# Data from the Arizona FACE (Free-Air $CO_2$ Enrichment) Experiments on Sorghum at Ample and Limiting Levels of Water Supply

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**Abstract:** In order to determine the likely effects of the increasing atmospheric $CO_2$ concentration on future sorghum productivity, two free-air $CO_2$ enrichment (FACE) experiments were conducted on sorghum (*Sorghum bicolor* (L.) Möench, a $C_4$ grain crop) at Maricopa, Arizona, U.S.A. during the 1998 and 1999 summer growing seasons. They were conducted at ample and limited (50% of ample) supplies of water. A large and varied set of data on plant, soil, and microclimatic responses to the elevated $CO_2$ and its interactions with the water supply was collected. The dataset assembled herein consists of many of these data, including those generally used for sorghum growth model validation, such as management, soils, daily and 15-minute weather, physiology (net photosynthesis, plant water potential, relative water content), phenology, biomass growth, leaf area, yield, canopy temperatures, energy balance, evapotranspiration, soil moisture, reflectance and vegetation indices, and absorption of photosynthetically active radiation. Partitioning of nitrogen between nitrate and cyanide, which affects toxicity of the sorghum forage to livestock, was measured. In addition, isotopic methods were used to trace carbon flows in both FACE and Control plots from atmosphere to plant material to soil carbon pools. Because the dataset is useful for validation of sorghum growth models with respect to their $CO_2$ responses, it can increase the accuracy of predictions of future sorghum productivity given projected global climate change.

**Keywords:** $CO_2$, carbon dioxide, sorghum, drought, free-air $CO_2$ enrichment, FACE, climate change, global change, carbon isotopes, cyanide, dhurrin.

## 1 BACKGROUND:

The increasing atmospheric $CO_2$ concentration (e.g. https://www.esrl.noaa.gov/gmd/ccgg/trends/) has caused concern regarding the effects on future agricultural crop productivity. This concern led to the development of free-air $CO_2$ enrichment technology (FACE), which was successfully demonstrated on cotton (*Gossypium hirsutum* L.) at Maricopa, Arizona from 1989-1991 (Hendrey, 1993). After cotton, the Maricopa group conducted four more FACE experiments on wheat (*Triticum aestivum* L.) from 1992-1997 (e.g., Kimball et al., 2017). The $C_3$ cotton was highly responsive to the FACE treatment (+40%), and the $C_3$ wheat was also responsive (+13%). However, it was not known in 1997 whether $C_4$ crops would also respond. Therefore, because $C_4$ sorghum (*Sorghum bicolor* (L.) Möench) is commonly grown in the Maricopa area, the next FACE experiments were conducted in 1998 and 1999 on sorghum.

Many scientists participated in the FACE Sorghum experiments, measuring leaf area, phenology, above-ground biomass, and yield (Ottman et al., 2001); apical and morphological development, photosystem energy use and quenching, and development of $C_4$ photosynthesis (Cousins et al., 2001, 2002, 2003); canopy reflectance, absorption of photosynthetically active radiation; canopy temperature, energy balance, and evapotranspiration (Triggs et al., 2004); soil water content (Conley et al., 2001); net assimilation rate, stomatal conductance, total leaf water potential and leaf relative water content (Wall et al., 2001); carbon isotope discrimination (Williams et al., 2001); soil $CO_2$ fluxes and changes in soil C storage from soil and plant C isotopes (Cheng, 2005; Cheng et al., 2007); stability of soil aggregates

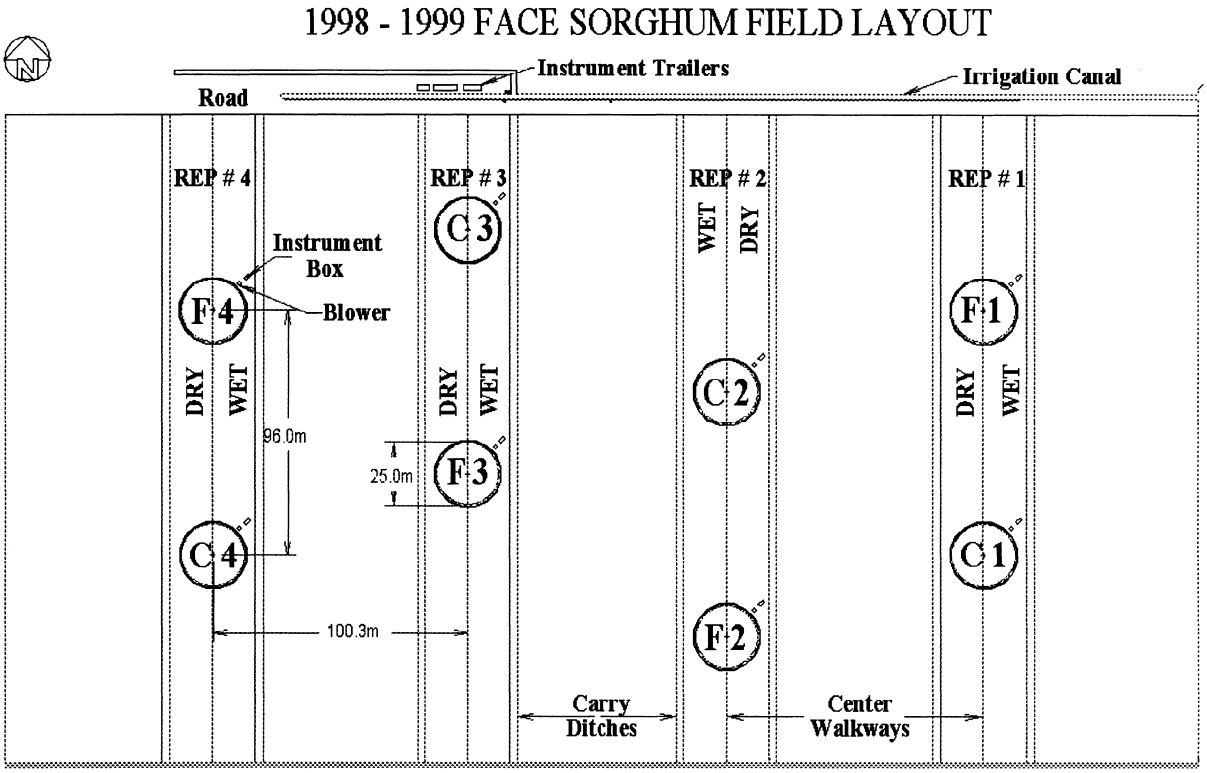
Rillig et al., 2001); $C_4$-$C_3$ competition between sorghum and cotton (Derner et al., 2003); and partitioning between cyanide and nitrate in leaves (Gleadow et al., 2016).
Many of the data collected in the FACE Sorghum experiments are useful for validating sorghum growth models, and to date, at least 2 papers have resulted from such model tests (Grant et al., 2004; Fu et al., 2016). The data herein are formatted in the ICASA Version 2.0 format (White et al., 2013) with some modifications under the umbrella of the AgMIP (Agricultural Model Inter-comparison and Improvement Project; http://www.agmip.org/). These data are included in this dataset in file "FACE Sorghum Maricopa growth management weather soil AgMIP.ods".

**2 METHODS:** Two experiments were conducted during the 1998 and 1999 summer growing seasons to determine the interactive effects of elevated $CO_2$ and limited soil water on grain sorghum (*Sorghum bicolor* (L.) Möench cv. Dekalb DK54) (Ottman et al., 2001). They were conducted at the University of Arizona Maricopa Agricultural Center (MAC), Maricopa, Arizona, USA (33.06° N latitude, -111.98 W longitude, 361 m elevation; Fig. 1). The soil was Trix clay loam [fine-loamy, mixed (calcareous), hyperthermic Typic Torrifluvents]; additional details about the soil properties are given by Post et al. (1988) and Kimball et al. (1992). A sorghum crop had been grown on the land in the summer-fall of 1997, and a cover crop of spring barley (*Hordeum vulgare* L.) had been grown in the winter-spring and harvested before maturity for hay at the beginning of April,1998.

**2.1 $CO_2$ TREATMENTS:** The free-air $CO_2$ enrichment (FACE) technique was used to enrich the air in circular plots within a sorghum field similar to prior experiments (e.g., Hendrey, 1993; Kimball et al., 2017; Fig. 1). Both the FACE and Control plots had blowers, toroidal plenums and vertical vent pipes with valves in order to provide similar air movement in all plots (Pinter et al., 2000). The FACE plots were enriched by 200 µmol $mol^{-1}$ above ambient (~ 370 µmol $mol^{-1}$ during daytime). A separate sequential sampling system was used to measure the concentration in all of the FACE and Control plots, as well as two additional sampling points. The minimum value from among the most recent observations of the four Control plots and the two ambient points was selected to provide *"THE"* system ambient value against which to reference the 200 µmol $mol^{-1}$ enrichment setpoint for the FACE plots. For 1998, the average daytime $CO_2$ concentrations in the FACE and Control plots were 556 and 363 µmol $mol^{-1}$, respectively, while the nighttime values were 603 and 428 µmol $mol^{-1}$. For 1999 the respective FACE and ambient Control concentrations were 566 and 373 µmol $mol^{-1}$, and at night they were 607 and 433 µmol $mol^{-1}$.
Recently, Allen et al. (2020) assembled data about the effects of fluctuating $CO_2$ (such as found in FACE plots) on the growth of $C_3$ plants compared to steady $CO_2$-enrichment. Their conclusions suggest that the responses of $C_3$ crops in FACE experiments need to be multiplied by a factor of about 1.5 to get the true values. The responses of our $C_4$ sorghum were small at ample water but substantial under limited water supply due to partial stomatal closure and some resultant water conservation (Wall et al., 2001; Conley et al., 2001; Triggs et al., 2004). In another recent paper, Bunce (2020) found that a square wave $CO_2$ oscillation reduced the stomatal conductance of $C_3$ plants but not $C_4$ plants. While not definitive, these few data suggest that the $CO_2$ fluctuations in our FACE sorghum plots probably did not significantly affect our results.

**2.2 IRRIGATION TREATMENTS:** Each of the main circular FACE and Control plots was split in semi-circular halves, with each half receiving either an ample (Wet) or a water-stress (Dry) irrigation regime (Ottman et al., 2001; Fig. 1). The water was applied using flood irrigation. "Carry ditches" (Fig. 1) were used to carry the irrigation water rapidly across the field and minimize the opportunity time for infiltration between the FACE and Control plots. As before (Kimball et al., 1999), the criterion used to decide when to irrigate the Wet plots was after 30% of the available water in the rooted zone was depleted; they were irrigated with an amount calculated to replace 100% of the potential evapotranspiration since the last irrigation, adjusted for rainfall (Fox et al., 1992). The Dry treatments received only two irrigations, at the start and near mid-season. The total amounts of irrigation plus rain applied during 1998 were 1218 and 474 mm to the Wet and Dry plots, respectively. In 1999, the amounts of irrigation plus rain were 1047 and 491 for Wet and Dry, respectively.

**Figure 1.** Field layout plan for the 1998 and 1999 FACE Sorghum experiments, where "F" indicates FACE plot, "C" indicates Control plot, and the 1, 2, 3, and 4 indicate replicate numbers. "WET" indicates the amply irrigated strips and "DRY" indicates the limited irrigation strips.




## 2.3 MEASUREMENTS

**2.3.1 PLANT SAMPLING:** Plants were sampled on a weekly basis from the 3 to 4 leaf stage until final harvest in order to develop relationships among plant growth parameters, $CO_2$, and water supply (see file "FACE Sorghum Maricopa growth management weather soil AgMIP.ods"). A total of eight plants were sampled per experimental unit in a pre-determined pattern. Four sampling areas were designated within each experimental unit that consisted of about 7.2 m of row arranged in two or three rows. Two plants were removed each week from the four sampling areas for a total of eight plants per experimental unit. The fourth plant beyond the spot of the last sampled plant was taken for the current sample. The plants were cut off at ground level and immediately placed in an ice chest. The plant samples were transported from the field to the lab in the ice chest. They were placed in a cooler set at 5 °C until processing could occur. Plant height was measured from the base of the plant to the longest extended leaf or to the tip of the head, whichever was longer. The number of tillers and their developmental stage was recorded. Leaves were removed from the stem at the collar and separated into green and brown leaves. Leaf area of green leaves was measured with a LI-COR leaf area meter (Model 3100, LI-COR Bioscience, Lincoln, NB, USA). Stem area (longitudinal section) was calculated as the product of stem length and mean stem diameter averaged from measurements taken at the base and top of the stem. Heads were removed from the stems. The stems, brown and green leaves, and heads were dried separately in an oven at about 65 °C for 2 to 4 days and then weighed. The mass of these various plant parts was calculated on an area basis using plant density determined at harvest. Leaf area index and stem surface area index was also calculated using plant density at harvest. Specific leaf weight was calculated by dividing green leaf weight by green leaf area.

Prior to heading, leaf developmental growth stages were determined on eight plants adjacent to the sampling areas. The fifth, tenth, and fifteen leaf were tagged on these plants for accurate determination of leaf appearance. Leaf number was based on appearance of the leaf collar. At heading, phenological stage was determined on plants sampled for biomass. Prior to heading, growth stages represent mean leaf number of all plants and not the most advanced 50% as was done after heading. After the vegetative period, the numbers during reproductive stages were 1 (50% of plants heading), 2 (anthesis), 3 (kernel watery), 4 (kernel milky), 5 (soft dough), 6 (hard dough), 7 (50% of plants at physiological maturity), and 8 (post-physiological maturity, 100% of the plants physiologically mature). In order to obtain more precise dates for heading and anthesis than possible with weekly sampling, once panicles began emerging, daily counts were made of plants with and without flowers along a pre-determined, 1.5m

segment of two plant rows within the final harvest area of each plot. Data were interpolated to determine the exact days when 50% heading and 50% anthesis were attained.
Yield and yield components were determined at final harvest to determine how these measurements relate to $CO_2$ and water supply. For the final harvest, grain yield was determined from a non-traffic area composed of six rows 3 m in length. Heads were removed from the plants, the heads were weighed, the heads were threshed, the grain was weighed, and samples of grain and chaff were saved for moisture determination. Grain moisture was determined with a digital moisture meter and chaff moisture was determined from wet and oven dry (65 °C) weights. Grain yield and chaff yield were calculated and adjusted to a dry weight basis. The biomass remaining after head removal in center two rows of the six row non- traffic area was harvested for stover determination. These stalks were cut at ground level, weighed, and sampled for moisture. Moisture was determined from wet and oven dry (65 °C) weights. Stover yield was defined as non-grain yield and was summed from plant yield after head removal chaff yield, or non-grain portion of the head. Total above ground biomass was summed from grain yield and stover yield. Harvest index was calculated by dividing grain yield by total yield. Kernel weight was determined from a 10 g sample of kernels. The number of heads in the final harvest area was counted. Kernels per head was calculated by dividing grain weight per head by kernel weight. Kernels per unit area was calculated by multiplying kernels per head by heads per unit area.

**2.3.2 WEATHER, CANOPY TEMPERATURE, ENERGY BALANCE AND EVAPOTRANSPIRATION:**
In order to document the weather conditions under which the experiments were conducted, a weather station (MARA; see tab in “FACE Sorghum Maricopa growth management weather soil AgMIP.ods” spreadsheet) was deployed in the sorghum field between the C3 and F3 plots (Triggs et al., 2004; Fig. 1). Solar radiation was measured with a pyranometer (Model 15, Eppley Laboratory Newport, RI), air dry and wet bulb temperatures were measured with shielded, aspirated psychrometers, and wind speed with cup anemometers (Model 12102D, R.M. Young Co., Traverse City, MI). Instruments were serviced weekly. Gaps were filled using data from the AZMET weather station (https://cals.arizona.edu/azmet/06.htm) about 1 km from the sorghum field. The weather data were observed every 10 s, and 15-minute averages were recorded and saved. Daily values were computed from the 15-minute data.
However, modelers using daily weather data should probably use MARB. MARB is based on data from the MARA weather station but adds 1.2 °C to TMIN. This was to account for the effect of blowers, which stirred the air over the plots (Pinter et al., 2000). It should also be mentioned that the FACE-Wet canopies were between about 1.0 and 1.4 °C warmer than the Control-Wet canopies at midday but no difference at night. The FACE-DRY plots were sometimes cooler than the Control-DRY plots due to earlier exhaustion of soil moisture in the Control-Dry plots (Triggs et al., 2004).
In order to determine the effects of elevated $CO_2$ on the crop microclimate and water use, evapotranspiration (ET) was determined in Replicates 3 and 4 (Fig. 1) from latent heat flux (λET) using the residual energy balance approach, whereby ET is the residual after subtracting measured sensible and soil heat fluxes from measured net radiation (Triggs et al., 2004) (see files “1998 15-min weather canopy & soil temperatures energy balance CO2.ods” and “1999 15-min weather canopy & soil temperatures energy balance CO2 O3.ods”). Sensible heat flux was determined from the difference between canopy surface temperatures and air temperature divided by aerodynamic resistance calculated from wind speed (Triggs et al., 2004). Canopy temperatures were measured with infrared thermometers (Model 4000a, Everest Interscience, Tucson, AZ). Soil heat fluxes were measured with four heat flux plates per plot at the 10 cm depth with heat storage above the plates determined from soil temperature measurements with thermocouples. Net radiations were determined with net radiometers (Model Q*6 with ventilators; Radiation and Energy Balance Systems, Seattle, WA). To minimize instrument bias, both net radiometers and infrared thermometers were interchanged weekly between FACE and Control plots within each replicate.

**2.3.3 SOIL MOISTURE:** Besides helping to decide when to irrigate the Wet plots (see Section 2.2), measurements of soil moisture were used to determine the effects of elevated $CO_2$ on the rates of water consumption of the sorghum plants. Soil moisture was measured using neutron probes (Hydroprobe Model 503 DR, Pacific Co., Martinez, CA, USA) (see file “FACE Sorghum Maricopa growth management weather soil AgMIP.ods”). Depths listed are from the soil surface to the middle of the sampled soil moisture region. The neutron probe measures a 30-cm-diameter sphere. Thus, depth ranges were not exact. Values of soil moisture were problematic for the uppermost soil layer because the neutron probe did not resolve small near-surface depth increments and because soil moisture is more dynamic and variable near the soil surface. The probes were calibrated from gravimetric soil water content and bulk density measurements taken in the same soil adjacent to the field plots using a wide range of soil

moisture contents. Measurements were taken at 0.3-m intervals to either 1.8 m or 3.0 m depths during the 1998 and 1999 seasons, respectively. In the 1998 season, the uppermost measurement was taken at 0.46m, whereas in 1999 it was at 0.23m. To facilitate year-to-year comparison of data, a simple model was developed to extrapolate water content for the upper 0.3m of soil for each dry-down cycle in 1998. This model used multiple regressions of the independent variables Growing Degree Days (GDD), Normalized Difference Vegetative Index (NDVI), Arizona Meteorological Network (AZMET) potential grass reference (modeled ET), and 0.46m 1999 data to estimate 0.23m data for 1998.

**2.3.4 GAS EXCHANGE AND PLANT WATER RELATIONS:** Data were collected to elucidate the effects of $CO_2$ enrichment and water supply on gas exchange properties and water relations of the sorghum, as described by Wall et al. (2001) (see file "FACE Sorghum physiology.ods"). In short, midday leaf net assimilation rates, stomatal conductance and transpiration rates were measured on the central portion of randomly selected fully expanded upper-canopy sunlit leaves (ligule emerged) with three portable closed-gas exchange (transient) systems (Model LI-6200, LI-COR Bioscience, Lincoln, NB, USA). Depending on leaf size either a 0.25-L or a 1-L transparent plexiglass cuvette was used. Leaf cuvette $CO_2$ concentrations were 370 ± 40 or 560 ± 40 μmol $mol^{-1}$ for Control and FACE, respectively. Use of three separate systems enabled replications 1, 2 and 3 (Fig. 1) to be measured simultaneously ~45 min from solar noon (1.5 h sample interval), thereby minimizing variation in gas exchange measurements due to diurnal changes in meteorological conditions.
Water relations measurements consisted of total leaf water potential and relative leaf water content. Blades of fully expanded upper-canopy sunlit leaves (ligule emerged) were excised ~5 mm apical to the leaf collar at midday (solar noon). They were sealed in a plastic bag containing a damp paper towel and stored in an insulated container. Total leaf water potential was measured with a pressure chamber apparatus (Model 3000, Soil Moisture Equipment Corp, Santa Barbara, CA, USA). Relative water content was determined using standard techniques as described previously by Wall et al. (2001).

**2.3.5 PAR ABSORPTION:** Photosynthetically Active Radiation (PAR, 0.4μm to 0.7μm) that is absorbed by plants for potential use in photosynthetic processes drives plant primary productivity and thus is an important parameter in any modelling activity. We measured incident, reflected, and transmitted PAR for sorghum in each of the $CO_2$ and irrigation treatments during the 1998 and 1999 seasons using an Accupar Light Interception Device (Model PAR80: Decagon, Pullman, WA, USA) (see file "PAR absorption.ods"). Observations were taken around solar noon near the center of each plot in an undisturbed area reserved for non-destructive measurements and final harvest. A light balance equation (Gallo and Daughtry, 1986; Pinter, 1993) was used to compute the fraction of PAR absorbed by the canopy (fAPAR). Fractional PAR closely parallels the development of green plant biomass, GLAI, and multispectral vegetation indices such as the Normalized Difference Vegetation Index (NDVI) and Ratio Vegetation Index (RVI) - see section 2.3.6 Canopy reflectance. Fractional PAR absorptance *per se* does not relate to productivity throughout the entire growing season because natural, end-of-season canopy senescence, disease, and frost resulted in a portion of PAR being absorbed by non-photosynthesizing tissues of the canopy.

**2.3.6 CANOPY REFLECTANCE:** Multispectral reflectance measurements can provide agricultural researchers with rapid, non-destructive methods for quantifying the growth, green leaf area index, and senescence of plant canopies throughout the season. They are also useful for characterizing the effects of various experimental treatments. We used a ground-based Exotech radiometer (Model 100BX, 15° field-of-view; Exotech, Inc., Gaithersburg, MD, USA) to measure canopy reflectance factors in 1998 and 1999 during the FACE Sorghum experiments (see file "Reflectance and vegetation indices.ods"). It was configured with four filters approximating the Landsat 4 Thematic Mapper satellite wavebands [*i.e.* TM1= 0.45-0.52 μm (blue); TM2=0.52-0.60μm (green); TM3=0.63-0.69μm (red); and TM4=0.76-0.90μm (near infrared, NIR). Signals from the radiometer were recorded on a portable data acquisition system (Polycorder Model 516; Omnidata International, Logan, UT, USA).
Observations were made from emergence until harvest at a frequency of from 2 to 5 times per week depending on weather conditions and rate of crop growth. The radiometer was handheld about 1.5m above the soil surface and oriented towards nadir. Twenty-four evenly spaced, overlapping measurements were averaged along a 6 meter transect in the final harvest areas of each treatment and replicate. Similar measurements were made in bare soil plots in the same field outside of the $CO_2$ manifolds south of Replicate 3. Reflectance factors were calculated as the ratio of radiance measured in each plot to incident irradiance inferred from a time-based interpolation of data collected over a calibrated, painted BaSO4 reference panel at 15- to 25-minute intervals using the same radiometer. Data collections required approximately 40 to 50 minutes to complete. A Normalized Difference

Vegetation Index (NDVI) and Ratio Vegetation Index (RVI) were computed from red and NIR reflectance factors. These data are presented in the associated "Reflectance and vegetation indices.ods" file along with ambient weather conditions and qualitative observations of cloud interference with direct beam solar irradiance, cloud cover, haze, wind speed, and dew on the canopy associated with each data set.

**2.3.7 MIDDAY CANOPY TEMPERATURE FROM ALL PLOTS:** Infrared thermometry has been widely adopted as a non-destructive, canopy level surrogate for assessing the response of agricultural crops to conditions that reduce plant transpiration (Pinter et al. 2003). Plants exposed to limited soil water due to reduced irrigation frequency or natural drought, disease, or elevated $CO_2$ typically display elevated temperatures when compared with those of well-watered or disease-free individuals (Pinter et. al. 1979, Hatfield and Pinter, 1994; Triggs et. al., 2004).
In the accompanying data (see file “Midday canopy temperature in all plots.ods”), we present midday measurements of apparent canopy temperatures (Tc) obtained using a roving, handheld infrared thermometer (IRT) during the 1998 and 1999 FACE Sorghum Experiments (see file “Midday canopy temperature in all plots.ods”). The data provide insight on canopy-level responses to the interactive effects of elevated $CO_2$ and irrigation frequency and amounts on grain sorghum growth and development, and they contribute to the overall modelling effort. They span the entire season from shortly after emergence through all growth stages to maturity and senescence.
Measurements of Tc were taken shortly after solar noon using a calibrated IRT having 10 to 12μm bandpass characteristics and a 15° field of view (IRT Model 110, Everest Interscience, Tucson, AZ, USA). Analog voltages from the IRT and measurement times were recorded on a portable data acquisition system (Polycorder Model 516; Omnidata International, Logan, UT, USA). The IRT was pointed in a nadir orientation from a height about 1.5 m above ground level. To obtain a representative average canopy temperature, 18 overlapping measurements were taken along a 6-m-long transect in the final harvest area of each treatment and replicate. The roving IRT was also used to measure the same canopy targets as the stationary IRTs in replicates 3 & 4 (see section 2.3.2) using approximately the same viewing angles (n=18).
Ancillary data included wet and dry bulb measurements of the air at ca. 1.5m height above the soil surface within the field at the start and finish of each data collection routine. These data were used to compute dew point and vapor pressure using standard psychrometric relations. IRT performance was checked against a thermistor-based black body calibration device (Everest Interscience, Tucson, AZ). Qualitative observations of weather (i.e., sun conditions, cloud type and cover, haze levels, wind speed and direction) were coded nominally and entered by hand into the Polycorder. Data collected during conditions that may have compromised their potential use because of moderate to heavy cloud cover, instrument malfunction, or operator error have been excluded.

**2.3.8 CARBON TRACING:** The distinct isotopic composition of the $C_4$ sorghum plants (compared to organic carbon already in the soils) and that of the commercial $CO_2$ chosen to elevate the concentration in the FACE plots provided a unique opportunity to trace carbon in the both the FACE and Control treatments, which has been much more difficult in FACE experiments with $C_3$ crops. The pure tank $CO_2$ added to FACE plots was $^{13}C$-enriched $CO_2$ derived from a geologic deposit with $\delta^{13}C$ = –4.7‰ to –4.8‰ (Cheng, 2005, Cheng et al., 2007) (see file “Soil carbon dynamics and isotopic tracing.ods”). The atmospheric $CO_2$ in the Control plots had an isotopic composition of $\delta^{13}C$ = –8.9‰ (1998) to –9.4‰ (1999), which is considered the C isotopic composition of the local background atmosphere and results in Control $C_4$-sorghum plants with $\delta^{13}C$ of ca. –11.9‰. Air in the FACE plots was composed of background air mixed with extra tank $CO_2$, resulting in its isotopic composition of ca. –7.6‰ (both years). Consequently, the $\delta^{13}C$ value of sorghum in FACE plots was about –10.4‰, only 1.0 to 1.4‰ less negative than that of Control sorghum. In both cases, however, the sorghum $\delta^{13}C$ was significantly $^{13}C$-enriched compared to $\delta^{13}C$ of resident soil organic carbon, so new carbon from the experiment could be traced in both FACE and Control plots, as described in the “Soil carbon dynamics and isotopic tracing.ods” file.

**2.3.9 NITROGEN PARTITIONING:** Cyanide can accumulate in sorghum forage, which then is toxic to livestock. Therefore, to determine the effects of elevated $CO_2$ and the drought treatments on cyanide, measurements were made of the partitioning between cyanide and nitrate in sorghum forage tissues (Gleadow et al., 2016) (see file “Sorghum cyanide and nitrate partitioning.ods”). In order to make meaningful ontogenetic comparisons across years, samples were taken from plants at the 10 leaf-stage (Day 237 in 1998 and Day 215 in 1999), and at the 19-leaf stage (Day 265 in 1998 and day 236 in 1999).

Foliar dhurrin (cyanogenic glucoside) concentrations were determined on leaves (i.e., leaf blade) and stems (comprising both the stem and the enclosing leaf sheaths) using the evolved cyanide method following Blomstedt et al. (2012). Exogenous -glucosidase (1.12 units $mL^{-1}$) from almond (EC 3.2.1.21, Sigma, St. Louis, MO, USA) was used to ensure that all dhurrin was converted to cyanide during incubation. Evolved HCN was assayed colorimetrically and expressed as cyanide (g HCN $g^{-1}$ dry weight). One gram of cyanide is equivalent to 11.9 g dhurrin. LC–MS analysis of the samples from the Maricopa experiment confirmed that cyanide was present as dhurrin and showed a very high correlation between evolved cyanide and the concentration of dhurrin measured directly by LCMS (y = 1.066x - 84.7, R2 = 0.85)(Gleadow et al., 2012).
Foliar nitrate was measured on dried tissue (Cataldo et al., 1975). Samples (50 mg) were extracted in MilliQ H2O, incubated at 45 °C for 1 h, centrifuged and the supernatant assayed colorimetrically following (Cataldo et al., 1975) as modified by O'Donnell et al. (2013) and the absorbance measured using an Lachat QuikChem 8000 autoanalyzer (Model 8000, Lachat QuickChem, Loveland, CO, USA). This was converted to nitrate per dry mass using the molar mass of nitrate to give milligram nitrate per gram plant tissue.
Elemental nitrogen concentration (Total N) was determined by combustion analysis in a C/N analyzer (Model 1500, Caarlo Erba, Cornaredo, Italy. Foliar N was within the expected range reported for well-fertilized sorghum at similar stages of development (ca. 2%) (Reuter et al., 1997).

## 3 DATA FORMAT AND STRUCTURE

**Table 1. Files and their content**

| File Name | Content |
|---|---|
| FACE Sorghum Maricopa growth management weather soil AgMIP.ods | Main spreadsheet with growth, growth stage, yield, daily weather, management, soil moisture, and other data generally used for plant growth model validation. |
| FACE Sorghum physiology.ods | Net assimilation rate, stomatal conductance, total water potential, relative water content |
| 1998 15-min weather canopy & soil temperatures energy balance CO2.ods | 15-minute average weather, $CO_2$ concentrations, canopy temperatures, soil temperatures, net radiation, soil heat flux, sensible heat flux, latent heat flux (evapotranspiration) for 1998. |
| 1999 15-min weather canopy & soil temperatures energy balance CO2 O3.ods | Ditto plus $O_3$ concentrations for 1999. |
| PAR absorption.ods | Fraction of photosynthetically active radiation absorbed by crop canopies |
| Reflectance and vegetation indices.ods | Measurements of canopy reflectance in blue, green, red, and near-infrared wave bands and resultant vegetation indices |
| Midday canopy temperature in all plots.ods | Canopy temperatures from portable infrared thermometer carried from plot to plot near midday on many days during the growing seasons |
| Soil carbon dynamics and isotopic tracing.ods | Air, plant, and soil carbon concentrations and isotopic compositions that trace carbon flows and sequestration |
| Sorghum cyanide and nitrate partitioning.ods | Nitrogen partitioning between cyanide and nitrate in sorghum forage tissues |

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