

A Mathematical Logistic Model Describes Both Global CO₂ Emissions and its Accumulation in the Atmosphere

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Abstract

A single kinetic model, of a logistic nature, is able to describe two different phenomena: the global emission of CO_2 due to the combustion of fossil fuels and the observed accumulation of CO_2 in the atmosphere. Unexpectedly, the analysis of the experimental data clearly shows that the two rates of emission and accumulation are almost exactly in phase and differ by a constant factor. The fraction of CO_2 that accumulates in the atmosphere is constantly equal to 65% of the emissions. The same percentage also applies to the rate of change of the two phenomena, i.e., the accelerations.

Introduction

The aim of this study is to carry out a comparative analysis between global anthropogenic CO_2 emissions resulting from the combustion of fossil fuels and the observed atmospheric accumulation of CO_2 . A logistic mathematical model is used for the comparative analysis. Research methods capable of detecting weak signals of changes in the rate of CO_2 accumulation are welcome, since the excess atmospheric concentration of CO_2 compared to the pre-industrial era is the main cause of the increase in the greenhouse effect, which in turn causes global warming. Research methods that can anticipate this type of information are of great scientific and managerial value. In a recent article, Hansen et al. (2023), [1] carried out this comparison using a different methodology. Studying the two phenomena simultaneously adds value that cannot be obtained by studying emissions and atmospheric accumulation of CO_2 separately.

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Investigation Procedure and Results

The construction of the logistic model starts from the material balance applied to global CO_2 emissions. We know that part of the CO_2 emissions accumulates in the atmosphere and part disappears, most likely due to the (diurnal) photosynthetic sequestration activity of terrestrial organisms, savannahs and tropical forests and marine organisms, according to the stoichiometric equation, Figure 1:

$$6 \operatorname{CO}_2 + 6 \operatorname{H}_2 \operatorname{O} \xrightarrow{h\nu} \operatorname{C}_6 \operatorname{H}_{12} \operatorname{O}_6 + 6 \operatorname{O}_2$$

Figure 1. Stoichiometric equation of photosynthesis.

Photosynthesis takes place in the presence of sunlight and produces glucose and oxygen from water and carbon dioxide. The reverse process (at night) produces CO_2 and H_2O . Not all the glucose takes part in the reverse process: a significant proportion is transformed into stable products (lignin, cellulose...) which actually bind the inorganic carbon of the CO_2 . In general, the three rates at which the three phenomena of emission, sequestration and accumulation of CO_2 occur will be different. Consequently, we will be able to write, provisionally, that the material balance must satisfy the block relation, Figure 2:



Figure 2. Block diagram of the material balance of CO_2 emissions. Numbers in brackets give the breakdown among the blocks, estimated in this work.

Photosynthesis plays a crucial role in the fate of CO_2 , in particular in the kinetics of its evolution over time: an increase in the atmospheric concentration of CO_2 will inevitably stimulate an increase in photosynthetic activity, probably with a certain delay. The analysis of experimental data will provide useful elements to evaluate this delay.

Note that we have primary experimental data on the emission rate (IEA data in Gt/year, [2]), but not on the accumulation rate. Instead, we have the primary experimental data, [3], [4], [5] of the Keeling curve, in ppmv, i.e. we have the primary data of the integral of the accumulation rate. Consequently, the comparison between the two kinetics, emission and accumulation, can only be made after the experimental data have

been made compatible, e.g. by calculating the derivative of the accumulation concentration in the atmosphere using a suitable method. For the analytical approximation of all the experimental data, a single logistic model is used which, in the differential formulation, serves to approximate the IEA data on the rate of global CO_2 emissions, while in the integral formulation it serves to approximate the data on CO_2 accumulation in the atmosphere, provided by the Keeling curve. Finally, the analytical derivative of this integral function approximating the Keeling curve will provide the rate of accumulation of CO_2 in the atmosphere. At this point, the two rates are comparable.

Unexpectedly, the analysis of the experimental data clearly shows that the two rates, emission and accumulation, are almost exactly in phase and differ from year to year by a constant factor of 0.65. In other words, the fraction of the rate of CO_2 accumulation in the atmosphere is equal to 65% of the rate of emissions. From the block diagram of the material balance in Figure 2, we can deduce that the rate of CO_2 sequestration is also in phase, i.e. there is no lag. Furthermore, we can clearly attribute CO_2 sequestration to photosynthetic activity. Since photosynthesis is proportional to the atmospheric/marine CO_2 concentration, it will increase each year with the resumption of vegetative activity, according to the air/water partition coefficient of CO_2 .

Logistic Mathematical Model

The description of the growth kinetics of global CO_2 emissions could be made by referring to classical models of population dynamics, but in this work, it was preferred to build a growth model by a judicious adaptation of Avrami's crystal growth theory [6]. According to this theory, any growth process can be described as the result of three phenomena: the birth of the growth nuclei of the specific phenomenon in the mass of possibilities (nucleation kinetics), the subsequent growth around these nuclei (actual growth) and the arrest of growth when the growing nuclei comes into contact with another interfering competitor. The obstruction means that there is no more free growth space available, as it has already been occupied by the approaching competitor. This third step is commonly referred to as "impingement". Under the special condition that both nucleation and growth kinetics obey the same rules of evolution (isokinetic hypothesis), it is possible to combine the three phenomena into a single equation for cumulative growth. To facilitate the analytical treatment of the equations, we will use the cumulative growth model developed by Tobin, [7]. Scheme 1 lists the model equations in both differential and integral formulations. Previously the author adapted this model to describe the global polypropylene market, [8] and the Covid19 coronavirus epidemic in China, [9].

$\chi = W_a/W_\infty$	(1)
$\frac{d\chi}{dt} = k \cdot f(\alpha, \chi)$	(2)
$f(\alpha,\chi) = \alpha \cdot \chi^{1-\frac{1}{\alpha}} \cdot (1-\chi)^{1+\frac{1}{\alpha}}$	(3)
$W_a(t) = W_{\infty} \cdot \frac{(kt)^{\alpha}}{1 + (kt)^{\alpha}}$	(4)
$\frac{d^2 X}{dt^2} = k \alpha \left(\frac{X}{1-X}\right)^{-\frac{1}{\alpha}} \left[\left(1-\frac{1}{\alpha}\right) - 2X\right] \frac{d\chi}{dt}$	(5)

Scheme 1

In the scheme 1, the dimensionless variable χ expresses the relationship between the current concentration of CO₂, described by the symbol W_a , and the concentration in the atmosphere reached at the end of the fossil fuel era, W_{∞} (Eq. 1). In other words, the parameter γ can take values between zero, at the beginning of the phenomenon, and one at the end, when it reaches the value W_{∞} . A first-order ordinary differential equation in the variable χ (Eq. 2) describes the kinetic growth rate of CO₂. The initial condition is: $\chi(0)$ = zero, i.e. zero concentration at the beginning of the phenomenon. Equation (2) describes the behavior of the absolute annual growth rate of CO_2 . The kinetic constant k has the dimensions of the inverse of a time and is a descriptor of the characteristic time of the temporal evolution of the growth phenomenon. The shape factor $f(\alpha, \chi)$ takes the analytical expression of equation (3). This function tells us that CO_2 grows proportionally to the value assumed by the concentration, with a sublinear trend given by the factor $\chi^{1-\frac{1}{\alpha}}$; it also tells us that the growth does not continue indefinitely, but gradually dies out as the concentration approaches the limit W_{∞} , with a superlinear trend given by the factor $(1-\chi)^{1+\frac{1}{\alpha}}$. The positive real number α is a convenient shape parameter for the initial and final curvature of the kinetics.

Equation (4) is the analytical integral of the growth kinetics. It gives the accumulation curve $W_a(t)$ up to time (t). This equation has the form of a logistic function: initially it grows rapidly, with the behavior of the power function $(kt)^{\alpha}$, then it gradually slows down and finally reaches a plateau. From the analytical solution we can see immediately that if the current time t is such that (kt) = 1, then the dimension of the phenomenon reaches the value $\chi = 1/2$, i.e. 50% of the maximum accessible value. The kinetic

constant (k) therefore corresponds to the inverse of the half-life of the growth phenomenon.

The curve described by equation (2) represents the rate of the phenomenon; therefore, we will use this equation to approximate the experimental global emissions of CO₂ into the atmosphere, (IEA data). Equation (4) gives the integral of the rate curve; therefore, we will use this equation to approximate the experimental data of CO₂ accumulation in the atmosphere (Keeling curve data). Both approximations of the experimental data require the knowledge of the three free parameters (W_{∞} , k, α), which can be obtained by an appropriate parameter identification procedure [10].

Analysis of Experimental Data: - Atmospheric CO₂ Accumulation

We will use the experimental data on CO_2 accumulation in the atmosphere, described by the Keeling curve in Figure 3, and approximate it analytically using the integral logistic equation (4). These data, together with the time when the phenomenon of CO_2 accumulation in the atmosphere began (around 1800), cover a period of more than 200 years and allow us to identify with sufficient reliability the three free parameters (W_{∞}, k, α) that allow the best approximation to the experimental data, Table 1.



Figure 3. Experimental data on the global accumulation of CO_2 in the atmosphere. Atmospheric CO_2 concentration (1750-1970) from ice cores taken from the Siple Antarctic station [3], [4] and direct measurements (1959-2023) from the Mauna Loa observatory [5].

$W_{\infty}(A)$	k	α
[ppmv]	[1/years]	[dimensionless]
1300	1/327	5.7

Table 1. Identified parameters of the global process of accumulation of CO_2 in the atmosphere described by the experimental points of the Keeling curve. Note that the half-life of the CO_2 accumulation is 327 years.

Inserting the identified parameters from Table 1 into the corresponding equation of scheme 1 allows the analytical calculation of both the accumulation, equation (4), and the rate of accumulation of CO_2 in the atmosphere, equation (2). The logistic model acts as a smoothing tool of the raw experimental data of the global amount of CO_2 . The continuous black curve in Figure 3 represents the analytical logistic approximation to the global amount of CO_2 , while the dashed black curve describes the analytical growth rate of CO_2 in the atmosphere. Calculating the growth rate by analytical derivation is a reliable and effective method. On the contrary, it is inadvisable to calculate the rate by direct numerical differentiation of raw experimental data.

Analysis of Experimental Data: - Global CO2 Emissions

Global emissions data represent the annual amount of CO₂ released into the atmosphere. They therefore have the character of a rate. The analytical approximation of these data requires the use of the differential logistic equation, (2). In principle, we could approximate the IEA, International Energy Agency, [2] data by leaving the three kinetic parameters ($W_{\infty}(E), k, \alpha$) completely free. However, it can be verified a posteriori that the experimental data, combined with the time when the phenomenon of CO₂ accumulation in the atmosphere began (around 1800), allow us to identify the three free parameters ($W_{\infty}(E), k, \alpha$) by varying only the intensive parameter $W_{\infty}(E)$, leaving the other two unchanged. The three parameters identified in Table 2 give the best analytical approximation (Figure 4) to the IEA experimental data [2].



Figure 4. Analytical approximation to IEA experimental data of global CO_2 emissions, [2], by the differential logistic function, Eq. (2).

$W_{\infty}(E)$	k	α
[ppmv]	[1/years]	[dimensionless]
2010	1/327	5.7

Table 2. Identified parameters of the differential logistic function, Eq. (2) which approximates experimental global CO₂ emissions, (IEA data, [2]). Note that the half-life of the emissions is 327 years.

Let us summarize the process of approximating the experimental data described above. The complete procedure required three steps:

1. Analytical approximation of the Keeling curve, (experimental data of CO_2 accumulation in the atmosphere), by identifying the three free parameters, $(W_{\infty}(A), k, \alpha)$, of the logistic integral function, equation (4).

2. Analytical derivation of the logistic curve to obtain the growth rate of CO_2 in the atmosphere, equation (2).

3. Analytical approximation to the IEA experimental data on global CO₂ emissions by a growth rate function of the same form as in step 2, but augmented by an appropriate constant factor. The identified emission parameters are now, $(W_{\infty}(E), k, \alpha)$, where $(W_{\infty}(A) = .65 \cdot W_{\infty}(E))$.

Comparing the Two Processes: Global Emissions and Atmospheric Accumulation of $\ensuremath{\text{CO}}_2$

It is of considerable interest to make a quantitative assessment of the rate of change of the two phenomena: emissions and atmospheric accumulation of CO_2 . This can be done by comparing the two differential logistic curves, which represent the rates of change of the two phenomena. The graph in Figure 5 shows the overlap between the two rates.



Figure 5. Comparison of the rates of emission, atmospheric accumulation and sequestration of CO_2 by the differential logistic function, Eq. (2).

By visual inspection of Figure 5, we can make the following observations: The accumulation rate of CO_2 in the atmosphere is always lower than the emission rate and is approximately equal to 65% of emissions. This fact indicates that an annual phenomenon

of absorption of part of the CO_2 emitted is active, most likely by photosynthetic terrestrial and marine organisms. This organic CO_2 fixation represents the annual sequestration rate.

The gap between the emission rate and the accumulation rate increases progressively until the year 2100, when emissions, accumulation and sequestration peak at 8.95 ppmv/year and 5.84 ppmv/year and 3.19 ppmv/year respectively (Hubbert's peak). They then begin to fall to zero, starting around 2100, at the Hubbert peak. The whole process takes several centuries.



Figure 6. Comparison of accelerations (CO_2 emission and accumulation) calculated using the second derivative of the logistic function, equation (5). Superimposing the growth rate graphs facilitates comparison.

The graphs in Figure 6 describe the second derivative of the differential logistic equation (5) together with the growth rates of the two phenomena: emissions and atmospheric accumulation of CO₂. Commenting on Figure 6, we can make the following observations: 1° - Around 2035, the accelerations reach their positive maximum, which coincides with the turning point of the growth rates. They then begin to fall to zero, starting around 2100, at the Hubbert peak, where growth rates reach their maximum value. From then on, the secular negative acceleration (deceleration) begins

symmetrically. 2° - Acceleration of CO_2 accumulation in the atmosphere is 65% of the acceleration of emissions. 3° - As mentioned in the introduction, Hansen et al., [1] estimated that the acceleration of accumulation is not much greater than 50% of the acceleration of emissions. This estimate is based on numerical calculation of derivatives from raw experimental data. Now, Numerical Calculus strongly advises against calculating numerical derivatives from raw data. In fact, this leads to unacceptable fluctuations of the calculated value compared to the true derivative value. In this paper, we have proceeded to analytically calculate these first derivatives (the CO_2 growth rate in the atmosphere) together with their second derivatives (accelerations) using the appropriate logistic mathematical model, thus obtaining an improved value of Hansen's estimate.

Critical Observations on the Model

The basic hypotheses of this work is that the differential equation (2) together with its integral, equation (4), can describe global CO₂ emissions and its atmospheric growth. The right-hand side of equation (2) is the product of a kinetic constant (k) and a shape factor $f(\alpha, \chi)$, which depends only on the current value of the variable (χ). In order to understand the scope and consequences of this choice, it is worth pausing for a moment to reflect:

1. Mathematical implications of the model: Because of this choice, the differential equation is independent of past history, but depends only on the present state (χ); in other words, the state of the system at any past time uniquely determines its state at any future time. In many real-world situations this is an obvious absurdity, and our situation is probably one of them! But it is useful, if patent, nonsense. The flaw in many mathematical models is not so much this kind of hypothesis, but the lack of awareness of its implications [10]. We should use a mathematical model of a real process as long as it makes predictions that are in reasonable agreement with observations. When one compares the complexity of the observed phenomenon with the simplicity of this mathematical model, it is not surprising that one is forced to modify the formulation from time to time in order to obtain results that are more accurate. However, it is remarkable how a deep understanding of many real processes can be achieved by using very rudimentary hypotheses!

2. Physical implications of the model: We have made the hypothesis that the shape factor takes the expression given by equation (3). The meaning of this function is that the

growth rate of the phenomenon is zero not only at the beginning of the process, when $\chi(0) = 0$, but also when $(1 - \chi) = 0$, i.e. at the end of the process. This implies that there is a phase of growth, the attainment of a maximum and then a decline in the rate to zero. From a physical point of view, the form factor explains the hypothesis that a finite system cannot grow infinitely, but tends to stabilise by reaching an appropriate value.

3. Predictive power of the model: The particular choice of the shape factor allows the analytic integration of the differential equation (2) to satisfy the initial condition $\chi(0) = 0$, thus obtaining the analytic expression of the CO₂ accumulation, equation (4). The historical data of the Keeling curve, [3], [4], [5], Figure 3, allowed the identification, by successive approximation, of the three free parameters (W_{∞}, k, α) of the logistic equation (4). By including the Antarctic data, the Keeling curve covers more than 200 years, i.e. about one third of the practical duration of the CO_2 accumulation phenomenon, as we can see a posteriori from Figure 3. This fact mitigates the major limitation highlighted in point 1, and thus mitigates the mathematical consequences outlined above. The parameter (k) has the character of a kinetic constant and determines the intensity of the rate of change of the phenomenon. It incorporates the effects of scientific and technological developments in energy production processes over time, and it is plausible that these developments will continue over time. In the case of CO_2 emissions, the parameter $W_{co}(E) = 16\,000\,Gt = 2010$ ppmv represents the total emissions throughout the fossil fuel era. It results from the product of three factors according to the relation:

$$W_{\infty}(E) = w_{\infty} \cdot \Delta t \cdot N_{\infty}, \tag{6}$$

where $w_{\infty} = 1.8 t/year$ is the average per capita emission, $\Delta t = 900$ years is the estimated duration of the CO₂ accumulation process and $N_{\infty} = 10 \cdot 10^9$ inhabitants is the estimated total population of the Earth at a future time, at the end of the fossil fuel burning era. The factor w_{∞} is an indicator of the impact of human presence on the Earth. In fact, it indicates the amount of CO₂ that each individual generates, directly or indirectly, to meet the needs of daily life. It is the average per capita footprint of CO₂ emissions for the entire duration of the fossil fuel era, also known as the secular fossil fuel carbon footprint.

All three factors will change over time. The world population is now about 7 billion and is likely to reach 10 billion in the future. The average annual per capita emission (2023) of CO₂ is about 5.26 t/year (i.e. about three times $w_{\infty} = 1.8$ t/year) and is strongly dependent on the geographical area considered, varying greatly from the USA and Europe to China and India. It is reasonable and desirable that w_{∞} is significantly lower than the average annual per capita CO₂ emission (2023) of 5.26 t/year. The variation of the three factors implies the variation of the value assumed by the parameter W_{∞} . The growth rate reaches its maximum, (Hubbert's peak), on the abscissa:

$$\chi_{Max} = \frac{1}{2} \left(1 - \frac{1}{\alpha} \right). \tag{7}$$

However, the time at which the maximum occurs can vary, according to the relationship:

$$(kt)^{\alpha} = \frac{\alpha - 1}{\alpha + 1}.$$
(8)

These considerations also point in the direction of improvements to this elementary model, in the spirit of a digital twin model of the Earth. Such improvements should include: the effects of developments in energy production technology on the kinetic constant k(t), the effects of competition between new technologies on the parameter w_{∞} and the effects of the dynamics of variation of the Earth's population on the parameter N_{∞} . As many equations as necessary will be added to the current formulation in order to describe these effects more precisely.

Conclusions

A single kinetic model was able to reproduce two different processes: CO_2 accumulation and emissions. The model is logistic with three free parameters (W_{∞}, k, α) . The two processes differ analytically by a constant factor given by the ratio $(W_{\infty}(A)/W_{\infty}(E) = .65)$. This factor corresponds to the ratio between two physically well-defined quantities: the total amount of CO_2 accumulated in the atmosphere, $W_{\infty}(A)$ and the total amount of CO_2 emitted, $W_{\infty}(E)$, from the beginning to the end of the fossil fuel era. The parameter (k) has the character of a kinetic constant and determines the intensity of the rate of change of the phenomenon. It incorporates the effects of scientific and technological developments in energy production processes over time, and it is plausible that these developments will continue over time. Improvements to this simple logistic model are readily feasible, in the spirit of digital twin models of the Earth. These improvements should include the effects of new energy production technologies on the kinetic constant, (k), the effects of competition between new technologies on the parameter w_{∞} , and the effects of population dynamics on the parameter N_{∞} . From time to

time, as many equations as necessary will be added to the current formulation in order to describe these effects more precisely.

Some of the results of this analysis are surprising: the half-life of the process of 300 years, the duration of the whole phenomenon of several centuries, the Hubbert's peak of the year 2100. These are all parameters that we would like to be closer to the more familiar parameter of the average human lifespan! However, the analysis has also produced results that are consistent with the average lifespan: Emissions, accumulation and sequestration of CO_2 are three processes that occur in phase with each other. Accumulation accounts for 65% of global emissions. Finally, we have begun a process of trying to anticipate changes in the balance between CO_2 accumulation and sequestration. Studying emissions and atmospheric accumulation of CO_2 simultaneously adds value that cannot be obtained by studying the two phenomena separately.

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