

MIT Joint Program on the Science and Policy of Global Change



**A Semi-Empirical Representation of the
Temporal Variation of Total Greenhouse Gas
Levels Expressed as Equivalent Levels of
Carbon Dioxide**

Jin Huang, Ray Wang, Ronald Prinn, and Derek Cunnold

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A Semi-Empirical Representation of the Temporal Variation of Total Greenhouse Gas Levels Expressed as Equivalent Levels of Carbon Dioxide

Jin Huang[†], Ray Wang[‡], Ronald Prinn^{†◊} and Derek Cunnold^{‡*}

Abstract

In order to examine the underlying longer-term trends in greenhouse gases, that are driven for example by anthropogenic emissions or climate change, it is useful to remove the recurring effects of natural cycles and oscillations on the sources and/or sinks of those gases that have strong biological (e.g., CO₂, CH₄, N₂O) and/or photochemical (e.g. CH₄) influences on their global atmospheric cycles. We use global observations to calculate monthly estimates of greenhouse gas levels expressed as CO₂ equivalents, and then fit these estimates to a semi-empirical model that includes the natural seasonal, QBO, and ENSO variations, as well as a second order polynomial expressing longer-term variations. We find that this model provides a reasonably accurate fit to the observation-based monthly data. We also show that this semi-empirical model has some predictive capability; that is it can be used to provide a reasonably reliable estimate of CO₂ equivalents at the current time using validated observations that lag real time by a few to several months.

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1. INTRODUCTION

With increasing public attention on changing climate, it is useful to have a “real-time” estimate of a single integrating metric that expresses the combined atmospheric levels of the long-lived greenhouse gases contributing to that change. Such a metric can help convey to the public how fast these levels are increasing, how close we are to the stabilization levels relevant to policy discussions, and the progress, or lack thereof, in slowing the rate of increase. Three key issues that arise in making such a calculation are: (1) long-lived greenhouse gases include multiple gases with varying lifetimes and radiative properties, (2) there are inevitable lags between the time measurements are taken to when they can be checked and assembled to produce an estimate of global average levels (usually expressed as mole fractions), (3) these mole fractions are subject to seasonal and other cyclical variations that need to be removed if we want to clearly reveal the underlying long term trends. In this technical paper, we address these issues by development of a model that fits a suitable integrating metric that is calculated using global network measurements for greenhouse gases. We then evaluate the accuracy with which

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this model can simulate the actual metric, and also provide “real time” estimates of the de-seasonalized metric using its values in the recent past.

First we need a procedure for converting the multiple gases to a common metric. Here we adopt the established approach that converts the observed global average mole fractions of CO₂ and non-CO₂ gases into the equivalent global average mole fraction of CO₂ alone (CO₂-eq in parts per million, ppm) that would yield the same total radiative forcing as the multiple gases (IPCC, 2007; Gohar and Shine, 2007). These CO₂-eq values, when computed on say monthly time scales, show important inter-monthly and inter-annual variations. These are associated with the effects of the natural seasonal cycles, and the natural quasi-biennial (QBO) and El Niño-Southern (ENSO) oscillations on the sources and/or sinks of these gases. This is especially true for gases that have strong biological (*e.g.* CO₂, CH₄, N₂O) and/or photochemical (*e.g.* CH₄) influences on their global atmospheric cycles.

A common approach for examining the underlying longer-term trends in a series with cycles is to calculate running means that extend over the cycle. A 12-month running mean would be needed for a series with an annual cycle, but an even longer running mean would be needed to be assured of removing or smoothing out other cycles. A clear drawback to such running means is that they necessarily lag real time by half of the averaging period. Added to this lag, is the fact that the measurement networks themselves generally report data with a lag of a number of months due to the need to carefully check the measurement precisions and absolute calibrations and to ship samples to central laboratories when air is collected in flasks rather than being measured on site in real time.

The approach we develop is to fit the measurement-based CO₂-eq using a model with basis functions that include the natural seasonal, QBO, and ENSO variations, as well as polynomials expressing longer-term variations. An advantage to this approach is that it provides both the basis for removing or smoothing out cycles in the data, and the remaining de-cycled trend also provides a method for extrapolating ahead to produce an estimate for the current time. The key questions are the accuracy of the model fit to the actual data, and the predictive skill of the model for extrapolations; that is can the model be used to provide a reasonably reliable estimate of CO₂-eq at the current time using validated observations that lag real time by several months or more.

In this technical paper, we use monthly data from NOAA/ESRL (2009a) for global average CO₂, and AGAGE (AGAGE, 2009; Prinn *et al.*, 2000) for global average non-CO₂ gases. We consider only the radiative forcing by those long-lived gases for which reliable continuous global measurements are currently available. For this and other reasons, we exclude shorter-lived radiatively important gases such as tropospheric and stratospheric O₃ and H₂O, aerosols (sulfate, black carbon, *etc.*), land-cover changes, and solar variations from our definition of radiative forcing. In section 2, we describe the process for converting the observed greenhouse gas (GHG) mole fractions into their CO₂ equivalent (which can be reported as either a global average mole fraction (parts per million [ppm] of CO₂-eq) or as a total mass in the atmosphere (metric tons or million grams of CO₂-eq). In section 3, we develop a model for the actual observation-based CO₂-eq that includes known cycles and oscillations in the greenhouse gases. Section 4

evaluates the accuracy of both the model-simulated CO₂-eq and the model projections needed to estimate current levels from past levels. Section 5 provides concluding remarks.

2. CALCULATION OF CO₂ EQUIVALENTS FROM OBSERVED MOLE FRACTIONS

The CO₂ equivalent mole fraction (CO₂-eq in ppm) calculation is made using the basic formula:

$$\text{CO}_2\text{-eq} = C_o \exp (RF_{total}/E_{CO_2}), \quad (1)$$

where C_o is the pre-industrial CO₂ mole fraction, $E_{CO_2} = 5.35 \text{ watts m}^{-2}$ and RF_{total} is the sum of the individual radiative forcings RF_i (watt m^{-2}) for all of the relevant gases (Gohar and Shine, 2007). Specific RF_i formulae are given below for CO₂, CH₄ and N₂O. The radiative efficiencies (E_i ; watt m^{-2}) of all other gases i needed to compute their RF_i values are taken from IPCC (2007). Specifically:

$$\left. \begin{aligned} RF_{CO_2} &= 5.35 \ln(C/C_o); \\ RF_{CH_4} &= 0.036 (\sqrt{M} - \sqrt{M_o}) - (f(M, N_o) - f(M_o, N_o)); \\ RF_{N_2O} &= 0.12 (\sqrt{N} - \sqrt{N_o}) - (f(M_o, N) - f(M_o, N_o)); \\ RF_i &= E_i (X_i - X_{i,0}). \end{aligned} \right\} \quad (2)$$

Here, $f(M, N) = 0.47 \ln [1 + 2.01 \times 10^{-5} (MN)^{0.75} + 5.31 \times 10^{-15} M(MN)^{1.52}]$, M is the CH₄ mole fraction (ppb), N is the N₂O mole fraction (ppb), C is the CO₂ mole fraction (ppm), X_i indicates the mole fractions of other greenhouse gases, i , and the subscripts, 0 , represent the unperturbed (pre-industrial) values. The pre-industrial mole fractions for all gases (see following list) are assumed zero, except for CO₂ ($C_o = 278$ ppm), CH₄ ($M_o = 715$ ppb), N₂O ($N_o = 270$ ppb) and CF₄ ($X_{CF_4,0} = 40$ ppt) (see IPCC, 2007, Table 2.1).

To supply information on how various sub-groups of gases contribute to radiative forcing we have broken the contributions into 5 subgroups:

1. CO₂;
2. CH₄ + N₂O;
3. HFC-23 + HFC-125 + HFC-134a + HFC-152a + SF₆ + CF₄ + C₂F₆;
4. CFC-11 + CFC-12 + CFC-13 + CFC-113 + CFC-114 + CFC-115 + CCl₄ + CH₃CCl₃ + HCFC-22 + HCFC-141b + HCFC-142b + Halon-1211 + Halon-1301 + Halon-2402;
5. HFC-143a + HFC-365mfc + PFC-218 + CH₃Br + HCFC-124 + CH₂Cl₂.

We provide results for CO₂-eq for 4 aggregations of these subgroups: (i) all 5 GHG subgroups together (denoted “All Gases”); (ii) subgroup 1 (denoted “CO₂ Only”); (iii) subgroups 1, 2 and 3 (denoted “Kyoto Gases”; these 3 subgroups contain the major GHGs that are regulated under the Kyoto Protocol for climate change mitigation as listed in Table 2.1, IPCC, 2007); and (iv) subgroups 1, 2, 3, and 4 (denoted “IPCC Gases”; these are the major Kyoto Protocol Gases plus the major GHGs that are regulated under the Montreal Protocol for protection of the ozone layer as listed in Table 2.1, IPCC, 2007). Subgroup 5 contains greenhouse and/or ozone-depleting gases measured by AGAGE but not included in IPCC (2007, Table 2.1).

The global average monthly-mean mole fraction observations used in our CO₂-eq calculations come from NOAA (2009a) for CO₂ and from AGAGE (2009) for all other gases. We use the AGAGE GC-Multi-Detector measurements of CH₄, N₂O, CFC-11, CFC-12, CFC-113, CCl₄ and CH₃CCl₃, and the AGAGE Medusa GC-MS measurements of all other non-CO₂ gases (which have low mole fractions but large E_i (and large Global Warming Potentials (GWPs)). Our calculations start for convenience in January 2004, which is the month when the Medusa measurements started at the Mace Head and Cape Grim AGAGE stations. Global average monthly mean mole fractions (X_i) for the AGAGE data used in the radiative forcing calculations are computed from the 5 primary AGAGE stations using the formula:

$$X_i = X_{i \text{ Mace Head-Ireland}} / 8 + X_{i \text{ Trinidad Head-California}} / 8 \quad (3)$$

$$+ X_{i \text{ Ragged Point-Barbados}} / 4 + X_{i \text{ Cape Matatula-Samoa}} / 4$$

$$+ X_{i \text{ Cape Grim-Tasmania}} / 4.$$

There are occasionally months with no measurements, particularly since the Medusa measurements at 3 of the 5 sites started after 2004. Missing data at Trinidad Head were equated with data from the other northern mid-latitude station at Mace Head and vice-versa. We have filled in for missing months at the tropical stations j (Ragged Point, Cape Matatula) using the formula:

$$X_{ij} = [X_{i \text{ Mace Head}} \langle X_{ij} \rangle / \langle X_{i \text{ Mace Head}} \rangle + X_{i \text{ Cape Grim}} \langle X_{ij} \rangle / \langle X_{i \text{ Cape Grim}} \rangle] / 2 \quad (4)$$

where the annual means $\langle X_{ij} \rangle$ were calculated centered on July 1, 2007 (annual means were calculated by interpolation if there were up to 3 missing monthly values). A minor disadvantage of this approach is the assumption that the ratios did not evolve with time (*i.e.* the annual mean latitudinal gradients did not evolve with time). While more accurate adjustments could be made by using results from a chemical transport model to correct for rapidly evolving latitudinal gradients, the contributions of the most rapidly evolving (percentage-wise) Medusa gases to CO₂-eq is relatively minor.

The radiative forcing (watt m⁻²) derived from observed mole fractions for each of the 5 subgroups is provided in **Figure 1**, and the total CO₂-eq derived from these observation-based radiative forcings is provided in **Figure 2** for the “CO₂ Only”, “Kyoto Gases”, and “IPCC Gases” aggregations. The separate CO₂-eq contributions from each of subgroups 2-5 are not provided in Figure 2 because all of the RF_i contributions must be summed before a CO₂-eq can be calculated. We could make approximate estimates by calculating the CO₂-eq values with and without each of the individual sub-groups, but in that case the individual contributions will not add to give the overall calculated CO₂-eq values due to the exponential dependence of CO₂-eq on RF . Using the total dry atmospheric mass of 5.132×10^{21} gm (Trenberth and Guillemot, 1994) and multiplying by the ratio of the molecular masses of CO₂ (44) and dry air (28.97), a mole fraction of 1 ppm CO₂-eq corresponds to 7.80×10^{15} gm = 7.81 Pg = 7.81×10^9 metric ton of CO₂-eq (see Figure 2 for results in ppm and metric tons).

We compare in **Table 1** our calculations of the total radiative forcing for 2005 with those reported in IPCC (2007, Table 2.1, pg. 141). The agreement between the two calculations is excellent.

Table 1. Radiative forcing (RF, watt m⁻²) and total CO₂ equivalents (ppm) in 2005 reported in IPCC (2007) and in this paper.

Species	IPCC	This paper
RF (CO ₂) (Subgroup 1)	1.66	1.655
RF (CH ₄ + N ₂ O) (Subgroup 2)	0.64	0.648
RF (Other "Kyoto Gases") (Subgroup 3)	0.017	0.018
RF (Montreal Gases) (Subgroup 4)	0.320	0.323
RF ("IPCC Gases") (Subgroups 1-4)	2.637	2.644 (2.646)*
CO ₂ -eq ("IPCC Gases")	455.10	455.70 (455.87)*

*Values for "All Gases" (Subgroups 1-5); these were not reported in IPCC (2007)

To estimate the uncertainty of our CO₂-eq values, we first calculate the standard deviations (1σ) for the global monthly mean mole fractions of all of the observed AGAGE species. For the NOAA global monthly mean CO₂ mole fractions, we use the CO₂ uncertainty from IPCC (2007) in this study (uncertainties are not explicitly stated by NOAA (2009a)). The reported mean and 90% confidence range (*i.e.* 1.645σ) for CO₂ in 2005 is 379 ± 0.65 ppm (Table 2.1, page 141, IPCC, 2007), corresponding to a 0.1% error. We therefore multiply the observed CO₂ mole fractions by 0.001 to estimate uncertainties (σ_{X_i} in ppm) for each month.

The radiative forcing and uncertainty (in watt m⁻²) from each individual compound, i , can then be calculated using equations (2). Specifically, we first calculate the mean radiative forcings by using the monthly mean mole fractions, X_i . A second set of radiative forcings is then calculated using $X_i + \sigma_{X_i}$ as the mole fractions. The differences between the two sets are taken as the uncertainties σ_{RF_i} in the calculated radiative forcings, RF_i . The total radiative forcing and its uncertainty then can be calculated using

$$\begin{aligned}
 RF_{total} &= \sum_{i=1}^n RF_i \\
 \sigma_{RF_{total}} &= \sqrt{\sum_{i=1}^n \sigma_{RF_i}^2}
 \end{aligned}
 \tag{5}$$

where n is the number of gases. The CO₂-eq values then can be calculated with equation (1). A second set of CO₂-eq values is then calculated by replacing RF_{total} with $(RF_{total} + \sigma_{RF_{total}})$, and the difference provides the estimated uncertainty (1σ) of CO₂-eq values in this study.

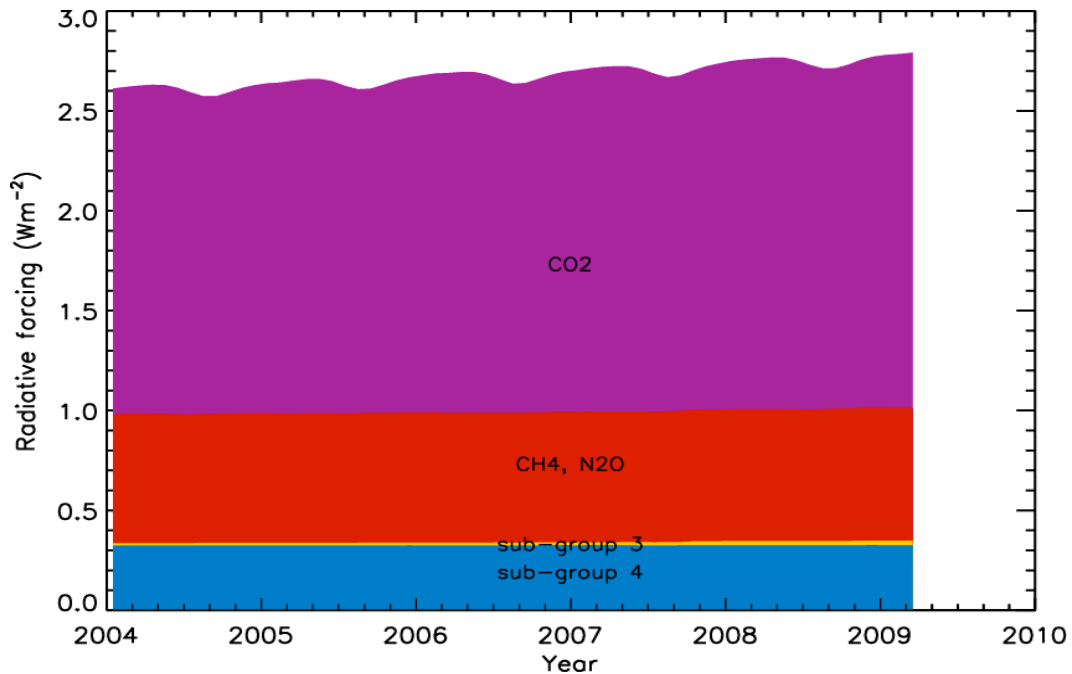


Figure 1. Radiative forcing by GHG sub-groups: (1) CO₂; (2) CH₄ + N₂O; (3) HFC-23 + HFC-125 + HFC-134a + HFC-152a + SF₆ + CF₄ + C₂F₆; (4) CFC-11 + CFC-12 + CFC-13 + CFC-113 + CFC-114 + CFC-115 + CCl₄ + CH₃CCl₃ + HCFC-22 + HCFC-141b + HCFC-142b + Halon-1211 + Halon-1301 + Halon-2402; (5) HFC-143a + HFC-365mfc + PFC-218 + CH₃Br + HCFC-124 + CH₂Cl₂. The radiative forcing by subgroup (5) is not resolved in the Figure since it accounts for only about 0.0016 watt m⁻² in 2004 and 0.0025 watt m⁻² in 2009.

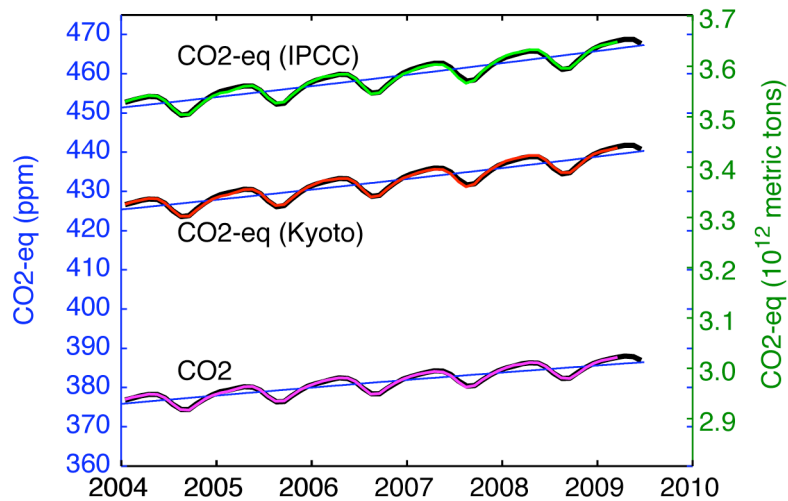


Figure 2. Total CO₂-eq (ppm on left-hand scale and metric tons on right-hand scale) from observed GHG mole fractions (oscillating colored lines), full 6-term equation (6) fit to the observations (oscillating black lines), and 3-term Legendre polynomial only fit to observations (smooth blue lines), for the “CO₂ Only”, “Kyoto Gases” and “IPCC Gases” cases. The “All Gases” case is only 0.2 ppm above the “IPCC-Gases” case and is not shown as it would be indistinguishable on the scale of the graph.

3. MODEL FOR OBSERVED CO₂-EQ VALUES AND APPLICATION TO EXTRAPOLATION TO CURRENT TIME

The monthly CO₂-eq values are fitted using the following 6-term semi-empirical function:

$$CO_2 - eq = F_0 \cdot P_0 + F_1 \cdot (nP_1) + F_2 \cdot \left(\frac{1}{3} n^2 P_2 \right) + F_3 \cdot Annual + F_4 \cdot ENSO + F_5 \cdot QBO. \quad (6)$$

Here, F_i are factors to be determined using optimal estimation, P_j are Legendre polynomials, n is the mid-point and t_0 is the starting-point of the time period of the available measurement-based CO₂-eq data (section 2), and

$$\left. \begin{aligned} P_0(x) &= 1, \\ P_1(x) &= x, \\ P_2(x) &= \frac{(3x^2 - 1)}{2}, \\ x &= \frac{t - t_0}{n} - 1. \end{aligned} \right\} \quad (7)$$

The Annual term is the time averaged annual cycle in the measurement-based CO₂-eq data, the ENSO term is the normalized monthly multivariate El Niño Southern Oscillation index (MEI) available from NOAA (2009b), and the QBO term is the normalized monthly quasi-biennial oscillation index available from NOAA (2009c).

A simple first order linear fit is obtained for the measurement-based CO₂-eq data and the coefficients from this fit are used as the first guess (*a priori*) estimates for the F_i factors. Optimal estimates of the F_i factors are then determined from the measurement-based CO₂-eq values and their errors in a subsequent recursive weighted least squares (Kalman filter) inversion (see *e.g.*, Prinn, 2000). The above empirical function with the optimally estimated F_i factors can then used to extrapolate the measurement-based CO₂-eq values to the present time.

The QBO and ENSO index reports usually lag real time, so the time-averaged monthly QBO indices and the most recent available monthly ENSO MEI indices are used whenever the actual measured indices are not available. This is not a significant issue since we find that the ENSO and QBO terms are relatively minor contributors to the CO₂-eq values for 2004-2009 compared to the other 4 terms. However, the 2004-2009 time period did not contain a significant El Niño so the importance of ENSO will need to be re-assessed when we enter a future El Niño by considering observations at least back to the last major El Niño in 1998 (note that we do not have continuous global observations of some of the sub-group 3-5 gases prior to 2004).

4. ACCURACY AND PREDICTIVE CAPABILITY OF MODEL

To measure how well the full 6-term expression (equation 6) for CO₂-eq compares to the monthly CO₂-eq computed from observations, the root mean square differences (RMSDs) have been calculated. For both the “All gases” and “Kyoto gases” cases, RSMD = 0.3 ppm, indicating that equation (6) provides a very good fit to the actual values. To examine whether the influences of the 3 oscillating terms in equation (6) integrate to approximately zero over time (*i.e.* that the

3-term polynomial expression by itself accurately simulates the longer-term trends in CO₂-eq (with the seasonal, QBO and ENSO oscillations removed), the sum of the differences between the full 6-term fit and the 3-term polynomial fit CO₂-eq values have been calculated. The summations of the differences are indeed negligible (0.1 ppm for both the “All gases” and “Kyoto-only” cases).

To estimate how accurately the 3 polynomial terms in equation (6) can forecast the equivalent observation-based CO₂-eq values (with oscillations removed) for 3 months into the future, we compared the 3-month forecasts with the values obtained when the next three months of observations were used to obtain an updated fit. The average differences between the forecasted and updated values using the 3-term polynomial CO₂-eq expression is only 0.05 ppm for both the “All gases” and “Kyoto Gases” cases. Thus, this 3-term expression provides a very accurate fit to the observation-based data with oscillations removed, and it has some predictive capability; that is it can be used to provide a reliable estimate of CO₂-eq at the current time using validated observations that lag real time by a few to several months.

5. CONCLUDING REMARKS

We have shown that a fit to monthly estimates of CO₂-eq from observations using basis functions that include the natural seasonal, QBO, and ENSO variations, as well as a second order polynomial expressing longer-term variations, provides a reasonably accurate fit to the observation-based data. We have also shown that this semi-empirical model has some predictive capability; that is it could be used to provide a reasonably reliable estimate of CO₂-eq at the current time using validated observations that lag real time by a few to several months.

In order to examine the underlying longer-term CO₂-eq trends (driven for example by anthropogenic emissions or climate change), it is useful to remove the recurring effects of the natural seasonal cycles, and the natural QBO and ENSO oscillations on the sources and/or sinks of gases that have strong biological (*e.g.*, CO₂, CH₄, N₂O) and/or photochemical (*e.g.*, CH₄) influences on their global atmospheric cycles. We have shown that the 3-term polynomial in equation (6) provides a reasonably accurate simulation of the longer-term trends in CO₂-eq with the seasonal, QBO and ENSO effects removed. We caution that the time period examined did not include a strong El Niño, so our current equation (6) coefficients (that show that the ENSO had only a small influence on CO₂-eq during 2004-2009) will need to be re-estimated should we enter a strong El Niño. We emphasize that total radiative forcing (watt m⁻²) or CO₂ equivalents (ppm or metric tons) refer to current and past greenhouse gas levels and their radiative effects. Because they do not explicitly take into account differences in the atmospheric lifetimes of GHGs, long-term forecasts (*i.e.* beyond the few to several month time scales addressed in this paper) require the use of models that incorporate explicit treatments of GHG sources and sinks. The use of GWPs (Global Warming Potentials) that convert emissions of non-CO₂ GHGs into equivalent emissions of CO₂ do approximately take into account these lifetimes, but they refer of course to GHG emissions not atmospheric levels. We also note that these estimates focus on the long-lived greenhouse gases and therefore do not include a number of other contributors to

radiative forcing. A major hurdle for extending our approach to these other contributors is the lack of relevant continuous and accurate global measurements for them. Metrics like the CO₂-eq addressed here can be useful in tracking the growing risks we face from climate change. The calculation of this metric underscores the value of existing observational networks, the need to maintain such networks, and the advantages of extending the continuous global observational capabilities to include as many contributors to forcing of climate change as possible.

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