[59], Jin Wu[60], Stan D. Wullschleger[61], Chonggang Xu[62], Zhengbing Yan[60], Dedi Yang[1]

Corresponding author

Kim S. Ely, kely@bnl.gov

Affiliations

[1]Department of Environmental and Climate Sciences, Brookhaven National Laboratory, Upton, NY 11973, USA, [2]Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA, [3]USDA ARS GCPRU, 1201 W. Gregory Drive, Urbana, IL 61801, USA, [4]Department of Biology, West Virginia University, Morgantown, WV 26506, USA, [5]Department of Bioclimatology, University of Goettingen, Goettingen, Germany, [6]School of Forestry and Wildlife Sciences, Auburn University, Auburn, AL 36849, USA, [7]Research group biology of plants under Mediterranean conditions, Department of Biology, University of Balearic Islands, Cra. de Valldemossa Km 7.5, Palma, 07122, Illes Balears, Spain, [8]ADC Bioscientific Ltd, Global

House, Geddings Road, Hoddesdon, Herts, EN11 0NT UK, [9]Department of Plant Sciences, UC Davis, Davis, CA 95616, USA, [10]USDA-ARS, Adaptive Cropping Systems Laboratory, Beltsville MD 20705, USA, [11]School of Biosciences, University of Birmingham, Birmingham, B15 2TT, UK, [12]School of Life Sciences, University of Essex, Colchester, CO4 3SQ, UK, [13]College of Science and Engineering, James Cook University, Cairns QLD 4879, Australia, [14]Earth and Environmental Sciences Area, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, [15]ARC Centre of Excellence for Climate Extremes, Sydney, NSW 2052, Australia; Climate Change Research Centre, University of New South Wales, Sydney, NSW 2052, Australia; Evolution & Ecology Research Centre, University of New South Wales, Sydney, NSW 2052, Australia, [16]Department of Earth & Environment, Boston University, Boston, MA 02215, USA, [17]Department of Biology, FFCLRP, University of São Paulo, Av. Bandeirantes 3900, 14040-901, Ribeirão Preto, Brazil, [18]Department of Biological and Environmental Sciences, University of Gothenburg, P.O. Box 461, SE-405 30 Gothenburg, Sweden, [19]Hawkesbury Institute for the Environment, Western Sydney University, Locked Bag 1797, Penrith NSW 2751, Australia, [20]Research School of Biology. The Australian National University, Canberra, ACT 2601, Australia, [21]NOAA/Geophysical Fluid Dynamics Laboratory, Princeton, NJ 08540, USA, [22]Smithsonian Tropical Research Institute, Apartado Postal 0843-03092, Panama City, Republic of Panama, [23]LI-COR Biosciences 4647 Superior St Lincoln, NE 68504, USA, [24]Virginia Commonwealth University, Department of Biology, Box 842012, 1000 W. Cary Street, Richmond, VA 23284, USA, [25]Department of Biological Sciences & Bjerknes Centre for Climate Research, University of Bergen, PO Box 7801, N-5020 Bergen, Norway, [26]UNM Biology, MSC03-2020, 219 Yale Blvd, Albuquerque, NM 87131, USA, [27]Department of Biology, Macalester College, 1600 Grand Ave, St Paul, MN 55105 USA, [28]Department of Biological Sciences, Florida International University, Miami, FL 33199, USA, [29]Climate and Ecosystem Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, [30]Max Planck Institute for Biogeochemistry, Hans Knöll Str. 10, 07745 Jena, Germany; German Centre for Integrative Biodiversity Research (iDiv) Halle-Jena-Leipzig, Deutscher Platz 5e, 04103 Leipzig, Germany, [31]Department of Environmental Science, Policy and Management, UC Berkeley, Berkeley, CA 94720, USA, [32]Department of Plant Sciences, University of Cambridge, Downing Street, Cambridge CB23EA, UK, [33]Plant Physiology Division, Coconut Research Institute of Sri Lanka, Lunuwila 61150, Sri Lanka, [34]Departments of Plant Biology and Crop Sciences, University of Illinois at Urbana-Champaign, 1206 W Gregory Dr, Urbana, IL 61801, USA, [35]College of Agriculture and Life Sciences, University of Arizona, Tucson, AZ 85721, USA, [36]Lancaster Environment Centre, Library Avenue, Lancaster University, Lancaster LA1 4YQ UK, [37]Pacific Northwest National Laboratory, PO Box 999, Richland, WA 99352, USA, [38]Carl R. Woese Institute of Genomic Biology, University of Illinois at Urbana-Champaign, 1206 W. Gregory Drive, Urbana, IL 61801, USA, [39]School of Natural Resources and the Environment, University of Arizona, Tucson, AZ 85721, USA, [40]Estonian University of Life Sciences, Kreutzwaldi 1, 51006 Tartu, Estonia, [41]Department of Animal and Plant Sciences, University of Sheffield, Sheffield S7 2NF, UK, [42]Atmospheric Science and Global Change

Division, Pacific Northwest National Laboratory, Richland, WA 99352, USA, [43]Plant Sciences (IBG2), Forschungszentrum Juelich GmbH, Juelich, Germany; Department of Biological Sciences, Macquarie University, North Ryde, NSW 2109, Australia, [44]US Geological Survey, Southwest Biological Science Center, 2290 S. West Resource Blvd, Moab, UT 84532, USA, [45]Department of Landscape Architecture and Rural Systems Engineering, Seoul National University, Seoul, South Korea, [46]Department of Crop, Soil and Environmental Sciences, Auburn University, Auburn, AL 36849, USA, [47]Department of Ecology, Evolution and Environmental Biology, Columbia University, New York, NY 10027, USA, [48]MSU-DOE Plant Research Laboratory, Michigan State University, 612 Wilson Rd, East Lansing, MI 48824, USA, [49]Department of Biological Sciences, Texas Tech University, Lubbock, TX 79409, USA, [50]School of Biological Sciences, Washington State University, Pullman, WA 99164, USA, [51]Department of Biological Sciences, Louisiana State University, Baton Rouge LA 70803, USA, [52]Forest Management Laboratory, National Institute for Amazon Research, Manaus, Amazonas, Brazil, [53]Department of Biology, University of New Mexico, Albuquerque, NM 87131, USA, [54]US Geological Survey, California Water Science Center, 6000 J St, Sacramento, CA 95819, USA, [55]Great Lakes Bioenergy Research Center, Michigan State University, East Lansing, MI, 48824, USA, [56]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, [57]Department of Plant Biology, Michigan State University, East Lansing, MI 48824, USA, [58]Department of Biology, University of Western Ontario, London, ON, N6A 5B7, Canada, [59]School of Renewable Natural Resources, Louisiana State University Agricultural Center, Baton Rouge, LA 70803, USA, [60]School of Biological Sciences, The University of Hong Kong, Pokfulam Road, Hong Kong, [61]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, [62]Earth and Environmental Sciences Division, Los Alamos National Laboratory, NM 87544, USA

Author emails and ORCIDs

Kim S. Ely, kely@bnl.gov, 0000-0002-3915-001X
Alistair Rogers, arogers@bnl.gov, 0000-0001-9262-7430
Deborah A. Agarwal, daagarwal@lbl.gov, 0000-0001-5045-2396
Elizabeth A. Ainsworth, lisa.ainsworth@usda.gov, 0000-0002-3199-8999
Loren Albert, loren.albert@mail.wvu.edu, 0000-0002-9674-6071
Ashehad Ali, ali.ashehad@gmail.com, 0000-0002-7328-306X
Jeremiah Anderson, jeanderson@bnl.gov, 0000-0003-1705-7823
Michael J. Aspinwall, aspinwall@auburn.edu, 0000-0003-0199-2972
Chandra Bellasio, chandra.bellasio@uib.es, 0000-0002-3865-7521
Carl Bernacchi, carl.bernacchi@usda.gov, 0000-0002-2397-425X
Steve Bonnage, sales@adc.co.uk
Thomas N. Buckley, tnbuckley@ucdavis.edu, 0000-0001-7610-7136

James Bunce, buncejames49@gmail.com, 0000-0002-6825-7510
Angela C. Burnett, aburnett@bnl.gov, 0000-0002-2678-9842
Florian A. Busch, f.a.busch@bham.ac.uk, 0000-0001-6912-0156
Amanda Cavanagh , a.cavanagh@essex.ac.uk, 0000-0001-5918-8093
Lucas A. Cernusak, lucas.cernusak@jcu.edu.au, 0000-0002-7575-5526
Robert Crystal-Ornelas, rcrystalornelas@lbl.gov, 0000-0002-6339-1139
Joan Damerow, JoanDamerow@lbl.gov, 0000-0003-2601-5043
Kenneth J. Davidson, kdavidson@bnl.gov, 0000-0001-5745-9689
Martin G. De Kauwe, mdekauwe@gmail.com, 0000-0002-3399-9098
Michael C. Dietze, dietze@bu.edu, 0000-0002-2324-2518
Tomas F. Domingues, tdomingu@gmail.com, 0000-0003-2857-9838
Mirindi Eric Dusenge, mirindi.eric.dusenge@bioenv.gu.se, 0000-0003-4218-0911
David S. Ellsworth, D.Ellsworth@westernsydney.edu.au, 0000-0002-9699-2272
John R Evans, john.evans@anu.edu.au, 0000-0003-1379-3532
Paul PG Gauthier, paul.pg.gauthier@gmail.com, 0000-0002-2893-7861
Bruno O. Gimenez, bruno.oliva.gimenez@gmail.com, 0000-0001-7336-9448
Elizabeth P. Gordon, elizabeth.gordon@licor.com, 0000-0002-5182-0143
Christopher M. Gough, cmgough@vcu.edu, 0000-0002-1227-7731
Aud H. Halbritter, aud.halbritter@uib.no, 0000-0003-2597-6328
David T. Hanson, dthanson@unm.edu, 0000-0003-0964-9335
Mary Heskel, mheskel@macalester.edu, 0000-0003-3227-2978
J. Aaron Hogan , Jamesaaronhogan@gmail.com , 0000-0001-9806-3074
Jason R. Hupp, jason.hupp@licor.com
Kolby Jardine, kjjardine@lbl.gov, 0000-0001-8491-9310
Jens Kattge, jkattge@bgc-jena.mpg.de, 0000-0002-1022-8469
Trevor Keenan, trevorkeenan@berkeley.edu, 0000-0002-3347-0258
Johannes Kromdijk, jk417@cam.ac.uk, 0000-0003-4423-4100
Dushan P. Kumarathunge, dkumarathunge@gmail.com, 0000-0003-1309-4731
Julien Lamour, jlamour@bnl.gov, 0000-0002-4410-507X
Andrew D.B. Leakey, leakey@illinois.edu, 0000-0001-6251-024X
David S. LeBauer, dlebauer@arizona.edu, 0000-0001-7228-053X
Qianyu Li, qli1@bnl.gov, 0000-0002-0627-039X
Marjorie R. Lundgren, m.lundgren@lancaster.ac.uk, 0000-0002-2489-3646
Nate McDowell, nate.mcdowell@pnnl.gov, 0000-0002-2178-2254
Katherine Meacham-Hensold, katmeach@illinois.edu, 0000-0003-1198-5389
Belinda E. Medlyn, b.medlyn@westernsydney.edu.au, 0000-0001-5728-9827
David J.P. Moore, davidjpmoore@email.arizona.edu, 0000-0002-6462-3288
Robinson Negrón-Juárez, robinson.inj@lbl.gov , 0000-0002-4691-2692
Ülo Niinemets, ylo.niinemets@emu.ee, 0000-0002-3078-2192
Colin P. Osborne , c.p.osborne@sheffield.ac.uk, 0000-0002-7423-3718

Alexandria L. Pivovaroff, alexandria.pivovaroff@pnnl.gov, 0000-0002-3104-1900
Hendrik Poorter, h.poorter@fz-juelich.de, 0000-0001-9900-2433
Sasha C. Reed, screed@usgs.gov, 0000-0002-8597-8619
Youngryel Ryu, ryuyr77@gmail.com, 0000-0001-6238-2479
Alvaro Sanz-Saez, sanz@auburn.edu, 0000-0002-7754-4618
Stephanie C. Schmiege, s.schmiege@columbia.edu, 0000-0001-9054-5538
Shawn P. Serbin, sserbin@bnl.gov, 0000-0003-4136-8971
Thomas D. Sharkey, tsharkey@msu.edu, 0000-0002-4423-3223
Martijn Slot, slotm@si.edu, 0000-0002-5558-1792
Nicholas G. Smith, nick.smith@ttu.edu, 0000-0001-7048-4387
Balasaheb V Sonawane, balasahebsonawane@gmail.com, 0000-0001-6539-5179
Paul F. South, pfsouth@lsu.edu, 0000-0001-7885-7096
Daisy C. Souza, daisysouza21@gmail.com, 0000-0001-5522-6494
Joseph Ronald Stinziano, jstinziano@unm.edu, 0000-0002-7628-4201
Ellen Stuart-Haëntjens, egoodrich-stuart@usgs.gov, 0000-0001-9901-7643
Samuel H. Taylor, s.taylor19@lancaster.ac.uk, 0000-0001-9714-0656
Mauricio D. Tejera , mauri@msu.edu, 0000-0003-1698-0501
Johan Uddling, johan.uddling@bioenv.gu.se, 0000-0003-4893-1915
Vigdis Vandvik , vigdis.vandvik@uib.no, 0000-0003-4651-4798
Charuleka Varadharajan, cvaradharajan@lbl.gov, 0000-0002-4142-3224
Anthony P. Walker, walkerap@ornl.gov, 0000-0003-0557-5594
Berkley J Walker, berkley@msu.edu, 0000-0001-5932-6468
Jeffrey M. Warren, warrenjm@ornl.gov, 0000-0002-0680-4697
Danielle A. Way, dway4@uwo.ca, 0000-0003-4801-5319
Brett T. Wolfe, wolfe1@lsu.edu, 0000-0001-7535-045X
Jin Wu, jinwu@hku.hk, 0000-0001-8991-3970
Stan D. Wullschleger, wullschlegsd@ornl.gov, 0000-0002-9869-0446
Chonggang Xu, cxu@lanl.gov, 0000-0002-0937-5744
Zhengbing Yan, zbyan@hku.hk, 0000-0002-5028-8167
Dedi Yang, dediyang@bnl.gov, 0000-0003-1705-7823

A reporting format for leaf-level gas exchange data and metadata

Abstract

Leaf-level gas exchange data support the mechanistic understanding of plant fluxes of carbon and water. These fluxes inform our understanding of ecosystem function, are an important constraint on parameterization of terrestrial biosphere models, are necessary to understand the response of plants to global environmental change, and are integral to efforts to improve crop production. Collection of these data using gas analyzers can be both technically challenging and time consuming, and individual studies generally focus on a small range of species, restricted time periods, or limited geographic regions. The high value of these data is exemplified by the many publications that reuse and synthesize gas exchange data, however the lack of metadata and data reporting conventions make full and efficient use of these data difficult. Here we propose a reporting format for leaf-level gas exchange data and metadata to provide guidance to data contributors on how to store data in repositories to maximize their discoverability, facilitate their efficient reuse, and add value to individual datasets. For data users, the reporting format will better allow data repositories to optimize data search and extraction, and more readily integrate similar data into harmonized synthesis products. The reporting format specifies data table variable naming and unit conventions, as well as metadata characterizing experimental conditions and protocols. For common data types that were the focus of this initial version of the reporting format, i.e., survey measurements, dark respiration, carbon dioxide and light response curves, and parameters derived from those measurements, we took a further step of defining required additional data and metadata that would maximize the potential reuse of those data types. To aid data contributors and the development of data ingest tools by data repositories we provided a translation table comparing the outputs of common gas exchange instruments.

Extensive consultation with data collectors, data users, instrument manufacturers, and data scientists was undertaken in order to ensure that the reporting format met community needs. The reporting format presented here is intended to form a foundation for future development that will incorporate additional data types and variables as gas exchange systems and measurement approaches advance in the future. The reporting format is published in the U.S. Department of Energy's ESS-DIVE data repository, with documentation and future development efforts being maintained in a version control system.

Keywords

Photosynthesis, carbon dioxide, irradiance, data reporting format, metadata, data standard

1. Introduction

The interface between plant and ecological sciences and research data infrastructure is rapidly evolving, with greater expectations for data preservation, reproducible and open research, and the potential to synthesize data across different studies maximizing investments in research. Moreover, publicly accessible data archiving is increasingly required by funding bodies and publishers. Numerous databases and repositories, and other data infrastructure, have been developed to fulfill these needs, including TRY (Kattge et al. 2020), Environmental Data Initiative (environmentaldatainitiative.org), Dryad (datadryad.org), figshare (figshare.com) and DataOne (dataone.org). Yet the reuse of these data resources remains hampered by the difficulty of locating, unifying and assessing the quality of data, and the absence of important metadata needed for inter-site comparison or synthesis. The challenges that must be addressed for data managers to best support scientific discoveries are summarized by the FAIR principles, a call to improve Findability, Accessibility, Interoperability and Reusability of data (Wilkinson et al. 2016).

Leaf-level gas exchange measurements quantify the flux of carbon dioxide (CO_2) and water vapor into and out of a leaf. Typically collected with infrared gas analyzer instruments, these measurements are used to determine a range of physiologically important fluxes and traits, principally the rates of net CO_2 assimilation, respiration and stomatal conductance. Gas exchange data are used to answer a wide variety of scientific questions regarding plant function and response to environmental change (Long et al. 1996; Long and Bernacchi 2003). They are the basis for estimating and scaling photosynthesis from the leaf to canopy (Yang et al. 2020), and are used to parameterize global biogeochemical models (Kattge et al. 2009). The products of photosynthesis are critical to society, as they provide renewable supplies of food, fuel, medicine,

and fiber (Vitousek et al. 1986). Understanding and improving photosynthesis, and water- and nutrient-use efficiencies are currently considered to be key targets to improve the resilience of crops to global change (Ainsworth, et al. 2008; Ort et al. 2015; Leakey et al. 2019; Simkin et al. 2019; López-Calcagno et al. 2020). Furthermore, plants play a critical and unique role in determining the response of the terrestrial biosphere to rising CO_2 concentration and in turn influence the rate of global change (Walker et al. 2020). Analyses have also shown that terrestrial biosphere model outputs are particularly sensitive to parameters derived from gas exchange data (Bonan et al. 2011; Booth et al. 2012; LeBauer et al. 2013; Sargsyan et al. 2014; Ricciuto et al. 2018) and that the use of derived parameters from gas exchange data can effectively constrain uncertainty in model simulations (Dietze et al., 2014). In short, gas exchange data are central to understanding, improving and modelling the response of plants to global and environmental change.

However, collection of these data requires specialist training, is time consuming, can involve elaborate logistics (Weerasinghe et al. 2014; Ellsworth et al. 2012), and often utilizes techniques adapted to particular experiments, instruments and environments. Thus, resulting data products are typical long-tail data, i.e. data are low volume, and have diverse and heterogeneous content, and are thus not easily shared (Wallis et al. 2013; Heidorn 2008). Currently, most data repositories that store diverse data typically focus on describing generic package-level metadata, and not metadata specific to the data type, which limits the use, search and data discovery services for long-tail data types (Limani et al. 2019). Our review of existing data repositories and plant trait databases revealed that where leaf-level gas exchange data are available, the data provided are limited and metadata required to properly interpret and reuse those data are often missing. The need for specialist data standards for disciplines is well recognized (Limani et al.

2019; Bruneau et al. 2019), and the importance of developing standards for the collection and storage of plant trait data has been the subject of several recent studies (Kissling et al. 2018; Schneider et al. 2019; Gallagher et al. 2020). Despite recent increases in compendia of gas exchange data (Lin et al. 2015; Keenan and Niinemets 2016; Kumarathunge et al. 2019; Smith et al. 2019; Niinemets et al. 2015; De Kauwe et al. 2016; Ali et al. 2015), and previous calls for standard archiving (Dietze 2014), there is no standardized reporting format that enables syntheses of these data.

Data archiving is only the first step towards maximizing the value of data. In order to be reused or incorporated into models or synthesis products, data must be both findable and accessible; these characteristics are optimized by appropriate, machine-readable search terms and persistent dataset identifiers. Currently, gas exchange instruments do not share a common output format, i.e., file structure, variable names, and units, and include column headers that are not machine readable. Additionally, reuse is enabled by including sufficient metadata to correctly interpret the data, and use of common formats and terms that allow processing multiple studies from different sites, with various measurement methods (Christianson et al. 2017). Currently, metadata associated with gas exchange data collections are largely limited to location and species (Kattge et al. 2020). Lack of documentation and metadata are recognized as data archiving risk factors (Mayernik et al. 2020), with the implication that without adequate metadata, data cannot be interpreted or used correctly. To reuse data, researchers often have to refer to original publications to access essential metadata or other key information (e.g. leaf temperature), which can be a prohibitively resource-intensive process, or, especially in the case of older work, impossible because information is unavailable. Also, as research data infrastructure moves towards advanced capabilities such as application programming interfaces (APIs) to facilitate

data upload and download, or support for data visualization and analytics, standardization of data and metadata in machine readable formats will become increasingly essential (Bruneau et al. 2019). For example, the Darwin Core standard for biodiversity data has enabled the global integration of hundreds of millions of species occurrence records through the Global Biodiversity Information Facility (GBIF, www.gbif.org), and has facilitated reuse of these data in countless studies (Ball-Damerow et al. 2019). However, specific guidance for leaf-level gas exchange data and metadata is lacking.

Here we present a new data and metadata reporting format for common types of leaf-level gas exchange data, reaching consensus among over 80 researchers in the field. We describe the process of development of these guidelines, for which the aim was to find the balance between maximizing the usefulness of the reporting format to the research community with ease of compliance when a data provider is preparing a new dataset. A key aspect has been engaging the community of leaf-level gas exchange experts in the development of this reporting format, with a concerted effort to reach as many potential data contributors and users as possible. Our goal with this initial focused effort on a leaf-level gas exchange reporting format was to develop a solid foundation for further development that could include a wider range of data types. An important component of this proposed reporting format is the public archive of complete instrument outputs. While we cannot foresee all future data uses or different processing methods, the preservation of the unprocessed instrument output is a way of future-proofing rare and valuable leaf-level gas exchange data sets (Rogers et al. 2017).

The creation of this reporting format for leaf-level gas exchange data was initiated by a call for community accepted data formats for the U.S. Department of Energy’s (DOE) Environmental

Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) data repository (Varadharajan et al. 2019). Accordingly, the reporting format described here is known as the 'ESS-DIVE reporting format for leaf-level gas exchange data and metadata', and referred to in this paper as 'the reporting format'. However, development of the format and documentation has considered global needs for these data. This paper presents a reporting format for leaf-level gas exchange data designed for wide adoption across ecological data repositories, and thus does not describe implementation in a specific repository or database. The reporting format is designed to complement, and not duplicate, other metadata requirements for sites, samples and additional relevant information, and when possible this format should be used in combination with such requirements. For example, in the ESS-DIVE data repository a data submission must also include package-level metadata (e.g. authors, keywords, publication date, spatial and temporal coverage) and sample-level metadata (e.g. sample material, latitude, longitude, elevation, biome). It is encouraged that, where available, this reporting format is used in conjunction with established ontologies, such as Darwin Core (Wieczorek et al. 2012), the Plant Ontology (Cooper et al. 2013) and the Environment Ontology (Buttigieg et al. 2013).

The scope of this reporting format for leaf-level gas exchange focused on defining data and metadata variables to describe the most common type of measurements and those that have been the focus of recent synthesis efforts, i.e. survey style measurements; the response of photosynthesis to CO_2 and irradiance; and parameters derived from these relationships. In this paper we 1) describe the process of developing the format, including review of existing standards and conventions, and community consultation; 2) provide details of the components of the reporting format, including the guidance for data and metadata fields, vocabularies, units and definitions; and 3) discuss challenges to reaching consensus, the future potential to include

additional measurement types and the use of this reporting format as a basis for the development of data management tools.

2. Methods

2.1 Review of existing standards and conventions

2.1.1 Search for published standards

Literature and web resources were searched to identify any published standards guiding best practice for the archive of leaf-level gas exchange data. A list of ecological trait databases was assembled, based on web searches, and a comprehensive table published by Schneider et al. (2019). Of these, databases and repositories identified as containing plant trait data were reviewed to determine if they included leaf-level gas exchange data, and if submission of data required adherence to any standards or formats (Supplementary Tables 1 & 2). A catalog of over 1400 data standards, including 17 categorized as concerning physiology, available at FAIRsharing (Sansone et al. 2019), was searched for standards that define variable names and metadata terms required to describe leaf-level gas exchange data.

2.1.2 Variable names and definitions

Existing data repositories, databases and synthesized datasets were reviewed, and the most commonly used variable terms and definitions were adopted into this reporting format (Supplementary Tables 1–3). The TRY plant trait database (Kattge et al. 2020) was identified as the most extensive publicly available plant trait database that contains leaf-level gas exchange data. Variable definitions in TRY are adopted from TOP, a thesaurus of plant characteristics (Garnier et al. 2017). Several relevant variables are included in BETYdb, the biofuel ecophysiological traits and yields database (LeBauer et al. 2018). Another resource for

measurement variable definitions are several published guides to standard measurement protocols, including ClimEx (Halbritter et al. 2020), the Plant Handbook (Pérez-Harguindeguy et al. 2013) and PrometheusWiki (Sack et al. 2010; Evans and Santiago 2014). The use of variable names in the large datasets including GlobResp (Atkin et al. 2015) and GlobAmax (Maire et al. 2015) were also considered. The default output from ten commercially available gas exchange instruments (manufactured by ADC Bioscientific, CID-Bioscience, LI-COR Biosciences, PP Systems and Walz; Supplementary Table 4) was assembled into a translation table to allow comparison and identify commonalities. Each variable was defined with a name, unit and description, and in some cases, an expected value range.

2.1.3 Metadata requirements

Many data repositories have existing metadata requirements to cover general experimental and sample parameters, such as characteristics of the location where measurements were conducted. Here we identified specific metadata parameters that would allow users of leaf-level gas exchange data to discriminate between data types, experimental protocols, and sample characteristics. We chose variables based on our collective expertise of conducting gas exchange measurements across diverse ecosystems and experimental designs, and of using those data in syntheses and meta-analysis. Our goal was to include metadata requirements for variables that would be most relevant for synthesis activities, including variables to distinguish data obtained from natural or cultivated plants, and to differentiate between common experimental manipulations and leaf sampling techniques. Controlled vocabularies—lists of preferred terms—were developed for each metadata variable to allow consistent metadata reporting. The selection of required metadata variables sought to find a balance between optimizing data discoverability and usability, while at the same time not placing undue burden on data contributors.

2.2 Community consultation

The draft reporting format was made available to the community of leaf-level gas exchange experts for suggestions and comment. Input was sought from data contributors, data scientists, data users, and instrument manufacturers. The invitation to participate was sent via direct email to 120 contacts, and reached a wider (unquantified) audience through encouraged sharing of the invitation to participate and social media. The development of this data reporting format was very well received by the community; eighty individuals contributed to the reporting format documentation, and thus this paper (Supplementary Figure S1).

An introduction to the purpose, structure and components of the reporting format was presented as a publicly accessible webinar hosted by ESS-DIVE in July 2020, followed by a month-long period of feedback and discussion. Follow up video conferences were scheduled to discuss refinements and solutions. Feedback was gathered in an open manner, with comments and suggestions available to view by all on a collaborative online document. The reporting format documentation was then migrated to a public GitHub repository, where additions and refinements can continue to be made, and version controlled releases will be freely available for use.

3. Results

There are a number of common conventions in use for reporting of leaf-level gas exchange data, however they are not universal, and our search did not discover any published standards for data reporting. This directed our efforts into the development of a new metadata and data reporting format to enable diverse data contributors to use unified terminologies and formats when publishing data, thus lowering the barrier for data reuse and harmonization. The range of

measurements that can be made with gas exchange instruments is broad. We have developed the foundation for a common reporting format by reaching consensus on a list of standard variable names and units for data tables, and metadata elements specific to leaf-level gas exchange measurements. Further guidance for data and metadata content is also proposed for data types that are commonly measured: survey style gas exchange measurements, dark adapted respiration measurements, CO_2 and light response curves, and parameters derived from those response curves.

The reporting format documentation comprises a number of elements relevant to all types of leaf-level gas exchange measurements; a list of variable names and units (Section 3.1) that should be used in data tables, a translation table of data outputs from commercial gas exchange instruments (Section 3.1.1) and comprehensive metadata requirements with controlled vocabularies (Section 3.2). For selected data types (Section 3.3), the reporting format also specifies the minimum required variables to be included in the data table, and a list of details to be included in the measurement protocol description. Each of these elements is described in more detail in the sections below. The reporting format templates and complete documentation is available for download from the ESS-DIVE repository (Ely et al, 2020) and an example data package following the reporting format guidelines is hosted on the NGEE-Arctic data archive (Rogers et al, 2019).

Here we use the term ‘data package’ to refer to a collection of data and metadata files to be published together in a data repository (Christianson et al. 2017). A data package of gas exchange data should contain formatted data tables, metadata tables and the complete instrument output. Any data package may also include additional data types and variables not yet covered by

the reporting format. Data packages should also include general metadata as required by the hosting data repository or database (e.g. author list and other citation information, data licensing terms). Figure 1 shows the relationship between the components of a data package and definition tables included in the reporting format documentation.

The documentation includes user guides and templates to present the methods metadata and instrument details. Data and metadata tables should be in comma separated value (.csv) format; additional materials can be also included as text if appropriate. All components of a data package should be in English language; other language translations can be included as an additional resource.

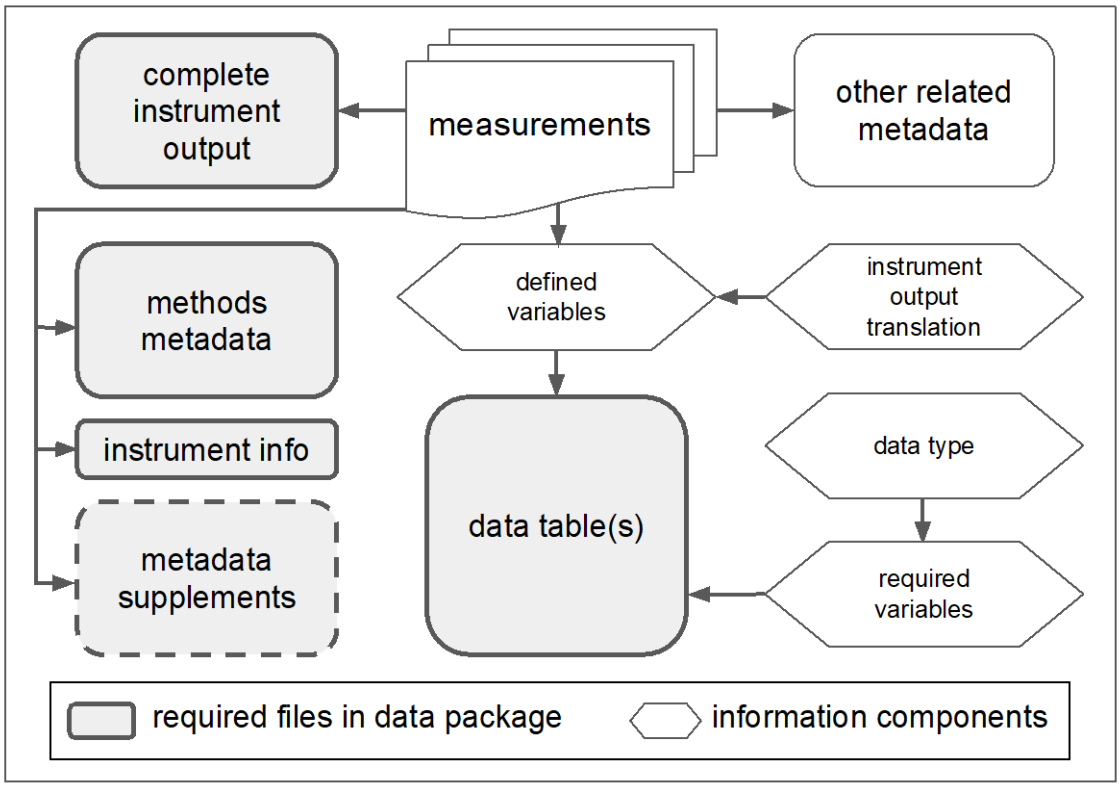

Figure 1. The relationships between gas exchange measurements and the components of this data and metadata reporting format. The characteristics of the 'measurements' (experimental design and recording of information) inform the content of metadata and data tables. Components shown in boxes should be included in a data package. Data tables, methods metadata, instrument details and the complete instrument output (if available) are required to be included in a data package (grey boxes with solid borders). Inclusion of metadata supplement tables will be dependent on the experiment (grey box with dashed border). The requirements for other related metadata (white box) could be set by a data repository, or be mandated by other specialist data standards or conventions; those details are not covered by this reporting format. Information components (hexagons) are reference tables to guide the format and content

requirements of the submitted data. Refer to the reporting format documentation for a complete list of variables, definitions and controlled vocabularies (Ely et al, 2020).

3.1 Variable names and unit specifications

Consistent use of variable names (also known as field names or headers) in data tables is a key element of generating standardized datasets that can be readily combined or imported into a database. A list of variables, including measured and calculated instrument outputs, calculated parameters, and constants, were designated as *variableName*, *variableUnit* and *variableDefinition* in the defined variables table. Note that the *camelCase* naming used here indicates variables defined in the reporting format documentation. These conventions for variables were reached based on the most common usage in existing publications, databases and instrument outputs. In cases where common usage had not already been established, *variableNames* were selected to be human and machine readable, and with no recognized conflicts with other uses. The units for each variable are listed separately, and are not included as part of the *variableName*. The measurement quantities are described in each *variableDefinition*, thus *variableUnits* are presented without information about the quantity, following NIST guidelines (Thompson & Taylor, 2008). For many *variableNames*, the reporting format also specifies an expected range of values resulting from common measurement approaches; these limits can be used to guide quality checking of data.

3.1.1 Instrument output translation table

A translation table of 23 measured and calculated output variables from ten commercially available gas exchange instruments (Supplementary Table 4) was compiled to assess the most common variable names and measurement units, and provided input into the process of defining

the variables for this reporting format. It was found that there is some variation among the output of different instruments, in both variable names and units used, and thus the default instrument outputs are not always exactly aligned with the proposed reporting format. For example, measurement of photosynthetic flux density (PPFD) incident on the leaf is variously labeled as Q, Qleaf, Qin, PAR, PARi or PARtop across the different instruments. The instrument output translation table provides a guide for conversion of results to standard *variableNames* and *variableUnits*, can assist data users to understand instrument output from unfamiliar instruments, and be used for future advances such as the development of automated tools for data upload. This compilation was based on current instrument manuals and software versions; users should note that future instrument and software updates may change the outputs. It is emphasized that re-labeling and conversion of variable names and units to match the format is not a requirement for the complete instrument output files.

3.2 Metadata

All published data packages that use this reporting format should include metadata to ensure that data are adequately described, in order to allow users to fully understand how the data were generated, and maximize findability of data with certain characteristics. The reporting format provides controlled vocabularies and template files for the required methods metadata (Section 3.2.1) and instrument details (Section 3.2.2). The inclusion of methods supplement tables (Section 3.2.3) and other related metadata (Section 3.2.4) will depend on the design of individual experiments; thus for these items the reporting format provides guidelines and recommendations only.

3.2.1 Methods metadata

The methods metadata is a record of data types, measurement protocols, experimental and sample characteristics, and details of data processing and calculation approaches, summarized in a single file. The reporting format includes a template file and controlled vocabularies to simplify metadata creation and ensure consistency across datasets. However, the diversity of experimental approaches is recognized, and flexibility is accommodated by allowing use of free text for many variables if the controlled vocabulary is not adequate.

Development of the methods metadata focused on important search filters for data users such as the growth conditions and treatments of the plants on which measurements were made; these should be indicated using the *growthEnvironment* and *experimentalManipulation* variables. For example, the *growthEnvironment* variable captures if the plants were grown in natural or controlled environments, while *experimentalManipulation* can be employed by data users to include or exclude common treatments such as atmospheric, water or nutrient manipulation. Further categorization is enabled by use of variables such as *canopyPosition*, *lightExposure*, *leafAge* and *plantAge*.

3.2.2 Instrumentation details

This data reporting format provides a template to record details of the instruments used for data collection, including model information, software version, type of chamber used, and a statement of instrument calibration. This will enable users of data to understand the data provenance, and achieve data equivalency in synthesis products.

3.2.3 Methods supplement tables

Leaf-level gas exchange data are often measured with the purpose of comparing between sample types or treatments; these discriminators are commonly included in data tables as codes to represent species, treatments, plots or other characteristics. The methods supplement tables component of this reporting format demonstrates how the explanation of these descriptors should be included in a data package with a range of examples. Inclusion of metadata supplements in a data package is highly dependent on the nature of the experiment, and as such, examples are provided as guidelines only and are not required by the reporting format.

3.2.4 Other related data and metadata

Gas exchange data are frequently associated with other measurements, e.g. leaf nitrogen content. We strongly encourage the use of unique, persistent sample identifiers to link gas exchange data and other data and metadata associated with the same sample. The unique sample identifier should be a column in the data file. Also, in simple cases associated data could be included as additional variables (i.e. columns) in a gas exchange data table and where data are collected in-line with gas exchange, e.g. fluorescence, logically they should be included in the same file. In cases where a *variableName* is not defined by this reporting format, data providers should follow other appropriate standards or conventions. Similarly, for experimental data not covered by the methods metadata variables, such as reporting of environmental, landscape, or climatic characteristics, or genotype variation, data providers should utilize published standards or formats for that data type. Metadata associated with the sample collection (e.g. location information, sample description) can be provided separately using a file that conforms to recognized sample reporting formats (e.g. Damerow et al 2020, Damerow et al in review).

3.3 Specific requirements for selected data types

Additional reporting guidelines are provided for seven data types identified as common gas exchange measurements (e.g. photosynthetic CO_2 response curves) and analytical approaches (e.g. one-point method) (Table 1). For each of these data types the reporting format includes a detailed description of the data type, a list of elements required in the protocol description, and the minimum required variables to include in the data table. For data types not described here, data creators should use a protocol and minimum variable requirements as judged appropriate for their data.

For each data type, a list of 5–8 required variables was developed in order to capture the result variable (e.g. V_{cmax}) and covariates required to interpret that result in context. Of the existing standards and databases reviewed, only the BETYdb specifies any required or optional covariates (LeBauer et al. 2018). Thus the minimum required variables presented in this reporting format are the result of an iterative feedback process involving both domain expert contributors and users. Data contributors may also include any other variables, using the *variableNames* defined in this reporting format. The data table should also include the sample identifier, and other sample variables (e.g. species, treatment) as required.

Table 1

The data types for which this reporting format makes specific recommendations for variables required in the data table, and protocol descriptions. Refer to the reporting format documentation for a detailed description of each data type.

Data type	Description
Survey	Single point measurement of leaf gas exchange.

Response of photosynthesis to intercellular CO_2 concentration (AC_i curves)	Sequential measurements on the same leaf material of photosynthetic rate with varying CO_2 concentration.
Photosynthetic parameters derived from AC_i curves	Results of fitting photosynthetic CO_2 response curves to derive parameters, e.g. apparent V_{cmax}, J_{max}, TPU.
V_{cmax} from one-point	Apparent V_{cmax} calculated from A_{sat} measurements using the one-point method.
Response of photosynthesis to irradiance (*AQ* curves)	Sequential measurements on the same leaf material of photosynthetic rate with varying irradiance.
Photosynthetic parameters derived from *AQ* curves	Results of fitting light response curves to derive parameters, e.g. quantum yield of CO_2 fixation.
Dark adapted respiration	Respiration rate of a dark adapted leaf.

3.4 Inclusion of instrument output data

The methods metadata and required variables are designed to capture adequate information to allow proper interpretation of datasets. However, not all possible data reuse can be foreseen. The inclusion of the complete instrument output (commonly referred to as ‘raw data’) in a data package is seen as the ultimate future-proofing for a dataset (Figure 1). Archiving of raw gas exchange data is recognized as good science practice and has been highlighted as important for the preservation and reuse of data (Dietze et al. 2014; Rogers et al. 2017). Ideally we would like to mandate archiving of quality controlled complete instrument output to allow reanalysis of highly valuable datasets as new knowledge, analytical approaches or data corrections are developed. The term ‘complete instrument output’ is used here to recognize that instrument data files with some quality control applied, such as correction of user input errors, are generally more valuable to data users than true raw data. However, this ideal has to be balanced by the need to ensure we do not create a barrier for data submission, particularly for older data sets where complete instrument output may no longer be available, or for data collected with custom built gas exchange systems.

4. Discussion

We have developed a reporting format for leaf-level gas exchange data and metadata with the goal of improving findability and the capacity to reuse these valuable data (Ely et al, 2020). This reporting format will be adopted by the ESS-DIVE data repository and be freely available to the community. We encourage its use by all data producers, repositories and databases. More than eighty data contributors, data users, manufacturers and data scientists contributed to the development of this effort, which we hope will form a foundation for future development by the community. The reporting format aims to provide a resource for data contributors to enhance the value of their data, reduce the overheads to re-using and synthesizing data, and provide prescribed metadata that will simplify parsing of data for analysis and synthesis (Figure 2).

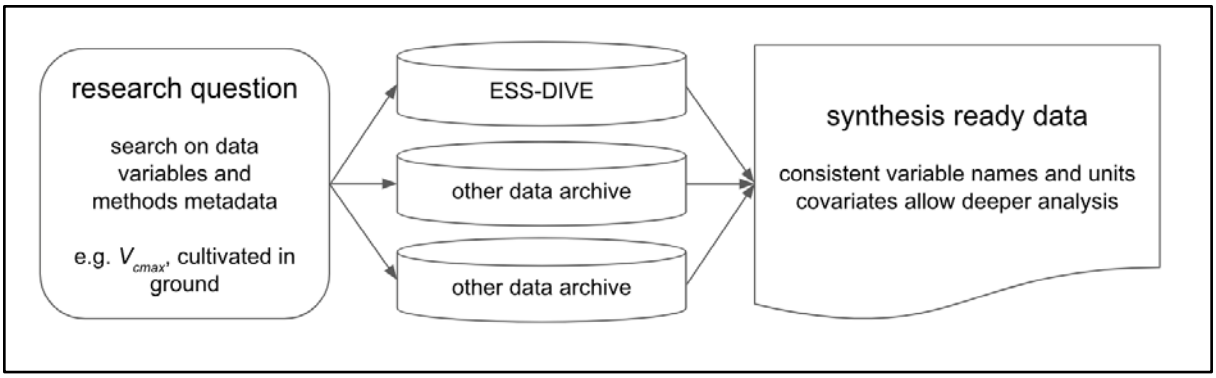

Figure 2. Schematic showing how the implementation of this data reporting format across data archives will facilitate data discovery and reuse.

4.1 Development of a community standard

Given the importance of gas exchange data, the effort taken to collect it, and the widespread use of gas exchange data in synthesis activities and model parameterization, it was surprising that a data standard did not yet exist. However, the need and desire for the development of a common reporting format was readily apparent. Both data contributors and data users were very supportive of the effort, were quick to contribute, and provided valuable input.

Data reporting formats, and the mandate by funding agencies to use them, burden the data contributor with the task of preparing and uploading their data. In contrast, the data user is hopefully relieved of the burden associated with finding and harmonizing datasets prior to analysis. Therefore there is a perception that data reporting formats and preservation of data in a repository offer little direct return for the contributor's effort. However, whilst not readily tangible, there are several benefits to contributors. These include the provision of a formal way to meet mandates for data preservation, defined data descriptions and units, and tools for data quality control (e.g. expected data ranges). Widespread adoption of a data reporting format will

also accelerate the development of data ingest tools that will benefit the contributor. Furthermore, sharing of data in an accessible and searchable format increases the impact of their data collection, jump-starts collaborations, and, with conscientious data users, can lead to invitations to co-author novel data syntheses where data contributors can share knowledge of their data and also gain additional insight from their collaborators (Allen and Mehler 2019; Cheruvelil and Soranno 2018). One issue that remains challenging for the field is formal recognition of datasets through citations and ensuring the continued recognition of a given contribution. For example, if the original dataset is combined with other data into a larger dataset the original association with the data contributor can be lost.

While a formal data format had not existed before we started this work, the vocabulary of leaf-level gas exchange was well established and was fairly similar across instruments. Therefore, incorporating many variables and definitions that are already in widespread use resulted in large parts of the reporting format being readily accepted by the community. Most feedback was focused on additional components, and fine tuning of definitions, rather than large changes to the first draft proposal. It was necessary to provide precise descriptive information to clearly communicate our goal of developing a data reporting format; in some instances this goal was conflated with documentation of measurement protocols, defining a gold standard method or building a database. The data reporting format does not attempt to constrain method choice by data contributors but is intended to be inclusive of all approaches and methodologies. However, there were several issues that garnered significant commentary and these are discussed further below.

4.2 Decisions and compromises

As expected there was a necessary compromise between the desire for additional metadata detail and the need for a relatively simple and manageable reporting format for data contributors. Many of the requests for increased metadata would increase the effort, and therefore the barrier, to format data for some contributors whilst providing only limited value for most data users. Experimental and sample details that are not covered by the methods metadata variables may be included in protocol descriptions or methods supplement tables. While not yet providing specific formats for data, methods metadata variables have been included to indicate the inclusion of canopy height information and additional data collected in-line with gas exchange. There are no restrictions preventing conscientious data contributors from including more metadata detail or data types. Similarly, when developing the required variables for each data type we resisted adding requirements for variables that are not essential to effectively reuse the data. We hope that by strongly encouraging (and perhaps, in time, mandating) the submission of complete instrument output we will preserve all data fields for the specialist data user, and for future, currently unanticipated uses of the data.

There were several comments about missing measurement types; in many cases this reflected the desire to expand the reporting format to cover more data types, e.g. temperature and vapor pressure deficit response curves, or porometer measurements of stomatal conductance. The combination of fluorescence with gas exchange data is very powerful and many instruments allow simultaneous collection of both data types. Whilst we recognize the value of including fluorescence data, developing common reporting formats for these data would have significantly expanded the scope of this initial effort. Development of a common data reporting format for fluorescence data presents some additional challenges, since these data are not always associated

with gas exchange data, they can be collected with a wider variety of instruments, and the vocabulary and protocols used are not as constrained as for gas exchange measurements (Baker 2008; Maxwell and Johnson 2000; Murchie and Lawson 2013).

Estimates of photosynthetic parameters derived from the response of photosynthesis to intercellular CO_2 concentration (C_i) provide apparent estimates of those parameters, i.e. the estimate assumes an infinite mesophyll conductance (g_m) and C_i is assumed to be equal to the CO_2 concentration inside the chloroplast (C_c)—the site of carboxylation. Whilst g_m and hence C_c can be estimated from gas exchange data (Sharkey et al. 2007; Ethier and Livingston 2004), the most robust approaches require in-line measurements of fluorescence or isotopic descrimination (Evans et al. 1986; von Caemmerer and Evans 1991; Bongi and Loreto 1989; Harley et al. 1992; Loreto et al. 1992; Busch et al. 2020). Estimates of photosynthetic parameters based on C_c are different from those that do not account for g_m, and the data can be used in different ways, so it is important to distinguish which data (C_i or C_c), were used to calculate the derived parameters. Additionally, for the specialist data user, knowledge of additional fluorescence or isotopic discrimination data collected in parallel with gas exchange data would be valuable. Therefore we added methods metadata requirements for photosynthetic CO_2 response data to capture assumptions about g_m and indicate the presence of additional data in the data package.

Specialist approaches of gas exchange measurements mean that equivalence cannot be assumed between different studies, even within the same lab, as protocols are adjusted for individual experiments, depending on species measured, ambient environmental conditions, and the experimental goals. The methods metadata categories have been defined to allow equivalency

between data sets to be recognized, and provide the required information to recalculate if necessary. Similarly, calculations of parameters such as maximum carboxylation capacity (V_{cmax}) are dependent on fitting approaches (Gu et al. 2010; Sharkey et al. 2007; Bernacchi et al. 2013), the choice of kinetic constants (Rogers et al. 2017), inclusion of mesophyll conductance (Warren 2006; Ethier and Livingston 2004) and whether and how investigators applied corrections for gasket diffusion leaks (Flexas et al. 2007; Rodeghiero et al. 2007). In some cases, capturing these metadata can enable data users to recalculate derived parameters using a common approach (e.g., Niinemets et al. 2015). Ideally data users should recalculate derived parameters from the underlying data.

4.3 Future developments

Development of this data reporting format highlighted the strong desire by the community for additional functionality to be added to repositories to aid data ingestion, search and compilation. For example, tools that would reduce the burden of curating instrument output files, enable data validation during upload, and enable full search and compilation of all measured and calculated instrument output variables. Whilst the creation of such tools is out of the scope of developing a data reporting format we considered these needs in our decision making processes. For example, we have provided an instrument output translation table that provides a column by column comparison of default output from commercially available gas exchange systems, have created and defined a machine readable vocabulary, defined units, and provided expected ranges for commonly measured variables that can aid validation and curation. Furthermore, we have mandated that data are published using a single non-proprietary file format (.csv) further reducing the challenge for long-term archival and cyberinfrastructure tool development.

To aid long-term development, the reporting format will be a dynamic document hosted as a public repository on GitHub, a version control platform (https://github.com/ess-dive-community/essdive-leaf-gas-exchange). This platform will allow the user community to flag issues, make suggestions, discuss amendments, and prioritize development of the reporting format, all in the open so the community can understand the motivation behind development and contribute to decision making. The published reporting format can be revised with minor edits, ensuring users can easily access the latest update. Contributors on the GitHub platform could also facilitate more substantial changes, such as the addition of new data types, leading to publication of a new version of this reporting format in the future.

We hope that widespread adoption of this first data reporting format for leaf-level gas exchange data will increase the preservation and reuse of these valuable, and hard won, data sets and elevate the importance of data storage in the mindset of data contributors. We also hope that this work will form the cornerstone for a more comprehensive effort by the community to expand and develop the reporting format, including expansion to include full consideration of additional data types that were beyond the initial scope of this effort.

CRediT author statement

Kim S. Ely and Alistair Rogers: Conceptualization, Investigation, Writing - Original draft preparation. All authors: Writing - Reviewing and Editing,

Acknowledgements

KSE and AR were supported by Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) community funds, through the Office of Biological and

Environmental Research in the Department of Energy, Office of Science. Further support was received from several additional projects funded by the Office of Biological and Environmental Research, including the Next Generation Ecosystem Experiments -Arctic (NGEE-Arctic) and -Tropics (NGEE-Tropics) projects and through the United States Department of Energy contracts No. DE-SC0012704, DE-AC02-05CH11231, and DE-AC05-00OR22725 to Brookhaven National Laboratory, Lawrence Berkeley National Laboratory, and Oak Ridge National Laboratory. In addition, ASS was supported by Alabama Agricultural Experiment Station and the Hatch program of the National Institute of Food and Agriculture, U.S. Department of Agriculture; BJW was supported by the Division of Chemical Sciences, Geosciences and Biosciences, Office of Basic Energy Sciences of the United States Department of Energy [Grant DE-FG02-91ER20021];JK was supported by the Biotechnology and Biological Sciences Research Council UK, grant reference BB/T007583/1; MJA was supported by the U.S. Department of Agriculture - National Institute of Food and Agriculture (Award number: 2019-67013-29161).

Supplementary materials

Supplementary figure S1, Supplementary tables S1 – S4

Full documentation of the reporting format is available on GitHub at the following links:

GitHub https://github.com/ess-dive-community/essdive-leaf-gas-exchange

GitBook (GitHub content in a user friendly webpage format) https://ess-dive.gitbook.io/leaf-level-gas-exchange/

References

Ainsworth, Elizabeth A., Alistair Rogers, and Andrew D. B. Leakey. 2008. "Targets for Crop Biotechnology in a Future High-CO2 and High-O3 World." *Plant Physiology*. https://doi.org/10.1104/pp.108.117101.

Ali, Ashehad A., Chonggang Xu, Alistair Rogers, Nathan G. McDowell, Belinda E. Medlyn, Rosie A. Fisher, Stan D. Wullschleger, et al. 2015. "Global-Scale Environmental Control of Plant Photosynthetic Capacity." *Ecological Applications*. https://doi.org/10.1890/14-2111.1.

Allen, Christopher, and David M. A. Mehler. 2019. "Open Science Challenges, Benefits and Tips in Early Career and beyond." *PLoS Biology* 17 (5): e3000246. https://doi.org/10.1371/journal.pbio.3000246.

Atkin, Owen K., Keith J. Bloomfield, Peter B. Reich, Mark G. Tjoelker, Gregory P. Asner, Damien Bonal, Gerhard Bönisch, et al. 2015. "Global Variability in Leaf Respiration in Relation to Climate, Plant Functional Types and Leaf Traits." *The New Phytologist* 206 (2): 614–36. https://doi.org/10.1111/nph.13253.

Baker, Neil R. 2008. Chlorophyll Fluorescence: A Probe of Photosynthesis *In Vivo Annual Review of Plant Biology* 59:1, 89-113. https://doi.org/10.1146/annurev.arplant.59.032607.092759

Ball-Damerow, Joan E., Laura Brenskelle, Narayani Barve, Pamela S. Soltis, Petra Sierwald, Rüdiger Bieler, Raphael LaFrance, Arturo H. Ariño, and Robert P. Guralnick. 2019. "Research Applications of Primary Biodiversity Databases in the Digital Age." *PloS One* 14 (9): e0215794. https://doi.org/10.1371/journal.pone.0215794.

Bernacchi, Carl J., Justin E. Bagley, Shawn P. Serbin, Ursula M. Ruiz-Vera, David M. Rosenthal, and Andy Vanloocke. 2013. "Modelling C_3 Photosynthesis from the Chloroplast to the Ecosystem." *Plant, Cell & Environment* 36 (9): 1641–57. https://doi.org/10.1111/pce.12118.

Bonan, Gordon B., Peter J. Lawrence, Keith W. Oleson, Samuel Levis, Martin Jung, Markus Reichstein, David M. Lawrence, and Sean C. Swenson. 2011. "Improving Canopy Processes in the Community Land Model Version 4 (CLM4) Using Global Flux Fields Empirically Inferred from FLUXNET Data." *Journal of Geophysical Research*. https://doi.org/10.1029/2010jg001593.

Bongi, G., and F. Loreto. 1989. "Gas-Exchange Properties of Salt-Stressed Olive (Olea Europea L.) Leaves." *Plant Physiology* 90 (4): 1408–16. https://doi.org/10.1104/pp.90.4.1408.

Booth, Ben B. B., Chris D. Jones, Mat Collins, Ian J. Totterdell, Peter M. Cox, Stephen Sitch, Chris Huntingford, Richard A. Betts, Glen R. Harris, and Jon Lloyd. 2012. "High Sensitivity of Future Global Warming to Land Carbon Cycle Processes." *Environmental Research Letters: ERL [Web Site]* 7 (2): 024002. https://doi.org/10.1088/1748-9326/7/2/024002.

Bruneau, Anne, Leonardo M. Borges, Robert Allkin, Ashley N. Egan, Manuel de la Estrella, Firouzeh Javadi, Bente Klitgaard, et al. 2019. "Towards a New Online Species-Information System for Legumes." *Australian Systematic Botany* 53: 1.

https://doi.org/10.1071/SB19025.

Busch, Florian A., Meisha Holloway-Phillips, Hilary Stuart-Williams, and Graham D. Farquhar. 2020. "Revisiting Carbon Isotope Discrimination in C Plants Shows Respiration Rules When Photosynthesis Is Low." *Nature Plants* 6 (3): 245–58. https://doi.org/10.1038/s41477-020-0606-6.

Buttigieg, Pier Luigi, Norman Morrison, Barry Smith, Christopher J. Mungall, Suzanna E. Lewis, and ENVO Consortium. 2013. "The Environment Ontology: Contextualising Biological and Biomedical Entities." *Journal of Biomedical Semantics* 4 (1): 43. https://doi.org/10.1186/2041-1480-4-43.

Cheruvelil, Kendra Spence, and Patricia A. Soranno. 2018. "Data-Intensive Ecological Research Is Catalyzed by Open Science and Team Science." *Bioscience* 68 (10): 813–22. https://doi.org/10.1093/biosci/biy097.

Christianson, Danielle S., Charuleka Varadharajan, Bradley Christoffersen, Matteo Detto, Boris Faybishenko, Bruno O. Gimenez, Val Hendrix, et al. 2017. "A Metadata Reporting Framework (FRAMES) for Synthesis of Ecohydrological Observations." *Ecological Informatics* 42 (November): 148–58. https://doi.org/10.1016/j.ecoinf.2017.06.002.

Cooper, Laurel, Ramona L. Walls, Justin Elser, Maria A. Gandolfo, Dennis W. Stevenson, Barry Smith, Justin Preece, et al. 2013. "The Plant Ontology as a Tool for Comparative Plant Anatomy and Genomic Analyses." *Plant & Cell Physiology* 54 (2): e1. https://doi.org/10.1093/pcp/pcs163.

Damerow J, Varadharajan C, Boye K, Brodie E, Chadwick D, Cholia S, Elbashandy H, Ely K, Goldman A, Hendrix V, Jones C, Jones M, Kakalia Z, Kemner K, Kersting A, Maher K, Merino N, O'Brien F, Perzan Z, Robles E , Snavely C, Sorensen P, Stegen J , Weisenhorn P, Whitenack K, Zavarin M , Agarwal D, 2020. "Sample Identifiers and Metadata Reporting Format for Environmental Systems Science". *Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE).* doi:10.15485/1660470

Damerow J, Varadharajan C, Boye K, Brodie E, Chadwick D, Cholia S, Elbashandy H, Ely K, Goldman A, Hendrix V, Jones C, Jones M, Kakalia Z, Kemner K, Kersting A, Maher K, Merino N, O'Brien F, Perzan Z, Robles E , Snavely C, Sorensen P, Stegen J , Weisenhorn P, Whitenack K, Zavarin M , Agarwal D (In Review). "Standardizing sample information to support efficient sample tracking, data integration, and reuse in Environmental Systems Science." *Data Science Journal.*

De Kauwe, Martin G., Yan-Shih Lin, Ian J. Wright, Belinda E. Medlyn, Kristine Y. Crous, David S. Ellsworth, Vincent Maire, et al. 2016. "A Test of the 'One-Point Method' for Estimating Maximum Carboxylation Capacity from Field-Measured, Light-Saturated Photosynthesis." *The New Phytologist* 210 (3): 1130–44. https://doi.org/10.1111/nph.13815.

Dietze, Michael C. 2014. "Gaps in Knowledge and Data Driving Uncertainty in Models of Photosynthesis." *Photosynthesis Research* 119 (1-2): 3–14. https://doi.org/10.1007/s11120-013-9836-z.

Ellsworth, David S., Richard Thomas, Kristine Y. Crous, Sari Palmroth, Eric Ward, Chris Maier, Evan DeLucia, and Ram Oren. 2012. "Elevated CO2 Affects Photosynthetic Responses

in Canopy Pine and Subcanopy Deciduous Trees over 10 Years: A Synthesis from Duke FACE." *Global Change Biology*. https://doi.org/10.1111/j.1365-2486.2011.02505.x.

Ethier, G. J., and N. J. Livingston. 2004. "On the Need to Incorporate Sensitivity to CO2 Transfer Conductance into the Farquhar-von Caemmerer-Berry Leaf Photosynthesis Model." *Plant, Cell and Environment*. https://doi.org/10.1111/j.1365-3040.2004.01140.x.

Ely K.S., Rogers A, Crystal-Ornelas R (2020): ESS-DIVE reporting format for leaf-level gas exchange data and metadata. Environmental Systems Science Data Infrastructure for a Virtual Ecosystem. doi:10.15485/1659484

Evans, John R., and Louis S. Santiago. 2014. "PrometheusWiki Gold Leaf Protocol: Gas Exchange Using LI-COR 6400." *Functional Plant Biology: FPB* 41 (3): 223–26. https://doi.org/10.1071/FP10900.

Evans, J. R., T. D. Sharkey, J. A. Berry, and G. D. Farquhar. 1986. "Carbon Isotope Discrimination Measured Concurrently with Gas Exchange to Investigate CO2 Diffusion in Leaves of Higher Plants." *Functional Plant Biology: FPB* 13 (2): 281. https://doi.org/10.1071/PP9860281.

Flexas, J., A. Díaz-Espejo, J. A. Berry, J. Cifre, J. Galmés, R. Kaldenhoff, H. Medrano, and M. Ribas-Carbó. 2007. "Analysis of Leakage in IRGA's Leaf Chambers of Open Gas Exchange Systems: Quantification and Its Effects in Photosynthesis Parameterization." *Journal of Experimental Botany* 58 (6): 1533–43. https://doi.org/10.1093/jxb/erm027.

Gallagher, Rachael V., Daniel S. Falster, Brian S. Maitner, Roberto Salguero-Gómez, Vigdis Vandvik, William D. Pearse, Florian D. Schneider, et al. 2020. "Open Science Principles for Accelerating Trait-Based Science across the Tree of Life." *Nature Ecology & Evolution* 4 (3): 294–303. https://doi.org/10.1038/s41559-020-1109-6.

Garnier, Eric, Ulrike Stahl, Marie-Angélique Laporte, Jens Kattge, Isabelle Mougenot, Ingolf Kühn, Baptiste Laporte, et al. 2017. "Towards a Thesaurus of Plant Characteristics: An Ecological Contribution." *The Journal of Ecology* 105 (2): 298–309. https://doi.org/10.1111/1365-2745.12698.

Gu, Lianhong, Stephen G. Pallardy, Kevin Tu, Beverly E. Law, and Stan D. Wullschleger. 2010. "Reliable Estimation of Biochemical Parameters from C3 Leaf Photosynthesis-Intercellular Carbon Dioxide Response Curves." *Plant, Cell & Environment*. https://doi.org/10.1111/j.1365-3040.2010.02192.x.

Halbritter, Aud H., Hans J. De Boeck, Amy E. Eycott, Sabine Reinsch, David A. Robinson, Sara Vicca, Bernd Berauer, et al. 2020. "The Handbook for Standardized Field and Laboratory Measurements in Terrestrial Climate Change Experiments and Observational Studies (ClimEx)." *Methods in Ecology and Evolution / British Ecological Society* 11 (1): 22–37. https://doi.org/10.1111/2041-210X.13331.

Harley, P. C., F. Loreto, G. Di Marco, and T. D. Sharkey. 1992. "Theoretical Considerations When Estimating the Mesophyll Conductance to CO2 Flux by Analysis of the Response of Photosynthesis to CO2." *Plant Physiology* 98 (4): 1429–36. https://doi.org/10.1104/pp.98.4.1429.

Heidorn, P. Bryan. 2008. "Shedding Light on the Dark Data in the Long Tail of Science." *Library Trends*. 57(2), 280-299. https://doi.org/10.1353/lib.0.0036.

Kattge, Jens, Gerhard Bönisch, Sandra Díaz, Sandra Lavorel, Iain Colin Prentice, Paul Leadley, Susanne Tautenhahn, et al. 2020. "TRY Plant Trait Database - Enhanced Coverage and Open Access." *Global Change Biology* 26 (1): 119–88. https://doi.org/10.1111/gcb.14904.

Kattge, Jens, Wolfgang Knorr, Thomas Raddatz, and Christian Wirth. 2009. "Quantifying Photosynthetic Capacity and Its Relationship to Leaf Nitrogen Content for Global-Scale Terrestrial Biosphere Models." *Global Change Biology*. https://doi.org/10.1111/j.1365-2486.2008.01744.x.

Keenan, Trevor F., & Niinemets, Ulo. (2016). The Canopy Trait Plasticity (CANTRIP) database v1.0.0 (Version V1.0.0) [Data set]. Zenodo. http://doi.org/10.5281/zenodo.164883

Kissling, W. Daniel, Ramona Walls, Anne Bowser, Matthew O. Jones, Jens Kattge, Donat Agosti, Josep Amengual, et al. 2018. "Towards Global Data Products of Essential Biodiversity Variables on Species Traits." *Nature Ecology & Evolution* 2 (10): 1531–40. https://doi.org/10.1038/s41559-018-0667-3.

Kumarathunge, Dushan P., Belinda E. Medlyn, John E. Drake, Mark G. Tjoelker, Michael J. Aspinwall, Michael Battaglia, Francisco J. Cano, et al. 2019. "Acclimation and Adaptation Components of the Temperature Dependence of Plant Photosynthesis at the Global Scale." *New Phytologist*. https://doi.org/10.1111/nph.15668.

Leakey, Andrew D. B., John N. Ferguson, Charles P. Pignon, Alex Wu, Zhenong Jin, Graeme L. Hammer, and David B. Lobell. 2019. "Water Use Efficiency as a Constraint and Target for Improving the Resilience and Productivity of C3 and C4 Crops." *Annual Review of Plant Biology*. https://doi.org/10.1146/annurev-arplant-042817-040305.

LeBauer, David, Rob Kooper, Patrick Mulrooney, Scott Rohde, Dan Wang, Stephen P. Long, and Michael C. Dietze. 2018. "BETYdb: A Yield, Trait, and Ecosystem Service Database Applied to Second-Generation Bioenergy Feedstock Production." *GCB Bioenergy* 10 (1): 61–71. https://doi.org/10.1111/gcbb.12420.

LeBauer, David S., Dan Wang, Katherine T. Richter, Carl C. Davidson, and Michael C. Dietze. 2013. "Facilitating Feedbacks between Field Measurements and Ecosystem Models." *Ecological Monographs*. https://doi.org/10.1890/12-0137.1.

Limani, Fidan, Atif Latif, Timo Borst, and Klaus Tochtermann. 2019. "Metadata Challenges for Long Tail Research Data Infrastructures." *Bibliothek Forschung Und Praxis*. https://doi.org/10.1515/bfp-2019-2014.

Lin, Yan-Shih, Belinda E. Medlyn, Remko A. Duursma, I. Colin Prentice, Han Wang, Sofia Baig, Derek Eamus, et al. 2015. "Optimal Stomatal Behaviour around the World." *Nature Climate Change*. https://doi.org/10.1038/nclimate2550.

Long, S. P., and C. J. Bernacchi. 2003. "Gas Exchange Measurements, What Can They Tell Us about the Underlying Limitations to Photosynthesis? Procedures and Sources of Error." *Journal of Experimental Botany* 54 (392): 2393–2401. https://doi.org/10.1093/jxb/erg262.

Long, S. P., P. K. Farage, and R. L. Garcia. 1996. "Measurement of Leaf and Canopy Photosynthetic CO2 exchange in the Field." *Journal of Experimental Botany*. https://doi.org/10.1093/jxb/47.11.1629.

López-Calcagno, Patricia E., Kenny L. Brown, Andrew J. Simkin, Stuart J. Fisk, Silvere Vialet-Chabrand, Tracy Lawson, and Christine A. Raines. 2020. "Stimulating Photosynthetic Processes Increases Productivity and Water-Use Efficiency in the Field." *Nature Plants* 6 (8): 1054–63. https://doi.org/10.1038/s41477-020-0740-1.

Loreto, Francesco, Peter C. Harley, Giorgio Di Marco, and Thomas D. Sharkey. 1992. "Estimation of Mesophyll Conductance to CO 2 Flux by Three Different Methods." *Plant Physiology* 98 (4): 1437–43. https://doi.org/10.1104/pp.98.4.1437.

Maire, Vincent, Ian J. Wright, I. Colin Prentice, Niels H. Batjes, Radika Bhaskar, Peter M. van Bodegom, Will K. Cornwell, et al. 2015. "Global Effects of Soil and Climate on Leaf Photosynthetic Traits and Rates: Effects of Soil and Climate on Photosynthetic Traits." *Global Ecology and Biogeography: A Journal of Macroecology* 24 (6): 706–17. https://doi.org/10.1111/geb.12296.

Maxwell, Kate, and Giles N. Johnson. 2000. "Chlorophyll Fluorescence—a Practical Guide." *Journal of Experimental Botany* 51 (345): 659–68. https://doi.org/10.1093/jexbot/51.345.659.

Mayernik, Matthew S., Kelsey Breseman, Robert R. Downs, Ruth Duerr, Alexis Garretson, and Chung-Yi Hou. 2020. "Risk Assessment for Scientific Data." *Data Science Journal*. https://doi.org/10.5334/dsj-2020-010.

Murchie, E. H., and T. Lawson. 2013. "Chlorophyll Fluorescence Analysis: A Guide to Good Practice and Understanding Some New Applications." *Journal of Experimental Botany* 64 (13): 3983–98. https://doi.org/10.1093/jxb/ert208.

Niinemets, Ülo, Trevor F. Keenan, and Lea Hallik. 2015. "A Worldwide Analysis of within-canopy Variations in Leaf Structural, Chemical and Physiological Traits across Plant Functional Types." *The New Phytologist* 205 (3): 973–93. https://doi.org/10.1111/nph.13096.

Ort, Donald R., Sabeeha S. Merchant, Jean Alric, Alice Barkan, Robert E. Blankenship, Ralph Bock, Roberta Croce, et al. 2015. "Redesigning Photosynthesis to Sustainably Meet Global Food and Bioenergy Demand." *Proceedings of the National Academy of Sciences*. https://doi.org/10.1073/pnas.1424031112.

Pérez-Harguindeguy, N., S. Díaz, E. Garnier, S. Lavorel, H. Poorter, P. Jaureguiberry, M. S. Bret-Harte, et al. 2013. "New Handbook for Standardised Measurement of Plant Functional Traits Worldwide." *Australian Journal of Botany* 61 (3): 167. https://doi.org/10.1071/BT12225.

Ricciuto, Daniel, Khachik Sargsyan, and Peter Thornton. 2018. "The Impact of Parametric Uncertainties on Biogeochemistry in the E3SM Land Model." *Journal of Advances in Modeling Earth Systems*. https://doi.org/10.1002/2017ms000962.

Rodeghiero, Mirco, Ulo Niinemets, and Alessandro Cescatti. 2007. "Major Diffusion Leaks of Clamp-on Leaf Cuvettes Still Unaccounted: How Erroneous Are the Estimates of Farquhar et al. Model Parameters?" *Plant, Cell & Environment* 30 (8): 1006–22. https://doi.org/10.1111/j.1365-3040.2007.001689.x.

Rogers, Alistair, Kim Ely, Shawn Serbin. 2019. Leaf Photosynthetic Parameters: Quantum Yield, Convexity, Respiration, Gross CO_2 Assimilation Rate and Raw Gas Exchange

Data, Barrow, Alaska, 2016. *Next Generation Ecosystem Experiments Arctic Data Collection*, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, USA. https://doi.org/10.5440/1482338.

Rogers, Alistair, Belinda E. Medlyn, Jeffrey S. Dukes, Gordon Bonan, Susanne von Caemmerer, Michael C. Dietze, Jens Kattge, et al. 2017. "A Roadmap for Improving the Representation of Photosynthesis in Earth System Models." *The New Phytologist* 213 (1): 22–42. https://doi.org/10.1111/nph.14283.

Sack, Lawren, Will K. Cornwell, Louis S. Santiago, Margaret M. Barbour, Brendan Choat, John R. Evans, Rana Munns, and Adrienne Nicotra. 2010. "A Unique Web Resource for Physiology, Ecology and the Environmental Sciences: PrometheusWiki." *Functional Plant Biology: FPB* 37 (8): 687. https://doi.org/10.1071/FP10097.

Sansone, Susanna-Assunta, Peter McQuilton, Philippe Rocca-Serra, Alejandra Gonzalez-Beltran, Massimiliano Izzo, Allyson L. Lister, Milo Thurston, and FAIRsharing Community. 2019. "FAIRsharing as a Community Approach to Standards, Repositories and Policies." *Nature Biotechnology* 37 (4): 358–67. https://doi.org/10.1038/s41587-019-0080-8.

Sargsyan, Khachik, Cosmin Safta, Habib N. Najm, Bert J. Debusschere, Daniel Ricciuto, and Peter Thornton. 2014. "Dimensionality reduction for complex models via Bayesian compressive sensing." *International Journal for Uncertainty Quantification*. https://doi.org/10.1615/int.j.uncertaintyquantification.2013006821.

Schneider, Florian D., David Fichtmueller, Martin M. Gossner, Anton Güntsch, Malte Jochum, Birgitta König-Ries, Gaëtane Le Provost, et al. 2019. "Towards an Ecological Trait-data Standard." *Methods in Ecology and Evolution*. https://doi.org/10.1111/2041-210x.13288.

Sharkey, Thomas D., Carl J. Bernacchi, Graham D. Farquhar, and Eric L. Singsaas. 2007. "Fitting Photosynthetic Carbon Dioxide Response Curves for C(3) Leaves." *Plant, Cell & Environment* 30 (9): 1035–40. https://doi.org/10.1111/j.1365-3040.2007.01710.x.

Simkin, Andrew J., Patricia E. López-Calcagno, and Christine A. Raines. 2019. "Feeding the World: Improving Photosynthetic Efficiency for Sustainable Crop Production." *Journal of Experimental Botany*. https://doi.org/10.1093/jxb/ery445.

Smith, Nicholas G., Trevor F. Keenan, I. Colin Prentice, Han Wang, Ian J. Wright, Ülo Niinemets, Kristine Y. Crous, et al. 2019. "Global Photosynthetic Capacity Is Optimized to the Environment." *Ecology Letters*. https://doi.org/10.1111/ele.13210.

Thompson, Amber and Taylor, Barry N. (2008), Guide for the Use of the International System of Units (SI) NIST Special Publication 811, 2008 Edition (version 3.2). [Online] Available: http://physics.nist.gov/SP811 [2020-08-28]. National Institute of Standards and Technology, Gaithersburg, MD.

Varadharajan, Charuleka, Shreyas Cholia, Cory Snavely, Valerie Hendrix, Christina Procopiou, Diana Swantek, William Riley, and D. Agarwal. 2019. "Launching an Accessible Archive of Environmental Data." *Eos* 100. https://doi.org/10.1029/2019EO111263.

Vitousek, Peter M., Paul R. Ehrlich, Anne H. Ehrlich, and Pamela A. Matson. 1986. "Human Appropriation of the Products of Photosynthesis." *Bioscience* 36 (6): 368–73. https://doi.org/10.2307/1310258.

von Caemmerer, S. V., and J. R. Evans. 1991. “Determination of the Average Partial Pressure of CO2 in Chloroplasts From Leaves of Several C3 Plants.” *Functional Plant Biology: FPB* 18 (3): 287. https://doi.org/10.1071/PP9910287.

Walker, Anthony P., Martin G. De Kauwe, Ana Bastos, Soumaya Belmecheri, Katerina Georgiou, Ralph Keeling, Sean M. McMahon, et al. 2020. “Integrating the Evidence for a Terrestrial Carbon Sink Caused by Increasing Atmospheric CO2.” *The New Phytologist*, August. https://doi.org/10.1111/nph.16866.

Wallis, Jillian C., Elizabeth Rolando, and Christine L. Borgman. 2013. “If We Share Data, Will Anyone Use Them? Data Sharing and Reuse in the Long Tail of Science and Technology.” *PloS One* 8 (7): e67332. https://doi.org/10.1371/journal.pone.0067332.

Warren, Charles. 2006. “Estimating the Internal Conductance to CO2 Movement.” *Functional Plant Biology*. https://doi.org/10.1071/fp05298.

Weerasinghe, Lasantha K., Danielle Creek, Kristine Y. Crous, Shuang Xiang, Michael J. Liddell, Matthew H. Turnbull, and Owen K. Atkin. 2014. “Canopy Position Affects the Relationships between Leaf Respiration and Associated Traits in a Tropical Rainforest in Far North Queensland.” *Tree Physiology* 34 (6): 564–84. https://doi.org/10.1093/treephys/tpu016.

Wieczorek J, Bloom D, Guralnick R, Blum S, Döring M, et al. (2012) Darwin Core: An Evolving Community-Developed Biodiversity Data Standard. PLoS ONE 7(1): e29715. https://doi.org/10.1371/journal.pone.0029715

Wilkinson, Mark D., Michel Dumontier, I. Jsbrand Jan Aalbersberg, Gabrielle Appleton, Myles Axton, Arie Baak, Niklas Blomberg, et al. 2016. “The FAIR Guiding Principles for Scientific Data Management and Stewardship.” *Scientific Data* 3 (March): 160018. https://doi.org/10.1038/sdata.2016.18.

Yang, Jinyan, Belinda E. Medlyn, Martin G. De Kauwe, Remko A. Duursma, Mingkai Jiang, Dushan Kumarathunge, Kristine Y. Crous, Teresa E. Gimeno, Agnieszka Wujeska-Klause, and David S. Ellsworth. 2020. “Low Sensitivity of Gross Primary Production to Elevated CO_2 in a Mature Eucalypt Woodland.” https://doi.org/10.5194/bg-17-265-2020.

A reporting format for leaf-level gas exchange data and metadata: Supplementary Figures and Tables

Links to full documentation of the reporting format

Full documentation of the reporting format is available on GitHub at the following links:
GitHub https://github.com/ess-dive-community/essdive-leaf-gas-exchange
GitBook (GitHub content in a user friendly webpage format) https://ess-dive.gitbook.io/leaf-level-gas-exchange/

Supplementary figure, S1

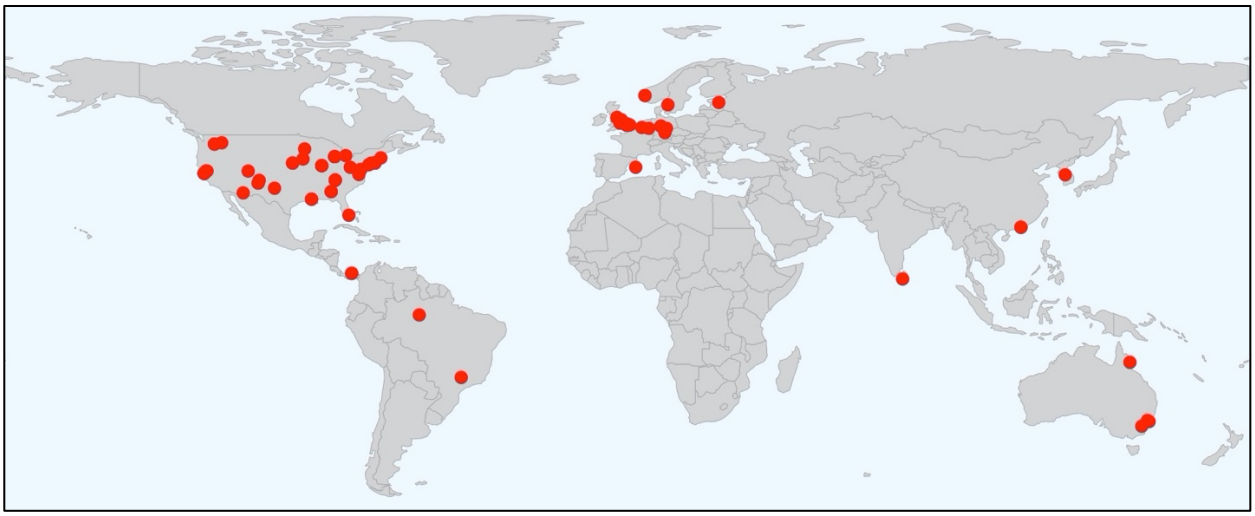

Figure S1. Input to development of the reporting format was received from gas exchange experts from around the world. Red circles indicate locations of contributors.

Supplementary tables, S1 – S4

Table S1
Ecological trait databases reviewed for leaf-level gas exchange data content. Databases sorted by relevance, with most relevant at the top.

Database	Web link	Relevant content?
TRY	www.try-db.org	Yes, variables and units considered in standard.
BETYdb	www.betydb.org	Yes, variables and units considered in standard.
EcoSIS	ecosis.org	Yes, but only as supporting data.
Botanical Information and Ecology Network (BIEN)	bien.nceas.ucsb.edu/bien/ Note: data not publicly available.	Yes, variables and units considered in standard.
Encyclopedia of Life - TraitBank	eol.org/traitbank	No gas exchange traits for plants.
LEDA	uol.de/en/landeco/research/leda	No gas exchange traits
BROT 2.0: A functional trait dataset	figshare.com/collections/BROT_2_0_A_functional_trait_database_for_Mediterranean_Basin_plants/3843841	No gas exchange traits
Data from: Three keys to the plants radiation of angiosperms into freezing environments	datadryad.org/stash/dataset/doi:10.5061/dryad.63q27	No leaf-level gas exchange traits
BioFlor	www.ufz.de/biolflor/index.jsp	No leaf-level gas exchange traits
Global Biotraits Database	biotraits.ucla.edu/	Published 2013. No longer available online.

Table S2
List of data repositories investigated for leaf-level gas exchange content.

Resource	URL	Type	Detailed metadata viewer?
Dryad	https://datadryad.org/	public data archive	no
NSF Environmental Data Initiative	https://environmentaldatainitiative.org/	public data archive	yes
Pangea	https://www.pangaea.de/	public data archive	no
Mendeley	https://data.mendeley.com/	public data archive	no
Figshare	https://figshare.com/	public data archive	datafile dependent
TERN	https://portal.tern.org.au	public data archive	yes
The Knowledge Network for Biocomplexity	https://knb.ecoinformatics.org/	public data archive	yes
Ag Data Commons	https://data.nal.usda.gov/	project data archive	yes
NSF Arctic Data Center	https://arcticdata.io/	project data archive	yes
ORNL DAAC	https://daac.ornl.gov/	project data archive	yes
DataONE	https://www.dataone.org/	archive and data search engine	yes

Table S3
Publications with large compiled datasets of leaf-level gas exchange measurements, showing type of data and how the presented data were incorporated into this data reporting format.

Publication reference	Data type	Data table available? Comment on incorporation into standards.
Atkin et al. 2015	respiration	Yes. GlobResp database. Fields considered for metadata variables.
De Kauwe et al. 2016	A-C_i	No
Gago et al. 2016	net photosynthesis (A), stomatal conductance to CO_2 (g_s), mesophyll conductance (g_m)	Yes. Considered for survey format.
Kumarathunge et al. 2019	A-C_i	No
Lin et al. 2015	stomatal conductance, g_s	Yes. Excellent interface on Figshare with fields clearly listed and defined.
Maire et al. 2015	A_{max}	Yes. GlobAmax database. Fieldsconsidered for metadata variables.
Niinemets et al. 2015	V_{cmax}, J_{max}	Yes, data fields only. Considered for V_{cmax} format.
Poorter et al. 2019	V_{cmax}, J_{max} and others	Yes, data fields only. Considered for V_{cmax} format.
Slot and Winter 2017	Temperature response, respiration, Q10, V_{cmax}, J_{max}	Yes, considered in defined variables.
Smith et al. 2019	V_{cmax}, from A-C_i and one point	No, but database fields are discussed (may not be a complete list). Fields considered for A-Ci format.
Walker et al. 2014	V_{cmax}, J_{max}, leaf chemistry	Yes, on ORNL DAAC. Considered for V_{cmax} format. Perhaps some extra constant fields that need consideration.
Way and Yamori 2014	net photosynthesis (A)	Compilation of 257 studies, listing units used for A. Considered for A_{max} variable definition..
Wright et al. 2004	Photosynthetic capacity (A), dark respiration rate (R)	Yes. GLOPNET database.

Table S4
Portable gas exchange instruments included in the Instrument Output Translation table.

Manufacturer	Model	Documentation version
ADC Bioscientific	iFL	Issue 2: 20 February 2020
ADC Bioscientific	LCi T	Version dated 2019
ADC Bioscientific	LCpro T	Issue 1-101 (2018)
CID Bio-Science	CI-340	Version dated 2019
LI-COR Biosciences	6800	Version 1.4 (2020)
LI-COR Biosciences	6400XT	Version 1.6 (2012)
PP Systems	CIRAS-3	Version 2.01 (2019)
PP Systems	CIRAS-2	Version 2.04 (2010)
PP Systems	TARGAS-1	Version 1.04 (2018)
Walz	GFS-3000	9th edition (2019)

References

Atkin, OK, KJ Bloomfield, PB Reich, MG Tjoelker, GP Asner, D Bonal, G Bönisch, et al. 2015. "Global Variability in Leaf Respiration in Relation to Climate, Plant Functional Types and Leaf Traits." *The New Phytologist* 206 (2): 614–36. https://doi.org/10.1111/nph.13253.

De Kauwe, MG, Y-S Lin, IJ Wright, BE Medlyn, KY Crous, DS Ellsworth, V Maire, et al. 2016. "A Test of the 'One-Point Method' for Estimating Maximum Carboxylation Capacity from Field-Measured, Light-Saturated Photosynthesis." *The New Phytologist* 210 (3): 1130–44. https://doi.org/10.1111/nph.13815.

Gago, J, D de Menezes Daloso, CM Figueroa, J Flexas, AR Fernie, Z Nikoloski. 2016. "Relationships of Leaf Net Photosynthesis, Stomatal Conductance, and Mesophyll Conductance to Primary Metabolism: A Multispecies Meta-Analysis Approach." *Plant Physiology* 171 (1): 265–79. https://doi.org/10.1104/pp.15.01660.

Kumarathunge, DP, BE Medlyn, JE Drake, MG Tjoelker, MJ Aspinwall, M Battaglia, FJ Cano, et al. 2019. "Acclimation and Adaptation Components of the Temperature Dependence of Plant Photosynthesis at the Global Scale." *The New Phytologist* 222 (2): 768–84. https://doi.org/10.1111/nph.15668.

Lin, Y-S, BE Medlyn, RA Duursma, IC Prentice, H Wang, S Baig, D Eamus, et al. 2015. "Optimal Stomatal Behaviour around the World." *Nature Climate Change* 5 (5): 459–64. https://doi.org/10.1038/nclimate2550.

Maire, V, IJ Wright, IC Prentice, NH. Batjes, R Bhaskar, PM van Bodegom, WK Cornwell, et al. 2015. "Global Effects of Soil and Climate on Leaf Photosynthetic Traits and Rates." *Global Ecology and Biogeography*. https://doi.org/10.1111/geb.12296.

Niinemets, Ü, TF Keenan, L Hallik. 2015. "A Worldwide Analysis of within-Canopy Variations in Leaf Structural, Chemical and Physiological Traits across Plant Functional Types." *The New Phytologist* 205 (3): 973–93. https://doi.org/10.1111/nph.13096.

Poorter, H, Ü Niinemets, N Ntagkas, A Siebenkäs, M Mäenpää, S Matsubara, T Pons. 2019. "A Meta-Analysis of Plant Responses to Light Intensity for 70 Traits Ranging from Molecules to Whole Plant Performance." *The New Phytologist* 223 (3): 1073–1105. https://doi.org/10.1111/nph.15754.

Slot, M, K Winter. 2017. "Photosynthetic Acclimation to Warming in Tropical Forest Tree Seedlings." *Journal of*

Experimental Botany 68 (9): 2275–84. https://doi.org/10.1093/jxb/erx071.

Smith, NG, TF Keenan, IC Prentice, H Wang, IJ Wright, Ü Niinemets, KY Crous, et al. 2019. "Global Photosynthetic Capacity Is Optimized to the Environment." *Ecology Letters* 22 (3): 506–17. https://doi.org/10.1111/ele.13210.

Walker, AP, AP Beckerman, L Gu, J Kattge, LA Cernusak, TF Domingues, JC Scales, G Wohlfahrt, SD Wullschleger, FI Woodward. 2014. "The Relationship of Leaf Photosynthetic Traits -VcmaxandJmax- to Leaf Nitrogen, Leaf Phosphorus, and Specific Leaf Area: A Meta-Analysis and Modeling Study." *Ecology and Evolution*. https://doi.org/10.1002/ece3.1173.

Way, DA., W Yamori. 2014. "Thermal Acclimation of Photosynthesis: On the Importance of Adjusting Our Definitions and Accounting for Thermal Acclimation of Respiration." *Photosynthesis Research*. https://doi.org/10.1007/s11120-013-9873-7.

Wright, IJ, PB Reich, M Westoby, DD Ackerly, Z Baruch, F Bongers, J Cavender-Bares, et al. 2004. "The Worldwide Leaf Economics Spectrum." *Nature* 428 (6985): 821–27. https://doi.org/10.1038/nature02403.