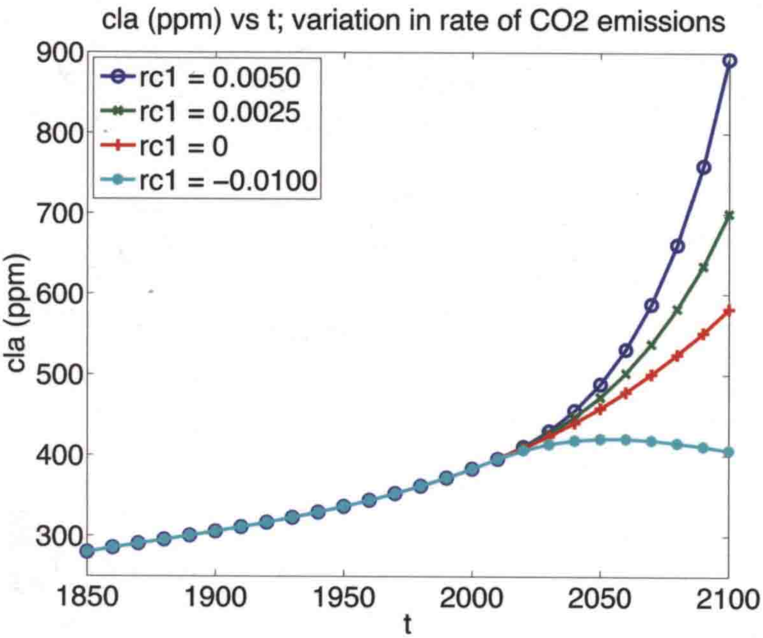
An Introductory Global CO_2 Model



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World Scientific

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with Companion Media Pack

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To Svante Arrhenius and Charles Keeling

PREFACE

The consequences of rising concentrations of atmospheric CO_2 are receiving increased attention in the news media as a major contributor to extreme climate change and global warming. For example, from the *New York Times* [12] and restated in Appendix D of this book:

> "Scientific monitors reported that the gas (CO_2) had reached an average daily level that surpassed 400 parts per million (ppm) — just an odometer moment in one sense, but also a sobering reminder that decades of efforts to bring human-produced emissions under control are faltering. The best available evidence suggests the amount of the gas in the air has not been this high for at least three million years, before humans evolved, and scientists believe the rise portends large changes in the climate and the level of the sea."

And from [14], "Climate-related disasters around the world (include): hurricanes and tornadoes, droughts and wildfires, extreme heat waves and equally extreme cold, rising sea levels and floods. Even when people have doubts about the causal relationship of global warming to these episodes, they cannot help being psychologically affected. Of great importance is the growing recognition that the danger encompasses the entire earth and its inhabitants. We are all vulnerable."

However, the CO_2 problem is not well understood quantitatively by a general audience. Although some measures of atmospheric CO_2 accumulation have been reported such as the 400 ppm from the 10 May 2013 *New York Times* noted above, other measures are less well understood, e.g., the increasing rate of CO_2 emissions, the movement of carbon to and from other parts of Earth's environmental system, particularly the oceans with accompanying acidification.

A mathematical model can be particularly informative and helpful for understanding what is happening. We therefore present an introductory global CO_2 model that gives some key numbers, for example, atmospheric CO_2 concentration in ppm and ocean pH as a function of time for the calendar years 1850 (preindustrial) to 2100 (a modest projection into the future).

The model is based on just seven ordinary differential equations (ODEs) and is therefore intended as an introduction to some basic concepts and as a starting point for more detailed studies. The ODEs are carbon balances for seven reservoirs: upper atmosphere, lower atmosphere, long-lived biota, short-lived biota, ocean upper layer, ocean deep layer and marine biosphere.

Basic calculus is the only required mathematical background, e.g., derivatives and integration, so that the model is accessible to high school students as well as beginning college and university students. Specifically, the ODEs define derivatives of the form dy/dt where y is a dimensionless reservoir carbon concentration and t is time as a calendar year over the interval $1850 \leq t \leq 2100$. The ODEs are integrated numerically to give $y(t)$. The solutions are presented numerically and graphically. The essential mathematical concepts are embedded in the fundamental theorem of calculus:

$$\int_{t_0}^{t} (dy/dt)\, dt = y(t) - y(t_0),$$

where $t_0 = 1850$ and $y(t_0)$ is the ODE initial condition (IC). The integration is carried out numerically by library initial-value ODE integrators.

Some background in computer programming would also be helpful, but not essential. The programming of the model is in R[1] and Matlab,[2] two basic, widely used scientific programming systems. Thus, it can be executed on modest computers and is generally

[1]R is an open source scientific programming system that can be downloaded (no cost) from the Internet.

[2]Matlab is a commercial product available from the Mathworks, Natick, MA. Octave is an open source (no cost) alternative that will run the Matlab code with minimal changes.

accessible and usable worldwide. The book could also be used by readers interested in Matlab and/or R programming or a translation of one to the other. This additional use is facilitated by a side-by-side format of sections of R and Matlab code with a comparison of the two.

The model includes ocean chemistry calculations that address acidification with ocean pH as an output, typically ranging from 8.2 to 7.8 (pH decreases with increasing acidity). These calculations illustrate some basic numerical procedures, such as a Newton solver applied to a fourth-order polynomial to calculate ocean pH and spline interpolation to provide additional model outputs. The problem of acidification has important implications for a major food source, deterioration of coral and the associated marine life, as well as ocean CO_2 uptake [9].

A basic global warming component has been added based on CO_2 buildup in the lower atmosphere but since climate change (e.g., warming) is still a controversial and uncertain area, the primary focus is on carbon buildup in the atmosphere and oceans which is being measured quantitatively and is therefore undisputed.

Our intention is to provide a quantitative introduction to the CO_2 problem so that the model is basic and educational, and is not a state-of-the-art research model. We hope that the model serves this educational purpose, and we welcome comments, questions about model implementation and use, and suggestions for improvements (directed to wes1@lehigh.edu).

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July 1, 2015

CONTENTS

1 INTRODUCTION

The anticipated changes in the Earth's climate that are now widely discussed are due in large part to the accumulation of so-called greenhouse gases (GHGs) in the Earth's atmosphere. The increase in GHGs causes a reduction in the re-radiation of energy from the Sun back into outer space. Since less energy leaves the Earth's atmosphere, heating of the atmosphere results in a temperature rise. This temperature rise, so-called global warming, is in turn a driving force for climate change.

Carbon dioxide (CO_2) is the major GHG, with increasing levels arising primarily from the burning of fossil fuels. Thus, changes in CO_2 level or concentration in the Earth's atmosphere is of paramount importance in understanding anticipated warming and climate change. A second aspect of CO_2 accumulation in the atmosphere that is not as generally recognized and appreciated as temperature rise is the accumulation of carbon (from CO_2) in the oceans that leads to ocean acidifcation. CO_2 dissolves in ocean water and undergoes a series of chemical changes that ultimately leads to increased hydrogen ion concentration, denoted subsequently as $[H^+]$, and thus acidification. This increase in $[H^+]$ is manifested as a decrease in pH; note that $[H^+]$ and pH move in opposite directions due to the basic relation[1]

$$pH = -log_{10}[H^+]. \tag{1.1}$$

[1] log_{10} indicates a base-10 logarithm. To briefly review, a number (real, nonnegative) can be expressed as $c = b^a$ where a is the logarithm (log) of c to the base b (e.g., 10; e = 2.718282, the base of the "natural" logarithm system). An important application of logs is to facilitate the multiplication or division

For example, if $[H^+] = 10^{-8}$, $pH = 8$ while if $[H^+] = 10^{-7}$, $pH = 7$.

As a point of notation, square brackets placed around a chemical formula, e.g., $[H^+]$, denotes a molar concentration. The units of concentration are typically mols/liter, millimols/liter or micromols/liter (where liter is a liter of aqueous solution). Since for H_2O one liter weighs one kilogram (kg) (because the density of H_2O is 1 g/milliliter = 1 g/cc with 1 liter = 1000 milliliters), these concentrations are also in reciprocal kg. For the purpose of using Eq. (1.1) to calculate pH, $[H^+]$ is in g mol/liter = kg mol/m^3.

Also, mols are taken specifically as g mols. One g mol of a chemical quantity has a weight equal to its atomic or molecular weight in g. For example, H_2O has a molecular weight of $2(1) + 16 = 18$ g. Thus, one g mol of H_2O is 18 g.

The causes for changing environmental CO_2 levels are complex and not completely understood. But increasing atmospheric CO_2 is clearly established through measurements over more than 50 years [8]. Enough is known about CO_2 accumulation[2] to begin to formulate quantitative descriptions of the various physical and chemical processes that determine CO_2 levels with the goal of projecting[3]

of numbers. For example, two numbers $c_1 = b^{a_1}, c_2 = b^{a_2}$ can be multiplied as $c_1c_2 = b^{a_1}b^{a_2} = b^{a_1+a_2}$, that is, the logs are merely added, followed by an antilog or inverse log (the common base b is raised to the power $a_1 + a_2$) to obtain the product. Similarly, for division, $c_1/c_2 = b^{a_1}/b^{a_2} = b^{a_1}b^{-a_2} = b^{a_1-a_2}$ so that the logs are subtracted to give the quotient c_1/c_2.

[2]The literature pertaining to CO_2 is extensive and expanding rapidly so that any attempt at a comprehensive survey of the literature would necessarily be limited and soon out of date. Therefore, only references that are used in the subsequent discussion of the model are included in the bibliography which also includes sources that the reader can access for the most current information, for example, the Carbon Dioxide Information Analysis Center, http://cdiac.esd.ornl.gov/. Other general sources of information include [1, 5, 6, 7, 10, 11, 13, 16–20, 22, 28–30]. The emphasis of the following discussion is therefore on the description and computer implementation of the model.

[3]The word *projection* is used rather than *prediction* to suggest that the model output reflects a plausible future scenario and not a certain outcome in the future. Various scenarios can then be considered based on postulated changes in the model, e.g., the CO_2 emissions rate.

how atmospheric CO_2 levels might be expected to increase in the future. To this end, we describe here an introductory global CO_2 model that elucidates at a basic level the mechanisms which determine CO_2 buildup in the Earth's atmosphere.

The model is necessarily a simplification of the physical and chemical processes at work that determine CO_2 levels. However, the model provides insight into CO_2 dynamics (the variation of CO_2 levels over time); specifically, it can be used to study the effect of various phenomena and parameters that determine CO_2 levels, and how they change with time.

In particular, the effect of variations in the rate of anthropogenic emissions can be assessed. This is accomplished by the numerical integration of a system of ordinary differential equations (ODEs) starting with known conditions in the past (for example, at 1850, but this starting year can easily be changed). The forward integration of the ODE model equations through time can be to an arbitrary point in the future (for example, to 2100, but this final year can also easily be changed). The details of the ODE model, and some representative output from the model, are discussed subsequently.

A major advantage of a computer-based mathematical model is the execution of the associated computer code[4] for the solution of the model equations to observe the effect of postulated conditions, e.g., the rate of anthropogenic CO_2 emissions. Thus, although only a limited set of model outputs is considered here, the code can easily be executed for other conditions to observe the effect of the model structure and parameters on projected CO_2 levels. Ideally, this process should elucidate the most relevant and sensitive conditions that determine future CO_2 levels, and thereby give an indication of plausible future CO_2 changes.

The model focuses only on CO_2. It does not have a climate component and it has only a basic global warming component consisting

[4]The coding is for two well established scientific computing systems: (1) Matlab, a commercially available programming system and (2) R, an open-source programming system available from the Internet. The details for using Matlab and R as applied to the CO_2 model are subsequently discussed in detail.

of multiplication of atmospheric CO_2 (in ppm) by a temperature sensitivity. While the current levels of CO_2 are relatively well known from measurements, the net effect of CO_2 on the Earth's climate is not well understood quantitatively at this point in time. Thus we have limited the model to CO_2 dynamics as a main determinant of global warming and climate, but we do not attempt to explain the resulting dynamics of anticipated global warming and climate change.

The model does, however, have as an output ocean H^+ and pH as a function of time. As with atmospheric CO_2, the long-term effects of ocean acidification are not completely understood at this point in time. However, two relatively well established effects can be observed:

- The ocean pH is decreasing and this can be measured.
- The effect of acidification on coral is being observed. We take $CaCO_3$ as the main component of coral, and the basic chemistry relating $CaCO_3$ and H^+ is considered toward the end of this discussion.

Of course, other important effects of acidification could be considered, for example, on the ocean biosphere, but they are not included in the model. No doubt these effects will be important and will be elucidated with future research.

2 MODEL STRUCTURE

The model structure [2], [27] is illustrated in Fig. 1.

- Seven reservoirs are used to represent the global CO_2 system:
  1. Upper atmosphere
  2. Lower atmosphere
  3. Short-lived biota
  4. Long-lived biota
  5. Upper ocean layer
  6. Deep ocean layer
  7. Marine biosphere

  These seven reservoirs were selected because each is considered to have an important effect on the global CO_2 dynamics. However, reservoirs can easily be added (or removed) from the mathematical model that is discussed subsequently.
- Within each reservoir, we consider CO_2 (and related carbon concentrations). As the most basic approach, we consider only one uniform CO_2 concentration in each reservoir. In other words, we neglect any spatial variation in CO_2 concentration. This assumed uniformity in space is, of course, an idealization and major research efforts are underway to elucidate spatial variations in CO_2 concentrations, particularly in the oceans. However, for our purpose of developing a basic model, we will assume spatial uniformity, sometimes termed perfect mixing or complete mixing [27].
- Thus, the CO_2 concentration in each reservoir varies only with time, and we are therefore using ODEs in time as the basic mathematical structure of the model (generally, ODEs have only one independent variable which in our analysis is time, denoted

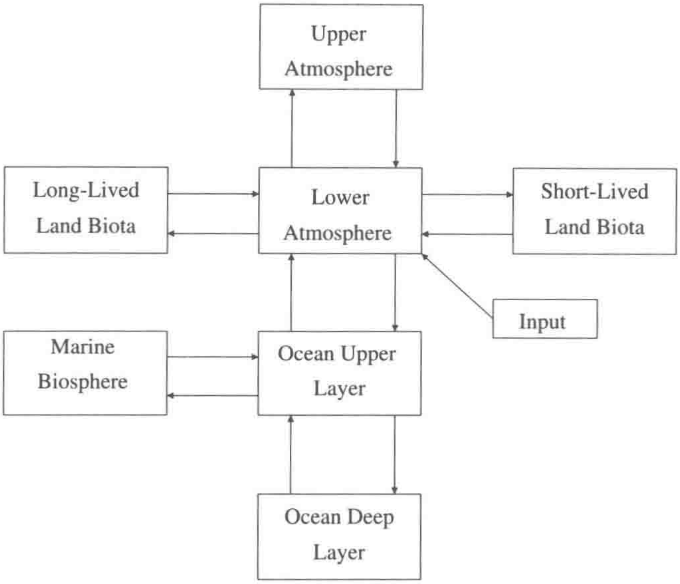

Figure 1: Diagram of the global CO_2 model

as t). Integration of the ODE system with respect to t gives the time variation of the reservoir concentrations, starting from an initial condition specified at the calendar year 1850.

- The time variation of the reservoir concentrations is driven through time by the anthropogenic emission of CO_2 to the lower atmosphere, identified as "input" in Fig. 1. This input is generally termed an emission rate.

3 MODEL EQUATIONS

As a significant simplification, only one CO_2 concentration in each reservoir is considered (by the perfect mixing assumption [27]), and the seven concentrations are identified mathematically as

Table 1: Model dependent variable concentrations

Concentration	**Reservoir**
$y_{ua}(t)$	upper atmosphere
$y_{la}(t)$	lower atmosphere
$y_{sb}(t)$	short-lived biota
$y_{lb}(t)$	long-lived biota
$y_{ul}(t)$	ocean upper layer
$y_{dl}(t)$	ocean deep layer
$y_{mb}(t)$	marine biosphere
t	time (calendar year)

The concentrations in Table 1 have the dimensionless form

$$y(t) = \frac{c_{\text{dim}}(t) - c_{\text{dim}}(t = 1850)}{c_{\text{dim}}(t = 1850)}, \tag{3.1}$$

where $c_{\text{dim}}(t)$ is a dimensional concentration with units, e.g., for the upper and lower atmospheres, the dimensional concentrations might be in parts per million, ppm (interpreted as μatm), or GtC (gigatons