

Article

Partitioning Uncertainty in Model Predictions from Compartmental Modeling of Global Carbon Cycle

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Abstract: Our comprehension of the real world remains perpetually incomplete, compelling us to rely on models to decipher intricate real-world phenomena. However, these models, at their pinnacle, serve merely as close approximations of the systems they seek to emulate, inherently laden with uncertainty. Therefore, investigating the disparities between observed system behaviors and model-derived predictions is of paramount importance. Although achieving absolute quantification of uncertainty in the model-building process remains challenging, there are avenues for both mitigating and highlighting areas of uncertainty. Central to this study are three key sources of uncertainty, each exerting significant influence: (i) structural uncertainty arising from inadequacies in mathematical formulations within the conceptual models; (ii) scenario uncertainty stemming from our limited foresight or inability to forecast future conditions; and (iii) input factor uncertainty resulting from vaguely defined or estimated input factors. Through uncertainty analysis, this research endeavors to understand these uncertainty domains within compartmental models, which are instrumental in depicting the complexities of the global carbon cycle. The results indicate that parameter uncertainty has the most significant impact on model outputs, followed by structural and scenario uncertainties. Evident deviations between the observed atmospheric CO₂ content and simulated data underscore the substantial contribution of certain uncertainties to the overall estimated uncertainty. The conclusions emphasize the need for comprehensive uncertainty quantification to enhance model reliability and the importance of addressing these uncertainties to improve predictions related to global carbon dynamics and inform policy decisions. This paper employs partitioning techniques to discern the contributions of the aforementioned primary sources of uncertainty to the overarching prediction uncertainty.

Keywords: compartmental model; uncertainty analysis; partitioning uncertainty



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1. Introduction

The real-world system is precise but complex; a model, which is a simplified representation of this system, may be imprecise but simple. This trade-off between precision and simplicity is the essence of the modeling process. The effectiveness of a model lies in its simplicity of use, as well as an understanding of the level of imprecision [1]. Because of the imprecision in the model, uncertainties exist in the conclusions derived from it. Perincherry et al. [1] point out that “Handling uncertainty is perhaps the most pervasive and the most difficult aspect in the analysis of systems”. Some investigators have a tendency to ignore the uncertainties since it simplifies the decision making process, but ignoring uncertainties may be disastrous. It is a duty of researchers to highlight the uncertainties associated with the inferences they make.

Uncertainties in model predictions stem from various sources, including the model structure representing the real-world system, the scenarios reflecting diverse future perspectives, and the uncertainties inherent in the model input factors. Conducting uncertainty analysis (UA) on global carbon cycle (GCC) models can help pinpoint carbon cycle components and processes with the highest sensitivities and uncertainties. This information is invaluable for assessing which uncertainties exert the most significant influence on future

atmospheric CO₂ concentrations. Furthermore, it guides targeted research efforts and data collection to effectively mitigate uncertainties. The insights acquired from UA can also inform the development of future models.

In this study, model uncertainty, scenario uncertainty, and input factor uncertainty within the framework of three distinct compartmental models of the GCC are scrutinized through sensitivity analysis. The examination of model and scenario uncertainties over input factor uncertainty, which was comprehensively explored in another publication (see [2]), is prioritized. Furthermore, this study presents the partitioning of overall prediction uncertainty in the atmospheric CO₂ content in the year 2100 into distinct components of uncertainty.

In the subsequent sections, a concise overview of compartmental system modeling is provided in Section 2. Section 3 introduces the three GCC models and the emission scenarios sourced from the existing literature. Section 4 explores the various categories of uncertainties inherent in GCC models. Following this, Section 4.1 elucidates the primary sources of uncertainty addressed in this study. In Section 5, the partitioning of uncertainty in model predictions among the identified sources is explored. Finally, the concluding remarks are presented in Section 6.

2. Modeling Compartmental Systems

Systems of real-world phenomena can be effectively modeled using compartmental models, which find extensive applications across various disciplines, including biology, biomedicine, pharmacokinetics, ecology, chemistry, and engineering [3–6]. Noteworthy texts such as those authored by Godfrey [4] and Jacquez [5] comprehensively cover both the theoretical underpinnings and practical applications of compartmental models. Additionally, articles by Brown [7] and Zierler [8] offer insightful reviews on compartmental analysis.

In a compartmental system, the system is partitioned into a finite number of subsystems known as *compartments*. Each compartment is assumed to be homogeneous and well-mixed, and it is further assumed that there is no creation or destruction of *material* within any compartment. The compartments of a system interact with each other and with the environment by exchanging material. The rate at which the quantity of material changes in the *i*th compartment can be written as the difference between the sum of all inputs into and the sum all outputs from that compartment, as follows:

$$\frac{dx_i}{dt} \equiv \dot{x}_i = \left(m_{i0} + \sum_{\substack{j=1 \\ j \neq i}}^c m_{ij} \right) - \left(\sum_{\substack{j=1 \\ j \neq i}}^c m_{ji} + m_{0i} \right), \quad (1)$$

$$0 \leq t < \infty, \quad x_i(0) = x_i^\circ, \quad i = 1, 2, \dots, c$$

where x_i is the state variable associated with compartment i ; $\dot{x}_i$ is the derivative of x_i with respect to time t ; x_i° is the initial value of x_i ; m is the rate at which material is transferred, and with the subscript ij read as ‘to compartment i from compartment j ’, subscript 0 refers to outside the system, and c is the number of compartments in the system. For a system being modeled using a linear compartmental model, it is assumed that the amount of material transferred between compartments follows linear kinetics, so that at any time point, the rate at which the material leaves a *source* compartment is a linear function of the amount present in the compartment. Hence, the possible flow of material from compartment j to compartment i , indicated by m_{ij} in Equation (1), is defined as $m_{ij} = k_{ij} x_j(t)$, $i = 0, 1, \dots, c$, $j = 1, 2, \dots, c$, $j \neq i$, where k_{ij} is the proportionality parameter that characterizes the rate of transfer from compartment j to compartment i . The term *transfer coefficient* is used to refer to the k_{ij} s. The set of c differential equations, which represents a c -compartment model given as Equation (1) takes the form

$$\frac{dx_i}{dt} = \dot{x}_i(t) = \sum_{\substack{j=1 \\ j \neq i}}^c k_{ij} x_j(t) - \sum_{\substack{j=1 \\ j \neq i}}^c k_{ji} x_i(t) - k_{0i} x_i(t) + w_i(t) \quad (2)$$

where $w_i(t)$ is used instead of m_{i0} to align with the change in notation.

3. Models and Emission Scenarios

3.1. The Three GCC Models

Three different GCC models, which are used to quantitatively describe the CO₂ distribution between atmosphere and oceans, atmosphere and terrestrial systems, and the responses of these reservoirs to the input resulting from fossil fuel burning and deforestation, are utilized in this study. Two of these models, referred to as Model I and Model II, offer a simpler representation with eight compartments each, albeit with structural differences. Conversely, Model III presents a more intricate framework, comprising 25 compartments. Within the context of these models, the release of CO₂ from fossil fuel combustion and forest clearing is construed as perturbations to an initial steady-state condition, while all other inputs to the models are assumed to be negligible.

The initialization of a carbon cycle model entails a crucial calibration phase wherein the model is configured to maintain a steady-state condition. This condition ensures that the flux of CO₂ leaving compartment i is equal to the flux of CO₂ entering that compartment, prior to introducing any perturbations to the system. Essentially, at the onset of model simulations in the year 1750, it is presumed that the rate of change in CO₂ concentration with respect to time dx_i/dt is zero. While the 25-compartment model incorporates an inherent calibration process within its computer code, the two 8-compartment models lack such a routine. In a separate investigation, utilizing one of these 8-compartment models, two computational methodologies were proposed to enforce the fundamental modeling assumption of the initial steady-state (refer to [2]).

After establishing steady-state conditions within each model, random sampling is employed to calculate the CO₂ content of each compartment. This calculation considers inputs from fossil fuel combustion and forest clearing. The time-dependent carbon releases span from 1750 to 2100, incorporating historical data from 1750 to 2014 and three emission scenarios outlined by the Intergovernmental Panel on Climate Change (IPCC), detailed in Section 3.2.

In many studies concerning sensitivity and uncertainty analyses experiments, when knowledge of the distributions followed by the model input factors is limited, assuming a uniform distribution for each input factor is often considered the most prudent approach. This methodology has been advocated for by several researchers in [9–12]. When establishing ranges of variability in the absence of specific information, various criteria are employed to determine the variability ranges for the model factors. For example, in [9], Campolongo and Saltelli adopt a range of $\pm 20\%$ of the nominal value for some factors in their study. Additionally, in the same article, they propose another criterion, $(\frac{1}{2}K_0; 2K_0)$, where K_0 represents the nominal value of the input factor. In this study, given the lack of information about the distribution of the model input factors for each GCC model under consideration, it is assumed that they all follow uniform distributions. As no reference values for the uncertainty ranges of the input factors are available, a criterion of $\pm 20\%$ of the nominal value is utilized to establish an uncertainty range for each input factor.

After assigning a range and an appropriate probability distribution to each input factor, the next step in sensitivity analysis (SA) is to generate a sample. Within the SA framework, several methods are commonly employed for this purpose, including simple random sampling (SRS), Latin hypercube sampling, and importance sampling. The primary objective of these techniques is to ensure comprehensive coverage of the sample space for the input factors. Helton and Davis [13,14] extensively discuss and compare the effectiveness of these sampling methods and their impact on results. Given the ease of implementation and explanation, alongside the relatively low computational cost of

evaluating the models considered in this study, SRS with a sample size of $N = 5000$ was chosen for the simulations.

The following subsections introduce the three GCC models used in this study. Due to space constraints, a concise overview of each model is provided. For readers seeking comprehensive details, including compartmental diagrams and dynamic equations, references for each model are provided for further exploration.

3.1.1. Model I

This model comprises 8 well-mixed compartments and 15 transfer coefficients, following the framework outlined in [15]. Among these compartments, two represent carbon in the ‘surface ocean’ and ‘deep ocean’. Carbon within living plants is divided into ‘tree’ and ‘ground vegetation’ compartments. The ‘tree’ compartment further distinguishes between ‘nonwoody parts of trees’ and ‘woody parts of trees’. To account for carbon in deceased terrestrial systems and their decomposers, two compartments are utilized. The ‘detritus/decomposers’ compartment encompasses litter and its decomposers on the soil surface, with carbon input derived from the death of above-ground vegetation. The ‘active soil carbon’ compartment includes carbon in soils and their decomposers, receiving carbon from the death and initial decomposition of below-ground vegetation parts, as well as the transport of decomposed material from the actively decaying litter layer.

The exchange of CO_2 among the eight compartments is described by a set of eight first-order linear differential equations, encompassing 23 uncertain model input factors (15 transfer coefficients and 8 initial conditions). These uncertain input factors are treated as random variables to ascertain the model’s sensitivity to their variations. The model’s state equations conform to Equation (2), where time (t) spans from 1750 to 2100, initial states are denoted as $x_i(t = 1750) = x_i^0$, with $i = 1, 2, \dots, 8$, and model outputs as $y_i(t) = x_i(t)$, with $i = 1, 2, \dots, 8$. The output from each compartment (i th) represents the CO_2 content in that specific compartment. Notably, CO_2 emissions originating from fossil fuel combustion and forest clearing enter the system solely through the atmosphere compartment, i.e., $w_i(t) = 0$ for all compartments except the atmosphere. The nominal values of the initial compartment contents, transfer coefficients, and their respective uncertainty ranges are detailed in Table 1.

3.1.2. Model II

This model, originally developed by Kelly et al. [16], is identical to that utilized by Bush et al. [17], McCartney [18], and Gazioğlu [19]. It is founded upon the GCC and primarily employed for predicting the potential impacts of ^{14}C discharges originating from the nuclear fuel cycle.

The model comprises a total of eight compartments, divided equally between the northern and southern hemispheres. Specifically, each hemisphere includes four compartments: ‘circulating carbon’, ‘surface ocean’, ‘deep ocean’, and ‘humus’ reservoirs. The ‘humus’ compartments encompass the entirety of the terrestrial ecosystem, including vegetation, both woody and nonwoody components of trees, detritus and the associated decomposers, as well as active soil carbon. This ensures that carbon pools within the terrestrial ecosystem are accurately accounted for within these compartments. Due to ^{14}C predominantly existing in the atmosphere as gaseous CO_2 and its significant involvement in various physical and biological processes, notably, photosynthesis and carbon cycle exchange, adherence to the nominal parameter values established by the model developers is maintained. Table 2 presents the detailed information regarding the initial contents of each compartment, along with the transfer coefficients and their associated uncertainty ranges.

The input into the circulating carbon compartments is presumed to be distributed in accordance with the current population distribution, with 80% allocated to the northern hemisphere (NH) and 20% to the southern hemisphere (SH), as outlined in [18].

Table 1. Model I reference case initial compartment contents and transfer coefficients for carbon transfer among compartments.

	Description	Input Factor	Nominal Value	Range	Unit
<i>Initial conditions</i>	(1) Atmosphere	x_1^o	622.40	497.92–746.88	Gt C
	(2) Surface ocean	x_2^o	667.37	533.90–800.84	Gt C
	(3) Deep ocean	x_3^o	37,542.00	30,033.60–45,050.40	Gt C
	(4) Nonwoody parts of trees	x_4^o	38.21	30.57–45.85	Gt C
	(5) Woody parts of trees	x_5^o	634.47	507.58–761.36	Gt C
	(6) Ground vegetation	x_6^o	59.32	47.46–71.18	Gt C
	(7) Detritus/decomposers	x_7^o	108.22	86.58–129.86	Gt C
	(8) Active soil carbon	x_8^o	1131.39	905.11–1357.67	Gt C
<i>Transfer Coefficients</i>	Atmosphere → Surface Ocean	k_{21}	0.1582	0.1266–0.1898	year ^{−1}
	Atmosphere → Nonwoody parts of trees	k_{41}	0.0354	0.0283–0.0425	year ^{−1}
	Atmosphere → Woody parts of trees	k_{51}	0.0408	0.0326–0.0490	year ^{−1}
	Atmosphere → Ground vegetation	k_{61}	0.0241	0.0193–0.0289	year ^{−1}
	Surface ocean → Atmosphere	k_{12}	0.1476	0.1181–0.1771	year ^{−1}
	Surface Ocean → Deep ocean	k_{32}	0.0473	0.0378–0.0568	year ^{−1}
	Deep ocean → Surface ocean	k_{23}	0.0008	0.0006–0.0010	year ^{−1}
	Nonwoody parts of trees → Detritus/decomposers	k_{74}	0.5758	0.4606–0.6910	year ^{−1}
	Woody parts of trees → Detritus/decomposers	k_{75}	0.0353	0.0282–0.0424	year ^{−1}
	Woody parts of trees → Active soil carbon	k_{85}	0.0047	0.0038–0.0056	year ^{−1}
	Ground vegetation → Detritus/decomposers	k_{76}	0.1667	0.1334–0.2000	year ^{−1}
	Ground vegetation → Active soil carbon	k_{86}	0.0862	0.0690–0.1034	year ^{−1}
	Detritus/decomposers → Atmosphere	k_{17}	0.4688	0.3750–0.5626	year ^{−1}
	Detritus/decomposers → Active soil carbon	k_{87}	0.0328	0.0262–0.0394	year ^{−1}
	Active soil carbon → Atmosphere	k_{18}	0.0103	0.0082–0.0124	year ^{−1}

Table 2. Model II reference case initial compartment contents and transfer coefficients for carbon transfer among compartments.

	Description	Input Factor	Nominal Value	Range	Unit
<i>Initial conditions</i>	Circulating carbon (NH) ¹	x_1^o	325.21	260.17–390.25	Gt C
	Surface ocean (NH)	x_2^o	448.31	358.65–537.97	Gt C
	Deep ocean (NH)	x_3^o	12,426.00	9940.80–14,911.20	Gt C
	Humus (NH)	x_4^o	1042.30	833.84–1250.76	Gt C
	Circulating carbon (SH) ²	x_5^o	291.59	233.27–349.91	Gt C
	Surface ocean (SH)	x_6^o	677.54	542.03–813.05	Gt C
	Deep ocean (SH)	x_7^o	21,983.00	17,586.40–26,379.60	Gt C
	Humus (SH)	x_8^o	356.21	284.97–427.45	Gt C
<i>Transfer Coefficients</i>	Circulating carbon (NH) → Surface Ocean (NH)	k_{21}	0.1400	0.1120–0.1680	year ^{−1}
	Circulating carbon (NH) → Humus (NH)	k_{41}	0.0160	0.0128–0.0192	year ^{−1}
	Circulating carbon (NH) → Circulating carbon (SH)	k_{51}	0.5000	0.4000–0.6000	year ^{−1}
	Surface ocean (NH) → Circulating carbon (NH)	k_{12}	0.1000	0.0800–0.1200	year ^{−1}
	Surface ocean (NH) → Deep ocean (NH)	k_{32}	0.0900	0.0720–0.1080	year ^{−1}
	Surface ocean (NH) → Surface ocean (SH)	k_{62}	0.1000	0.0800–0.1200	year ^{−1}
	Deep ocean (NH) → Surface ocean (NH)	k_{23}	0.0032	0.0026–0.0038	year ^{−1}
	Deep ocean (NH) → Deep ocean (SH)	k_{73}	0.0050	0.0040–0.0060	year ^{−1}
	Humus (NH) → Circulating carbon (NH)	k_{14}	0.0050	0.0040–0.0060	year ^{−1}
	Circulating carbon (SH) → Circulating carbon (NH)	k_{15}	0.5600	0.4480–0.6720	year ^{−1}
	Circulating carbon (SH) → Surface ocean (SH)	k_{65}	0.2300	0.1840–0.2760	year ^{−1}
	Circulating carbon (SH) → Humus (SH)	k_{85}	0.0061	0.0049–0.0073	year ^{−1}
	Surface ocean (SH) → Surface ocean (NH)	k_{26}	0.0660	0.0528–0.0792	year ^{−1}
	Surface ocean (SH) → Circulating carbon (SH)	k_{56}	0.1000	0.0800–0.1200	year ^{−1}
	Surface ocean (SH) → Deep ocean (SH)	k_{76}	0.0900	0.0720–0.1080	year ^{−1}
	Deep ocean (SH) → Deep ocean (NH)	k_{37}	0.0028	0.0022–0.0034	year ^{−1}
	Deep ocean (SH) → Surface ocean (SH)	k_{67}	0.0028	0.0022–0.0034	year ^{−1}
	Humus (SH) → Circulating carbon (SH)	k_{58}	0.0050	0.0040–0.0060	year ^{−1}

¹ NH: Northern Hemisphere. ² SH: Southern Hemisphere.

3.1.3. Model III

In contrast to the previously discussed GCC models, the model presented here offers a more intricate portrayal of the carbon cycle dynamics. Adopted from a technical report [20]

commissioned by the United States Department of Energy, this model initially aimed to forecast the future scope of the greenhouse effect.

The model comprises three primary components: the atmosphere, oceans, and terrestrial systems, delineated into 25 compartments. The atmosphere is represented by a singular compartment, while the oceans are segmented into 19 globally averaged layers based on depth. Within the ocean component, the ‘surface ocean’ encompasses waters above 75 m, while the ‘deep ocean’, partitioned into 18 horizontal layers, corresponds to depths ranging from 75 to 4500 m. This segmentation is grounded in the relationship between the ocean’s horizontal cross-sectional area and the carbon concentration at various depths. The surface ocean compartment interacts with the atmosphere to exchange carbon, while the deep ocean compartment solely exchanges carbon with the surface ocean.

The terrestrial component allocates carbon among five compartments: ‘nonwoody parts of trees’, ‘woody parts of trees’, ‘ground vegetation’, ‘detritus/decomposers’, and ‘active soil carbon’. In this model, CO₂ is emitted into the atmosphere through fossil fuel combustion, while deforestation contributes to carbon transfer directly from tree compartments to the atmosphere, as well as to the ‘detritus/decomposers’ compartment. The relative magnitudes of carbon transfers from the atmosphere to tree and ground vegetation compartments are adjusted to reflect changes in land use patterns, such as deforestation and reforestation, which alter the distribution and amount of vegetation cover.

The descriptions of the 30 independent input factors that are subject to uncertainty, their nominal values, variability ranges, and units, are provided in Table 3. Among these factors, six pertain to the initial conditions of the atmosphere and terrestrial biota compartments, seven describe land-use practices, while others pertain to the chemical and physical parameters of the oceans. The remaining input factors determine coefficients that regulate fluxes between the terrestrial components of the model.

Table 3. Model III input factors selected for sensitivity analysis.

Description	Input Factor	Nominal Value	Range	Unit
<i>Initial conditions:</i>				
Atmosphere (c_1^o)	CA0	548.80	510.7–596.0	Gt C
Nonwoody parts of trees (c_{21}^o)	CF0	38.20	30.0–46.0	Gt C
Woody parts of trees (c_{22}^o)	CW0	634.50	507.0–762.0	Gt C
Ground vegetation (c_{23}^o)	CG0	59.30	47.0–72.0	Gt C
Detritus/decomposers (c_{24}^o)	CD0	108.20	86.0–130.0	Gt C
Active soil carbon (c_{25}^o)	CSL0	1131.00	905.0–1348.0	Gt C
<i>Forest clearing:</i>				
Fraction of forest clearing carbon transferred to atmosphere (φ_A)	PHIA	0.5	0.4–0.6	—
Fraction of forest clearing carbon transferred to detrit./decomp. (φ_D)	PHID	0.5	0.4–0.6	—
Ratio of soil to detrit./decomp. flux to forest clearing flux (ψ_S)	PSIS	0.1	0.08–0.12	—
Fraction of forest clearing release that serves to decrease capacity for carbon storage in trees (ξ_T)	SXIT	0.5	0.4–0.6	—
<i>Reforestation:</i>				
Rate of re-establishment of tree compartments (σ_T)	SIG	1.0×10^{-6}	0.8×10^{-6} – 1.2×10^{-6}	year ^{−1}
Rate coefficient controlling the time required for trees to dominate ground vegetation (κ_S)	SS	0.2	0.16–0.24	year ^{−1}
Fraction of the change in capacity for carbon storage in trees that causes a change in capacity for storage in ground vegetation (ϵ)	EPS	0.5	0.4–0.6	—

Table 3. Cont.

Description	Input Factor	Nominal Value	Range	Unit
<i>Physical and Chemical ocean:</i>				
Depth of surface ocean	HM	75.0	60.0–90.0	m
Area of surface ocean	AREA	3.61×10^{14}	2.88×10^{14} – 4.33×10^{14}	m ²
Temperature change in surface ocean as a result of doubling atm. carbon content (<i>DT</i>)	DELTP	3.0	1.5–4.5	K
Total boron concentration in surface ocean (ΣB)	SIGB	4.1×10^{-4}	3.27×10^{-4} – 4.90×10^{-4}	mol/L
Initial temperature of surface ocean (T_0)	TEMP0	292.75	290.75–294.75	K
Chlorinity of surface water (<i>Cl</i>)	CL	19.24	15.0–23.0	mL ^{−1}
Relative humidity in atmosphere (<i>RH</i>)	RELHUM	0.75	0.6–0.9	—
<i>Terrestrial turnover times:</i>				
Nonwoody parts of trees (τ_{21})	TF	1.75	1.4–2.1	year
Woody parts of trees (τ_{22})	TW	25.00	20.0–30.0	year
Ground vegetation (τ_{23})	TG	4.00	3.2–4.8	year
Detritus/decomposers (τ_{24})	TD	2.00	1.6–2.4	year
Active soil carbon (τ_{25})	TSL	100.00	80.0–120.0	year
<i>Soil-forming fractions:</i>				
Woody parts of trees (θ_{22})	THW	0.1180	0.094–0.14	—
Ground vegetation (θ_{23})	THG	0.3330	0.26–0.40	—
Detritus/decomposers (θ_{24})	THD	0.0625	0.05–0.075	—
<i>Intrinsic recovery times:</i>				
Nonwoody parts of trees (ν_T)	TT2	20.0	16.0–24.0	year
Ground vegetation (ν_V)	TV2	4.0	3.2–4.8	year

The three GCC models calculate carbon levels in the atmosphere, oceans, and terrestrial systems. The primary dynamic variables, also known as state variables, are the total carbon masses within each compartment. Commencing from a pre-industrial steady-state, the models produce results at annual time scales. Historical global annual CO₂ emissions data, spanning from 1751 to 2014, sourced from Boden et al. [21], serve as inputs for the models. As for the future CO₂ predictions spanning from 2015 to 2100, the models rely on the three scenario estimates provided by the Intergovernmental Panel on Climate Change (IPCC), as outlined in the subsequent section. Masses of CO₂ are measured in gigatons (1 Gt = 10¹² kg), time in years, and atmospheric CO₂ concentration in parts per million by volume (ppmv).

3.2. Emission Scenarios

The Intergovernmental Panel on Climate Change (IPCC) was jointly established by the World Meteorological Organization and the United Nations Environmental Programme in 1988. The primary objectives of IPCC's three working groups are: to assess the available information on climate change, to assess the environmental and socio-economic impacts of climate change, and to formulate response strategies.

Despite trends indicating a significant increase in net greenhouse gas emissions over the next century, the IPCC asserts that “significant reductions . . . are technically possible and can be economically feasible” (as cited in [22]). In 1992, the IPCC developed six alternative emission scenarios, known as the IS92a-to-f scenarios, based on various assumptions about factors influencing future CO₂ emissions. Factors such as population and economic growth, structural changes in economies, energy prices, technological advances, and fossil fuel supplies were considered (see [22]). These scenarios extend to the year 2100 and encompass emissions of other greenhouse-related gases alongside CO₂. In this study, three of these scenarios (IS92a, IS92c, and IS92e) for the years 2015–2100 are utilized as input scenarios.

Scenario IS92a, known as the ‘business-as-usual’ scenario, represents a middle-of-the-range scenario with modest and largely offsetting changes in the underlying assumptions. Scenario IS92c, identified as a ‘low’ emission scenario, features a CO₂ emissions path that

eventually decreases below its initial value, driven by assumptions such as a decline in population by the middle of the next century, low economic growth, and severe constraints on fossil fuel supply. On the other hand, scenario IS92e, described as a ‘high’ emission scenario, exhibits the highest greenhouse gas emissions, assuming moderate population growth, high economic growth, ample fossil fuel availability, and a phased-out nuclear power. For further details on these scenarios, please refer to Ref. [22].

Figure 1 illustrates the projected future CO₂ emissions associated with the three selected scenarios, alongside the historical record of CO₂ emissions.

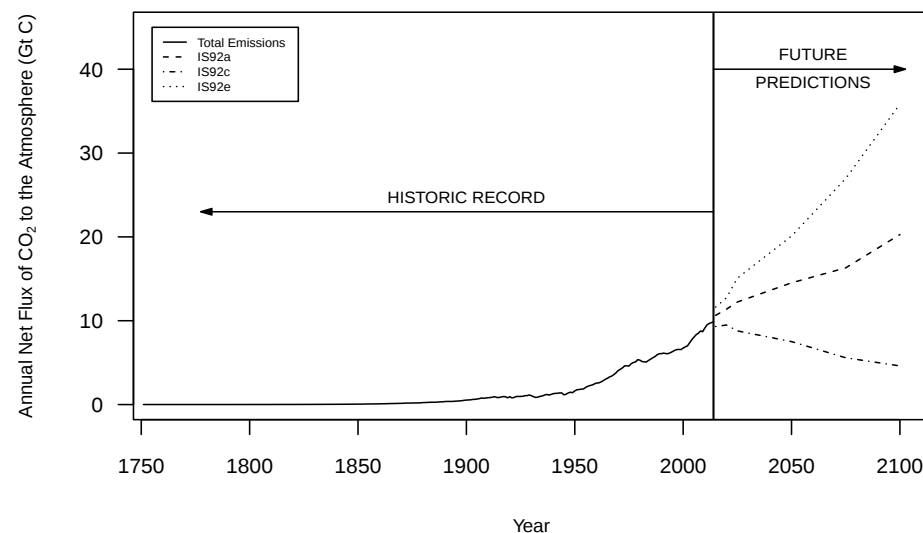


Figure 1. Historic and future global CO₂ emissions. The 1751–2014 historic emission record is from Ref. [21]. The 2015–2100 future predictions are from Ref. [22].

4. Uncertainties in GCC Models

The acknowledgment of inherent uncertainty within environmental and climatic systems is widespread [23–25]. The future role of terrestrial and oceanic systems in the GCC remains uncertain. Regarding the terrestrial system, scientific consensus on whether terrestrial vegetation acts as a source or sink for CO₂ is lacking [26–28]. Additionally, the amount of carbon stored in terrestrial systems varies significantly, ranging from 420 to 830 Gt, depending on the methodologies employed.

Although oceans possess a considerable capacity for CO₂ storage, uncertainties persist regarding their overall impact on the oceanic environment and the repercussions of injected CO₂.

In a general sense, Draper [29] identifies three primary sources of uncertainty in any problem as: (i) predictive uncertainty, which is conditional on the scenario and model; (ii) scenario uncertainty regarding the inputs to the models; and (iii) model uncertainty (conditional on the scenario) regarding how to translate the inputs into forecasts.

In another article, Draper et al. [30] elaborate on the sources of uncertainty in complex prediction problems, which encompass six ingredients: past data, future observables, scenarios, model (or structural), parametric, and predictive uncertainty.

Uncertainties in computer models can stem from various sources, necessitating attention to the magnitude of uncertainty associated with model behavior. As modern computing power enables consideration and comparison of an increasing number of models, the challenge of addressing uncertainties in models grows more pronounced, as noted by Chatfield [31]. This concern is further emphasized by Kennedy and O’Hagan [32], who highlight the need to quantify uncertainties in model results. They identify various sources of uncertainty in computer models, such as parameter uncertainty, model inadequacy, code uncertainty, and observation error.

In the realm of climate modeling, King and Sale [33] identify three primary sources of uncertainty: scenario uncertainty, model uncertainty, and input factor uncertainty. Scenario uncertainty pertains to uncertainties in future energy and land-use emissions, while model uncertainty arises from the structural and conceptual differences among models representing the GCC. Input factor uncertainty encompasses errors and uncertainties in the parameters and variables within a specific model.

This paper aims to assess the uncertainty in model predictions resulting from these three main sources through SA. The subsequent subsections delineate these sources of uncertainty within the GCC modeling framework. Firstly, the three main sources of uncertainty are outlined. Then, input factor uncertainty within models and scenarios, scenario uncertainty within models, and model uncertainty within scenarios are examined.

4.1. Main Sources of Uncertainty

4.1.1. Input Factor Uncertainty

In any model, the output is usually the focal point. However, our understanding of the input factors driving the model equations is imperfect, as their values can only be approximated from the real-world system. Consequently, these input factors are characterized by uncertainty, leading to uncertainties in the output. As articulated in [13], UA aims to address the question: “What is the uncertainty in the model response given the uncertainty in the input factors?”.

This uncertainty manifests as a distribution of input factor values. Mitigating uncertainty in influential factors, identifiable through SA, can substantially reduce uncertainty in model predictions. In Figure 2, the illustration demonstrates how decreasing uncertainty in a significant input factor leads to reduced prediction uncertainty. This demonstration is based on the atmosphere compartment of Model III. The prior research (see [19]) indicates that the surface ocean’s area (i.e., the input factor AREA) exerts the most substantial influence on the atmosphere compartment. Figure 2 underscores the considerable impact of reducing uncertainty in AREA (i.e., setting it to its best estimate) on the uncertainty in the predicted atmospheric CO₂ content.

It is important to note that while the findings in this study are derived from $N = 5000$ model simulations, the figure below exclusively showcases results from $N = 100$ simulations. This deliberate choice aims to enhance clarity in illustrating the time-dependent behavior of the model output. Additionally, it should be mentioned that in this figure and throughout the paper, carbon stocks are represented as CO₂ and measured in units of Gt C (gigatons of carbon).

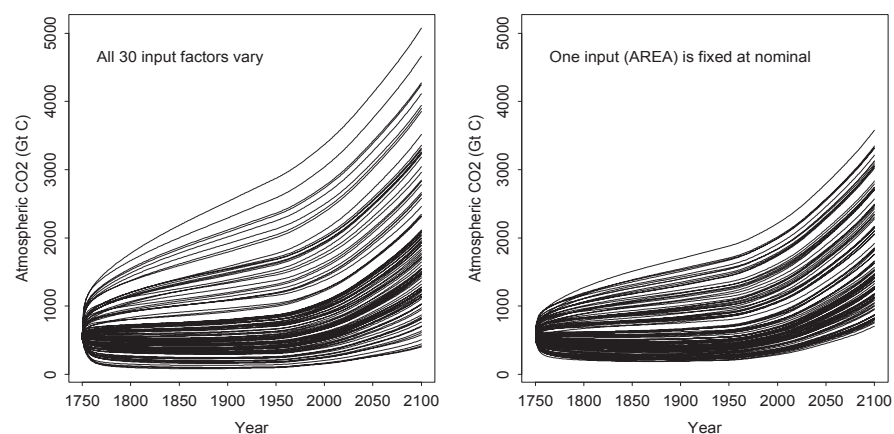


Figure 2. An example of prediction uncertainty bands, illustrating how reducing uncertainty in influential input factors (here, AREA) decreases uncertainty in atmospheric CO₂ predictions. This demonstration uses Model III’s atmosphere compartment under the IS92a emission scenario, with 100 model simulations. Each line in the graph represents a single model simulation.

4.1.2. Scenario Uncertainty

One significant source of uncertainty in GCC models stems from the inherent challenge of accurately predicting future conditions due to limited knowledge. Factors such as population growth, structural shifts in economies, fluctuations in energy prices, availability of fossil-fuel resources, and income levels collectively contribute to the complexity of forecasting future levels of CO₂ emissions, with substantial uncertainty surrounding each [22]. To address this uncertainty, scientists, including those contributing to the Intergovernmental Panel on Climate Change (IPCC) reports, have developed various scenarios depicting potential future emission trajectories. These scenarios serve as essential inputs for climate models. The IPCC reports involve extensive contributions from a broad scientific community worldwide, compiling and synthesizing the research on emissions scenarios and their implications for climate modeling (see [22,34–38]).

4.1.3. Model Uncertainty

As Kennedy and O’Hagan [32] put it: “No model is perfect”. Even in scenarios where input factors are precisely known, the predicted value of a process may deviate from its actual value due to what they term ‘model inadequacy’.

Moreover, uncertainty stemming from model structure compounds this inherent imperfection, as there exists no singular methodology to encapsulate a real system within a limited set of variables and equations. Numerous factors contribute to uncertainty in GCC models, including but not limited to, physical assumptions and the potential omission of relevant processes. Despite multiple GCC models endeavoring to represent the same system, disparities in results frequently arise due to uncertainties pertaining to model assumptions, initial conditions, and structural intricacies.

In addressing model uncertainty, a thorough examination and comparative analysis of the three GCC models employed within this study are conducted. Assessing the magnitude of model uncertainties frequently requires comparing model outputs with empirical observations. However, it is important to recognize that observations themselves can introduce significant uncertainty.

In Figure 3, the atmospheric CO₂ predictions of the three GCC models are presented alongside observed data from the Mauna Loa Observatory (MLO) record spanning from 1959 to 2023. This dataset originates from precise measurements initiated by Charles D. Keeling in March 1958 at MLO in Hawaii. Notably, these measurements constitute the largest continuous record of atmospheric CO₂ concentrations globally.

The atmospheric CO₂ concentrations from the three GCC models are projected using their respective model codes with parameters set at nominal values, as detailed in Tables 1–3. Historical emission records from 1959 to 2014 (referenced from Ref. [21]) and the IPCC’s middle-of-range emission scenario IS92a for the years from 2015 to 2023 (cited from Ref. [22]) are utilized as inputs into the models through the atmospheric compartment. This setup facilitates a comparison between the three model predictions and the observed MLO data throughout the record period.

The MLO data provide a robust and highly accurate record of atmospheric CO₂ concentrations. MLO is strategically located in the central Pacific Ocean, far from significant local pollution sources, allowing it to capture baseline atmospheric conditions that are reflective of global trends. This makes MLO an ideal benchmark for comparing model predictions with observed CO₂ levels.

Although the GCC models do not explicitly account for spatial variability, their outputs are designed to represent global average CO₂ concentrations. The use of historical emission records and the IPCC’s IS92a emission scenario ensures consistency across all three models and aligns their predictions with the global trends observed at MLO. This approach provides a valid framework for comparing the model predictions with the observed MLO data, as both represent overarching global patterns in atmospheric CO₂ concentrations.

The annual averages of the data collected at MLO demonstrate a consistent upward trend in atmospheric CO₂ concentrations, rising from 315.98 ppm in 1959 to 421.08 ppm in

2023 [39]. However, despite this observed increase, all three GCC models tend to underestimate the observed CO₂ levels. Model III, in particular, exhibits a slight overestimation in atmospheric CO₂ levels during the last decade.

Model I predicts atmospheric CO₂ concentrations of 308.16 ppm in 1959 and 353.80 ppm in 2023. Similarly, Model II predicts these concentrations to be 302.27 ppm and 339.48 ppm during the same years. While Models I and II initially exhibit closer alignment with the observed data compared to Model III, their deviation from observed values accelerates over time. Model III predicts atmospheric CO₂ concentrations of 295.12 ppm in 1959 and 429.89 ppm in 2023.

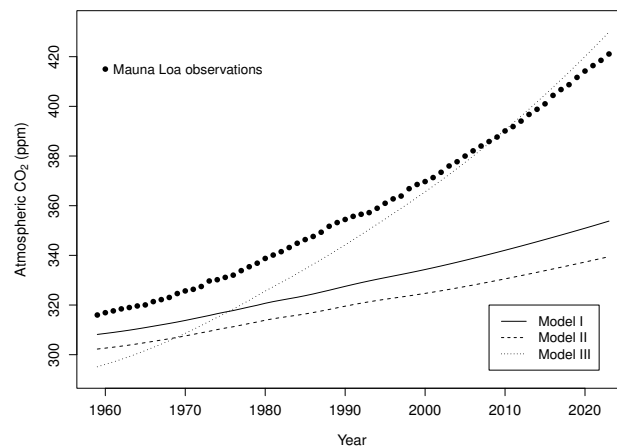


Figure 3. Comparison of predicted atmospheric CO₂ concentrations from the three GCC models and the measured atmospheric CO₂ concentrations from Mauna Loa Observatory: 1959–2023 [39].

The observed rise in atmospheric carbon content lags behind the emissions from fossil fuel combustion and land-use changes due to the complex carbon exchange between the atmosphere and other compartments within the system. Models I and II, characterized by their highly linear mathematical structures, exhibit rapid carbon uptake across all model compartments. Consequently, these models project a relatively slow increase in atmospheric CO₂ levels. These models are constructed using a linear, time-invariant compartmental modeling formulation and neglect the physical processes of global climate change (GCC), leading to substantial uncertainty. In contrast, Model III is believed to provide a more realistic representation of carbon cycle processes. For instance, it considers the turnover mechanism of carbon in the oceans, the storage of non-labile carbon in terrestrial biota, and the depth distribution of ¹⁴C, among other factors, resulting in a more accurate portrayal of atmospheric carbon dynamics [20].

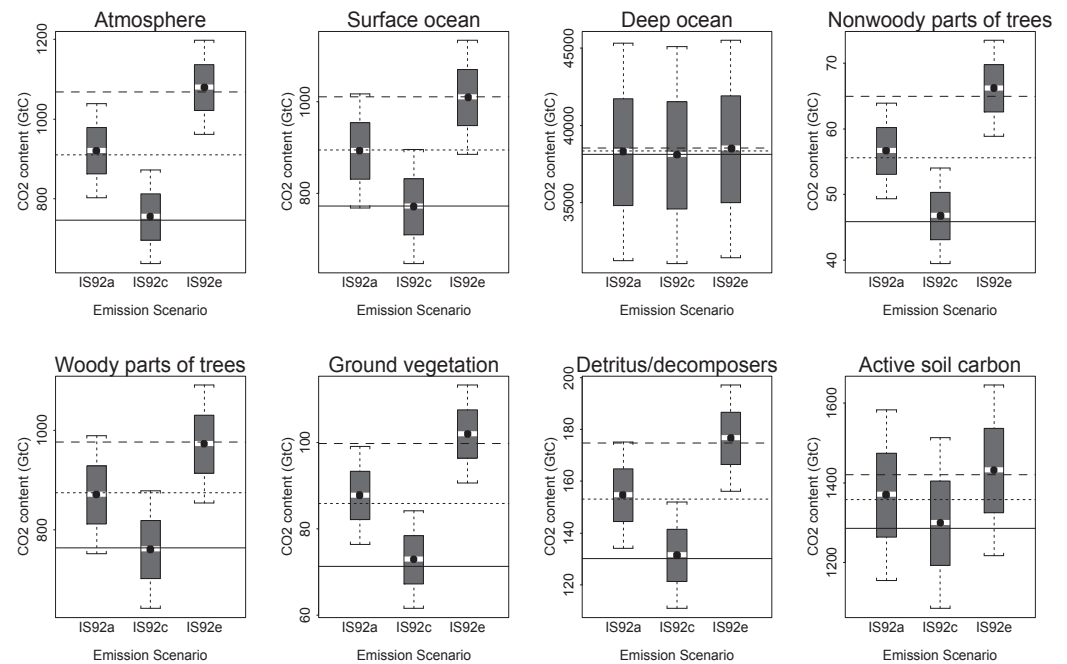
4.2. Delving Deeper into Primary Uncertainty Sources

4.2.1. Input Factor Uncertainty within Models and Scenarios

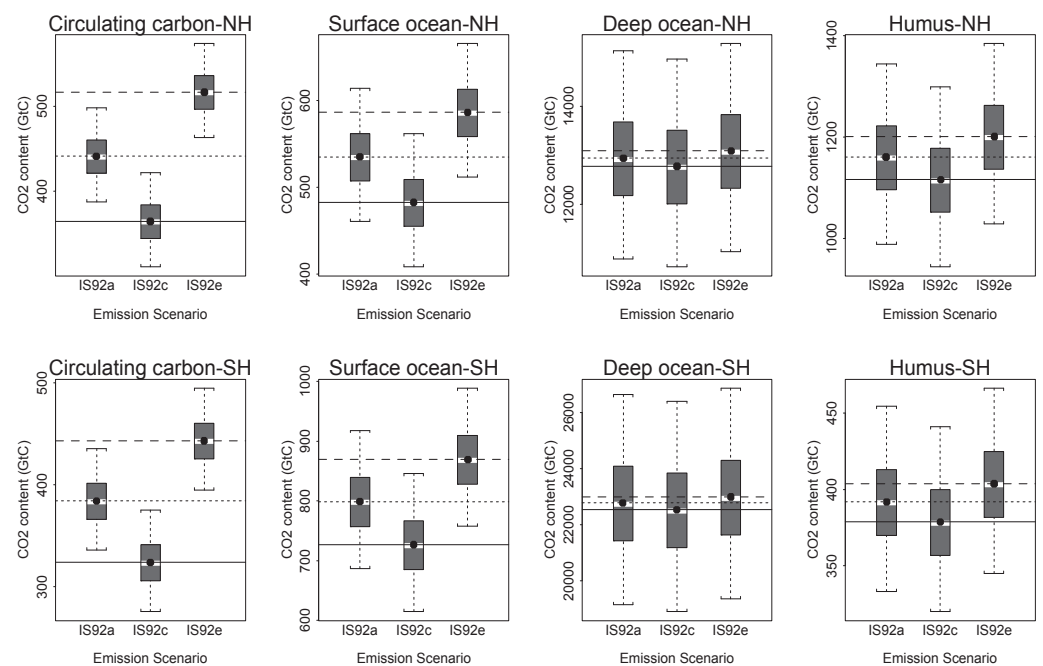
Next, considering input factor uncertainty and varying factors within assigned ranges from a uniform distribution within each model, an examination of the results across three emission scenarios is undertaken. In simulations, the same set of input values is used with each scenario to facilitate direct comparison. Compartmental predictions are evaluated in year 2100. Boxplots in Figures 4 and 5 provide a concise summary of the output variable distributions for the three models. The horizontal lines represent baseline values for each compartment in 2100 under respective scenarios (dotted line: IS92a; solid line: IS92c; dashed line: IS92e). Estimated mean values are indicated by solid circles in the boxplots.

In Figure 4, the boxplots of Models I and II show considerable overlap, indicating that distinguishing between predictions for the three scenarios based on overall output uncertainties is challenging. Similarly, in Figure 5, the boxplots for Model III display notable overlap among compartments. Specifically, for the deep ocean—layer13 compartment

and all five terrestrial compartments, output distributions exhibit similar behavior across emission scenarios.



(a) Model I



(b) Model II

Figure 4. Boxplots showing the distribution of CO₂ predictions for the year 2100 from (a) Model I and (b) Model II, considering three IPCC emission scenarios and 5000 simulations with uniform distribution for all input factors. Horizontal lines represent the baseline CO₂ content of each compartment in 2100 under each scenario: · · · IS92a; —IS92c; - - IS92e. Solid circles indicate the means.

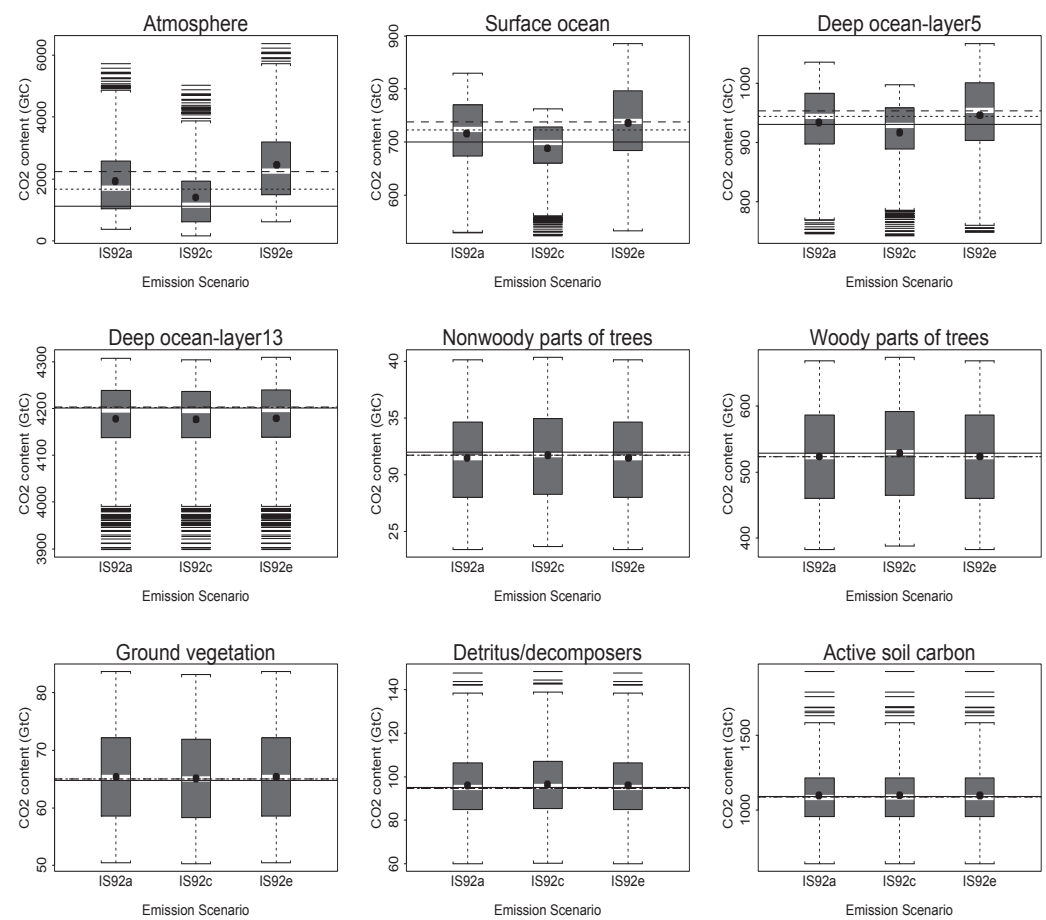


Figure 5. Boxplots showing the distribution of CO₂ predictions in the year 2100 from Model III, considering three IPCC emission scenarios and 5000 simulations with uniform distribution for all input factors. Horizontal lines represent the baseline CO₂ content of each compartment in 2100 under each scenario: ··· IS92a; —IS92c; - - IS92e. Solid circles indicate the means.

The contribution of input factor uncertainties to prediction uncertainties appears to be considerable within each model. In Table 4, alongside the baseline values of each compartment's year 2100 predictions under the three scenarios, the uncertainty ranges resulting from scenario uncertainty alone and from both scenario and input factor uncertainties are presented.

As observed in the table, the inclusion of input factor uncertainties alongside scenario uncertainty leads to a significant expansion of overall uncertainty ranges, particularly evident in Model III. Notably, in the atmosphere compartment, the minimum increase surpasses 450%. Models I and II also experience substantial changes in uncertainty ranges across all compartments, with a pronounced impact on deep ocean compartments when integrating input factor uncertainties alongside scenario uncertainty. In the deep ocean compartment of Model I, the minimum increase exceeds 3500%. Additionally, for Model II, the minimum increase reaches nearly 1350% for the northern hemisphere (NH) and approximately 1648% for the southern hemisphere (SH).

Table 4. Scenario baseline values in 2100; uncertainty ranges of compartmental predictions from 2100 as a result of scenario uncertainty; and uncertainty ranges of compartmental predictions from 2100 as a result of both scenario and input factor uncertainties (in Gt C).

Compartment		IS92a	IS92c	IS92e	Scenario ^a Uncer. Range	Sce. and In. Factor ^b Uncer. Range
Model I	Atmosphere	746.7	910.51	1067.97	321.27	560.31
	Surface ocean	771.80	894.42	1011.44	239.64	488.65
	Deep ocean	38,130.16	38,342.57	38,527.41	397.25	14,445.26
	N.woody parts trees	45.87	55.63	64.99	19.13	34.05
	Woody parts trees	763.19	874.18	976.54	213.35	449.04
	Ground vegetation	71.26	85.85	99.80	28.54	51.86
	Detritus/decomposers	130.09	153.10	174.80	44.71	86.12
	Active soil carbon	1285.88	1357.38	1420.06	134.19	561.41
Model II	Circulating carbon (NH)	364.43	441.26	516.85	152.42	263.44
	Surface Ocean (NH)	482.58	535.00	586.07	103.49	256.56
	Deep ocean (NH)	12,773.49	12,940.26	13,087.97	314.49	4557.71
	Humus (NH)	1115.79	1160.47	1200.78	84.99	440.27
	Circulating carbon (SH)	323.85	384.00	443.10	119.25	218.80
	Surface Ocean (SH)	726.43	798.86	869.32	142.90	374.23
	Deep ocean (SH)	22,526.45	22,768.65	22,981.94	455.49	7961.98
	Humus (SH)	378.71	391.91	403.76	25.04	146.50
Model III	Atmosphere	1109.99	1674.90	2238.98	1128.99	6212.12
	Surface ocean	700.44	723.01	737.92	37.48	361.94
	Deep ocean—layer5	931.13	944.70	953.98	22.85	324.50
	Deep ocean—layer13	4201.45	4202.53	4203.30	1.85	410.52
	N.woody parts trees	31.97	31.72	31.72	0.25	16.96
	Woody parts trees	528.82	523.55	523.55	5.28	291.39
	Ground vegetation	64.79	65.05	65.05	0.26	33.40
	Detritus/decomposers	95.13	94.68	94.68	0.46	88.48
	Active soil carbon	1089.23	1088.24	1088.24	0.99	1283.69

^a Uncertainty ranges as a result of scenario uncertainty. ^b Uncertainty ranges as a result of scenario and input factor uncertainties.

Subsequently, considering input factor uncertainty and focusing on the predictions for the year 2100 from the three models under the three emission scenarios, the mean and coefficient of variation (CV) of the three components are computed. The outcomes, derived from 5000 model iterations, are presented in Table 5. Due to disparities in modeling assumptions, initial conditions, and model structures, the estimated average CO₂ content of the three reservoirs varies across the three models. Given the similarities between Models I and II, it is appropriate to compare the estimated means and CVs associated with these models. Both the average CO₂ content and the CV of all components in 2100 appear to be higher with Model I compared to Model II.

The comparison of the coefficients of variation (CVs) for each component of the three models reveals that for the atmosphere component, Model III exhibits the highest variability (with a CV of approximately 58% for IS92a, 71% for IS92c, and 49% for IS92e), while Model II displays the lowest variability (with CVs ranging from approximately 5 to 7% across all scenarios). Concerning the ocean component, Model III demonstrates the least variability, with a CV of approximately 3% across all three emission scenarios, whereas Model I exhibits the highest variability, with a CV of approximately 10% under all three scenarios. As for the terrestrial component, the variability is greatest with Model III (approximately 13% across all scenarios) and lowest with Model II (approximately 7% across all scenarios).

Table 5. Comparison of mean and coefficient of variation (CV) values for atmosphere, ocean, and terrestrial ecosystem components projected for the year 2100 using three GCC models under IPCC- IS92a, c, and e scenarios (in Gt C). Calculations are derived from 5000 model simulations.

	Model Component	Model I		Model II		Model III	
		Mean	CV	Mean	CV	Mean	CV
IS92a	Atmosphere	920.89	7.29	825.25	5.86	1926.86	57.69
	Ocean	39,212.26	10.38	37,043.26	7.53	38,628.22	2.89
	Terr. Ecosys.	2540.40	8.33	1551.92	7.06	1813.54	12.64
IS92c	Atmosphere	755.42	8.88	688.26	7.03	1402.77	70.94
	Ocean	38,878.15	10.46	36,509.43	7.64	38,418.11	2.61
	Terr. Ecosys.	2311.30	9.16	1494.04	7.33	1820.23	12.60
IS92e	Atmosphere	1079.93	6.21	959.93	5.04	2455.73	48.78
	Ocean	39,513.22	10.30	37,525.79	7.43	38,778.30	3.10
	Terr. Ecosys.	2749.78	7.70	1604.07	6.83	1813.54	12.64

4.2.2. Scenario Uncertainty within Models

This section investigates the impact of uncertainty inherent in the three scenarios on model predictions. Initially, assuming zero uncertainty regarding input factors by setting them to their nominal values, baseline CO₂ predictions for each compartment within the three models across the aforementioned IS92 scenarios have been computed. These baseline predictions are visually depicted in Figures 6–8.

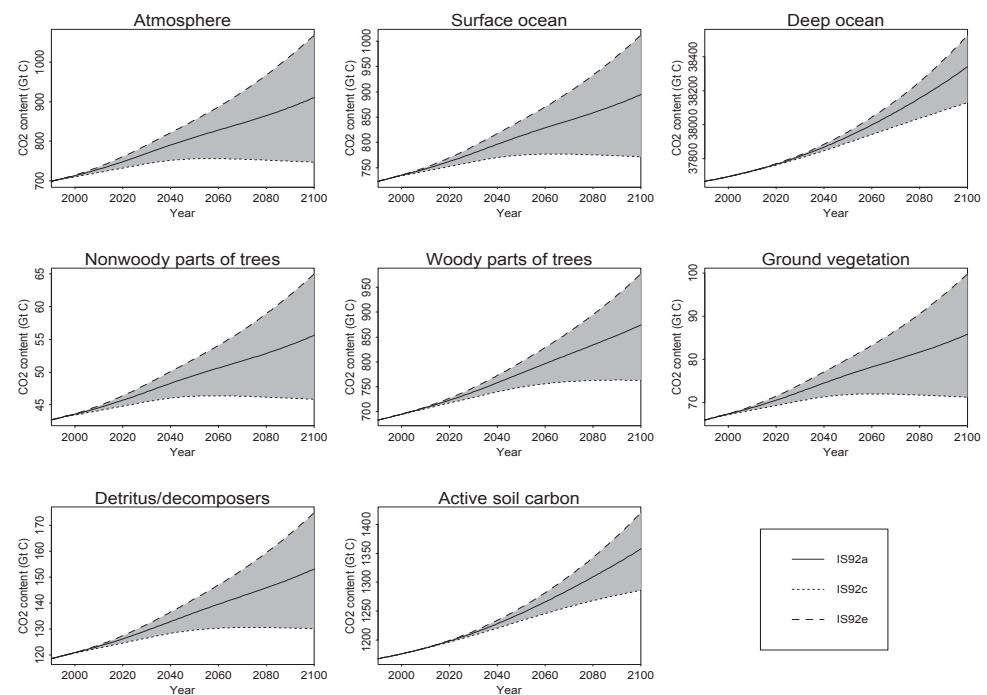


Figure 6. The prediction range of CO₂ baseline predictions of each compartment of Model I, with IPCC-IS92a, c, e emission scenarios and all model input factors set to their nominal values.

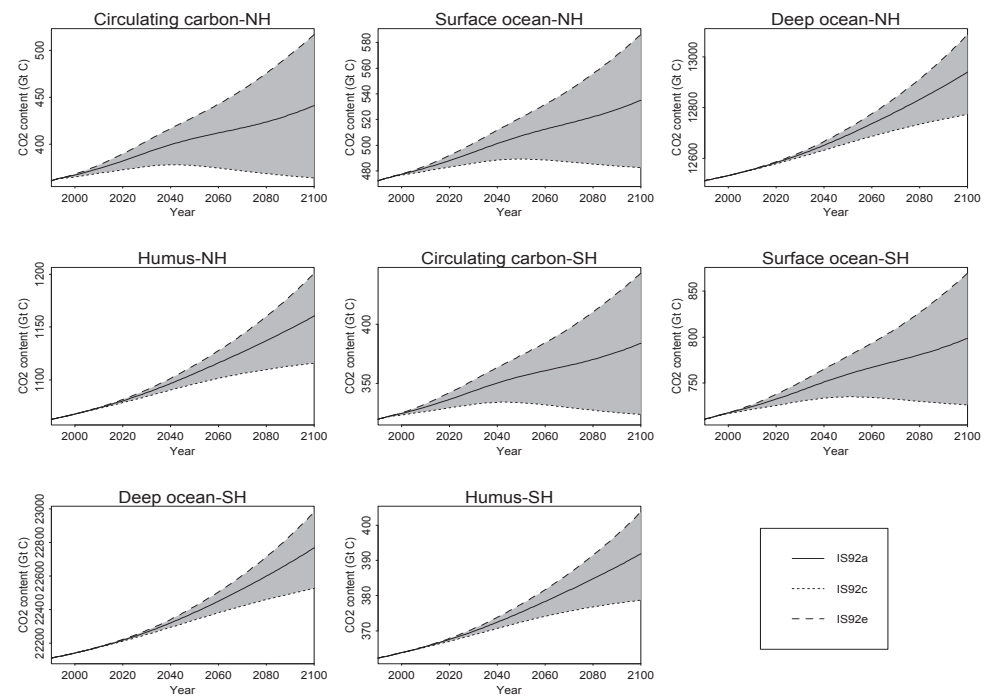


Figure 7. The prediction range of CO₂ baseline predictions of each compartment of Model II, with IPCC-IS92a, c, e emission scenarios and all model input factors set to their nominal values.

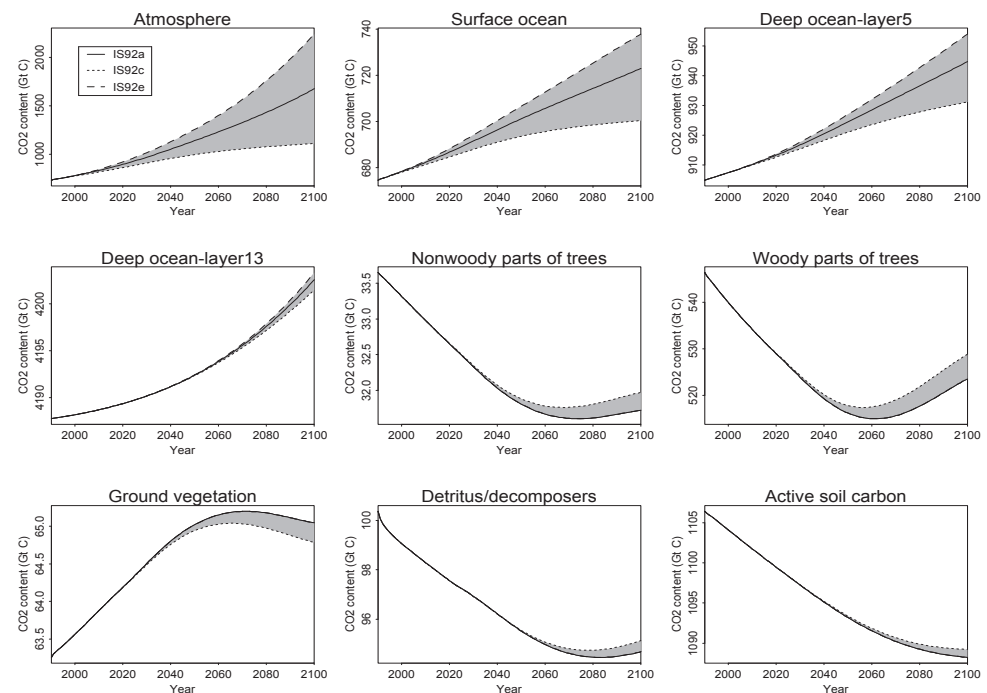


Figure 8. The prediction range of CO₂ baseline predictions of the nine compartments of Model III, with IPCC-IS92a, c, e emission scenarios and all model input factors set to their nominal values.

Figures 6 and 7 present the results for all eight compartmental CO₂ outputs of both Models I and II, respectively. The IS92e scenario yields a high estimate, IS92a a median estimate, and IS92c a low estimate of compartmental CO₂ contents across the entire time frame (1995 to 2100). However, in the case of Model III (refer to Figure 8), this pattern is observed only in the atmosphere and three of the ocean compartments under consideration.

In the ground vegetation compartment of Model III, IS92a and IS92e estimations show a pronounced increase compared to IS92c, while for other terrestrial compartments, IS92c produces notably higher estimates, whereas IS92a and IS92e scenarios indicate lower estimates. The impact of emission scenarios on deeper layers of the ocean and terrestrial ecosystems is less immediate than on the atmosphere, surface layer, and upper ocean layers. It is important to mention that due to space constraints, this study presents results from only two layers of the deep ocean compartments, specifically layer 5 and layer 13 (referred to as compartments 7 and 15 in the model diagram as shown in [20]).

4.2.3. Model Uncertainty within Scenarios

Assuming zero uncertainty for model input factors by setting them to their nominal values, our focus shifted to future projections. Compartmental CO₂ predictions were calculated for each model under three emission scenarios. After conducting Monte Carlo simulations, the compartments of the three models were aggregated into atmosphere, ocean, and terrestrial ecosystem components, with each model considered in isolation. The time-dependent behavior of the predictions for these model components between the years 2000 and 2100 is illustrated in Figure 9.

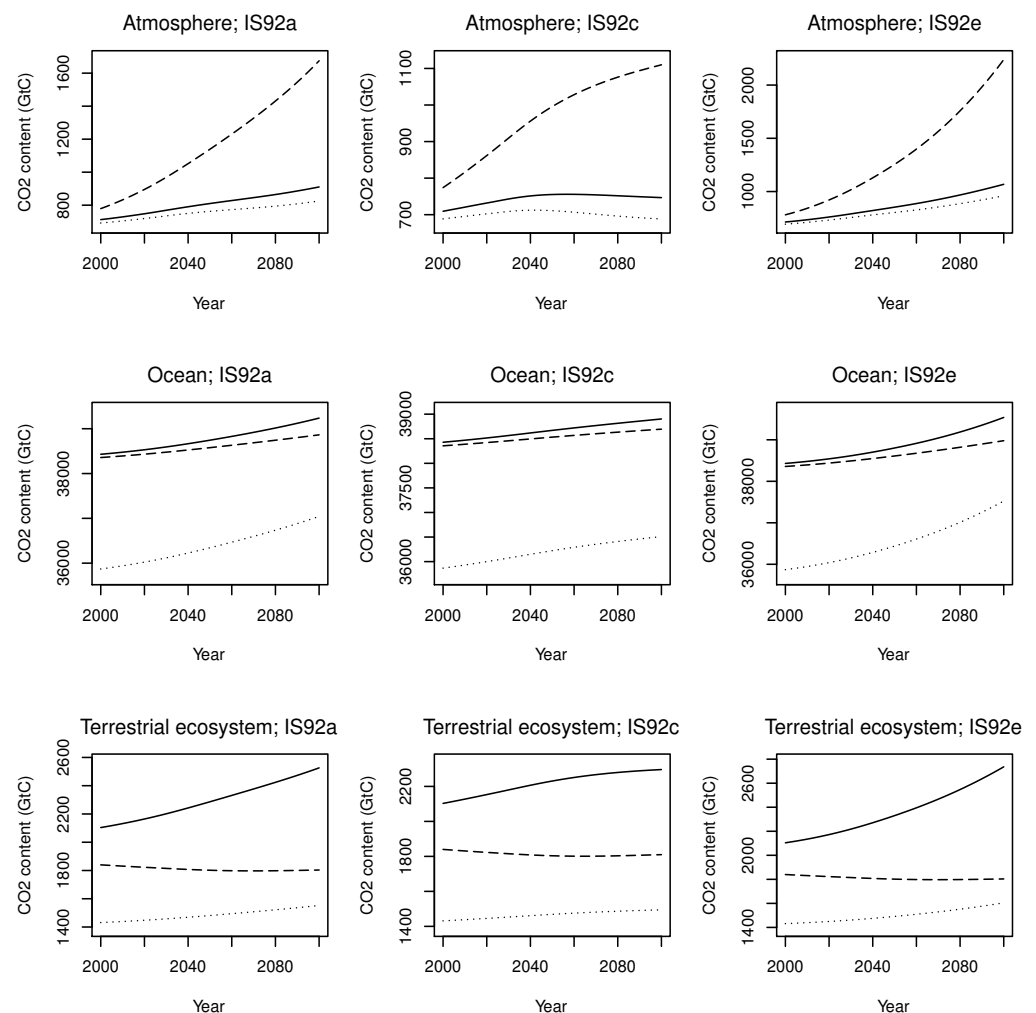


Figure 9. Baseline predictions from the three GCC models (—Model I; ··· Model II; - -Model III) with the IS92a, c, e emission scenarios for the time period 2000–2100. These calculations are based on model simulations in which all model input factors are set to their nominal values.

For the atmosphere component, Models I and II show comparable results across all three scenarios. Under the IS92a emission scenario, for example, Model I predicts that atmospheric CO₂ content will reach 910.50 Gt C by the year 2100, representing a 28% increase from 2000. In comparison, Model II projects a slightly lower increase, with atmospheric CO₂ reaching 825.27 Gt C by 2100, reflecting approximately a 20% increase. However, the 25-compartment model forecasts a significantly higher atmospheric CO₂ content of 1674.90 Gt C by 2100, corresponding to an approximate 114% increase.

The predictions of CO₂ content in the ocean component from Models I and III are relatively close, whereas Model II predicts significantly lower values. However, all three models project an increase in oceanic CO₂ over time, with Model II indicating a more rapid rise.

Model III's baseline curve illustrates a decrease in the CO₂ content of the terrestrial ecosystem, from 1839.96 Gt C in 2000 to 1803.24 Gt C in 2100. Conversely, both Models I and II predict an increase in terrestrial ecosystem CO₂ content over time, with Model I showing a more rapid increase compared to Model II.

It is notable that the models demonstrate consistent behavior across scenarios when input factors are set to their nominal values.

5. Partitioning Uncertainty

The disparities observed between the actual data and the predicted atmospheric CO₂ content highlight significant sources of uncertainty. To pinpoint these sources, it is imperative to conduct an analysis to discern their contributions. By identifying the primary sources of uncertainty, subsequent research endeavors can focus on minimizing output uncertainties. Initially, by setting input factors at their nominal values and focusing solely on the atmosphere compartment, the three GCC models across three emission scenarios are utilized to delineate the overarching uncertainty range over time. Figure 10 illustrates the shaded area, representing the maximum uncertainty range (MUR_t) of atmospheric CO₂ content spanning the period from 1995 to 2100.

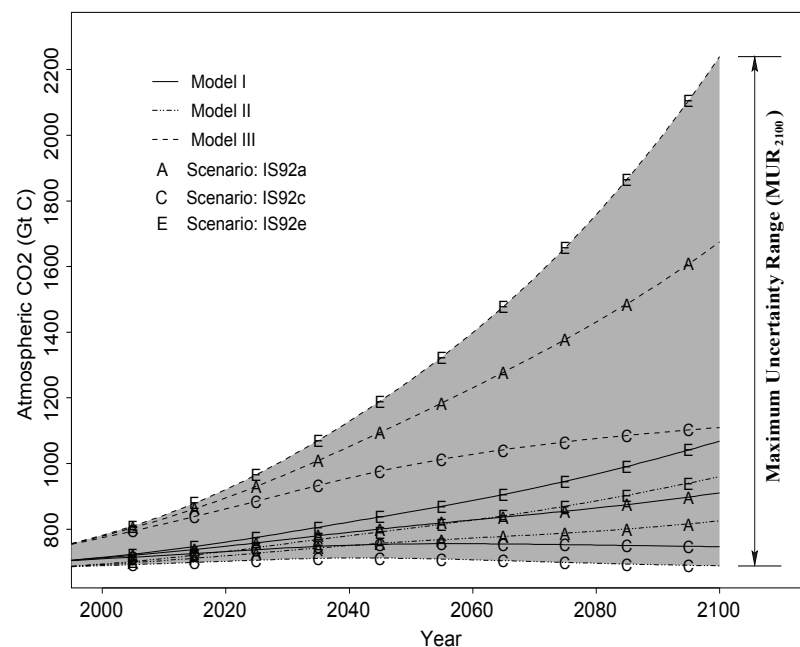


Figure 10. Maximum uncertainty range of Atmospheric CO₂ predictions derived from three GCC models using the IS92a, c, and e emission scenarios for the period 1995–2100. Model simulations maintain all input factors at their nominal values.

The maximum uncertainty range MUR₂₁₀₀, encompassing both model and scenario uncertainties for the year 2100 (highlighted in Figure 10), is calculated as 1550.71 Gt C,

derived by subtracting the minimum value of 688.28 from the maximum of 2238.99. The uncertainty range (UR_i) can be further refined when certain models and/or scenarios are excluded. For instance, the reduced UR_{2100} when Model III is omitted indicates that this model contributes 76% to the MUR_{2100} ; without its influence, the MUR_{2100} diminishes to 379.68. Notably, the exclusion of Model I, considered the ‘median’ model, does not alter the MUR_{2100} . Conversely, Model II contributes only 4% to the MUR_{2100} .

Shifting focus to scenarios, it is evident that IS92e exerts the most significant influence on the MUR_{2100} (approximately 36%), while IS92c contributes 9%. Excluding scenario IS92a, identified as the ‘median’ scenario, does not affect the MUR_{2100} .

Employing a methodology pioneered by Draper (see [29]), termed the “model uncertainty audit”, the comprehensive predictive uncertainty surrounding y is partitioned into two components: ‘between scenario (BS)’ and ‘due to input factors within scenario (WS)’. The latter component represents uncertainty arising from the lack of knowledge about specific input factors.

In preceding sections, the complexities of input factor uncertainty within models and scenarios, scenario uncertainty within models, and model uncertainty within scenarios were explored. Now, the focus shifts to discerning the contribution of each of these sources to the overall uncertainty surrounding an output variable. Initially, an investigation was conducted to determine whether disparities in predictions primarily stem from scenario variations or differences in input factors for a given model. The analysis centers on the atmospheric CO_2 content in the year 2100 (referred to as $y_{Atm}(t = 2100)$), denoted as y for brevity in this section.

With y as the output variable and scenario i occurring with probability p_i , leading to estimated mean ($\hat{\mu}_i$) and standard deviation ($\hat{\sigma}_i$) of y , the overall mean and variance of the output variable are calculated as follows:

$$\hat{\mu} = E_S[\hat{E}(y|S)] = \sum_{i=1}^s p_i \hat{\mu}_i \quad (3)$$

and

$$\hat{\sigma}^2 = V_S[\hat{E}(y|S)] + E_S[\hat{V}(y|S)] = \sum_{i=1}^s p_i (\hat{\mu}_i - \hat{\mu})^2 + \sum_{i=1}^s p_i \hat{\sigma}_i^2 = \hat{\sigma}_{BS}^2 + \hat{\sigma}_{WS}^2 \quad (4)$$

Here, S stands for scenario, and $s = 3$ represents the three emission scenarios (IS92a, IS92c, and IS92e), BS indicates ‘between scenario’, and WS denotes ‘within scenario’. For each of the three models, the scenario-specific means and standard deviation (SD) estimates are provided in Table 6, along with two possible vectors of scenario probabilities. The first vector (Case 1) assigns a probability of 0.9 to the IS92a (business-as-usual scenario) and 0.05 to each of the IS92c and IS92e scenarios. Another case (Case 2) considers equal probabilities for all three scenarios. These cases are chosen for demonstration purposes; however, in practice, expert opinion should guide the determination of possible scenario probability vectors.

The estimates presented in Table 6 are based on 5000 model simulations, assuming all model input factors follow a uniform distribution within their assigned ranges. Following this, employing Equations (3) and (4) alongside the estimates from Table 6 for each of the two scenarios yields the summarized outcomes as presented in Table 7.

For Model III, it is noteworthy that the proportion of variance attributed to scenario uncertainty is relatively small across both scenario probability cases: approximately 2% in Case 1 and 13% in Case 2. This finding echoes observations from Figure 5, where minimal variation was apparent in prediction uncertainty due to different scenarios for this specific model.

As for Models I and II, Table 7 illustrates that in Case 1, the contributions of scenario and input factor uncertainties to the overall uncertainty are approximately equal, with input factor uncertainty slightly outweighing scenario uncertainty. However, in Case 2,

where scenarios are assumed to have equal probability of occurrence, the scenario uncertainty becomes predominant. Specifically, the percentage of variance arising from scenario uncertainty rises significantly to approximately 80% with Model I and 84% with Model II.

Table 6. Estimated scenario-specific means and standard deviations of Atmospheric CO₂ content in 2100 from all three models (in Gt C), accompanied by two sets of scenario probabilities.

Model	Scenario	Mean ($\hat{\mu}_i$)	SD ($\hat{\sigma}_i$)	Scenario Probability (p_i)	
				Case 1	Case 2
Model I	IS92a	920.9	67.0	0.90	1/3
	IS92c	755.4	67.0	0.05	1/3
	IS92e	1079.9	67.0	0.05	1/3
Model II	IS92a	825.2	48.1	0.90	1/3
	IS92c	688.3	48.1	0.05	1/3
	IS92e	959.9	48.1	0.05	1/3
Model III	IS92a	1926.9	1111.7	0.90	1/3
	IS92c	1402.9	995.3	0.05	1/3
	IS92e	2455.6	1198.0	0.05	1/3

Table 7. Partitioned uncertainty analysis of predicted atmospheric CO₂ content in 2100, delineating contributions from ‘between scenarios’ and ‘due to input factors within scenarios’ components, contingent upon scenario probabilities. Results presented for all three models.

Model	Summary of the Results	Results with Scenario Probabilities	
		Case 1	Case 2
Model I	Overall mean ($\hat{\mu}$)	920.58	918.73
	Overall variance ($\hat{\sigma}^2$)	7122.46	22,041.39
	Between-scenario variance ($\hat{\sigma}_{BS}^2$)	2633.46	17,552.39
	Within-scenario variance ($\hat{\sigma}_{WS}^2$)	4489.00	4489.00
	% of variance between scenarios	37.0	79.6
	% of variance due to input factors within scenarios	63.0	20.4
Model II	Overall mean ($\hat{\mu}$)	825.09	824.47
	Overall variance ($\hat{\sigma}^2$)	4157.88	14,608.31
	Between-scenario variance ($\hat{\sigma}_{BS}^2$)	1844.27	12,294.7
	Within-scenario variance ($\hat{\sigma}_{WS}^2$)	2313.61	2313.61
	% of variance between scenarios	44.4	84.2
	% of variance due to input factors within scenarios	55.6	15.8
Model III	Overall mean ($\hat{\mu}$)	1927.14	1928.47
	Overall variance ($\hat{\sigma}^2$)	1,261,285.00	1,405,265.00
	Between-scenario variance ($\hat{\sigma}_{BS}^2$)	27,704.93	184,697.40
	Within-scenario variance ($\hat{\sigma}_{WS}^2$)	1,233,581.00	1,220,568.00
	% of variance between scenarios	2.0	13.0
	% of variance due to input factors within scenarios	98.0	87.0

Having partitioned the prediction uncertainty between scenarios and input factors within scenarios for each individual model, the aim now is to delve deeper and partition the prediction uncertainty into three components: between scenarios, between models within scenarios, and between input factors within models and scenarios, following Draper’s model uncertainty audit approach. This endeavor, aimed at dissecting the overall uncertainty about y into three distinct components, presents a slightly more intricate scenario.

There are three scenarios ($s = 3$) and three models ($m = 3$), each given equal weights ($w_1, w_2, w_3 = \frac{1}{3}, \frac{1}{3}, \frac{1}{3}$). Using the scenario index i and model index j , the nine values of atmospheric CO₂ content for the year 2100 ($\hat{y}_{ij}$) are computed. Table 8 presents the scenario-specific means $\hat{\mu}_i = \sum_{j=1}^m w_j \hat{y}_{ij}$ and standard deviations $\hat{\sigma}_i = \left[\sum_{j=1}^m w_j (\hat{y}_{ij} - \hat{\mu}_i)^2 \right]^{1/2}$ based on these predictions, alongside the probability assessments (p_1, p_2, p_3) for the three scenarios. As previously, two cases with different sets of scenario probabilities are examined.

Table 8. Estimated scenario-specific means and standard deviations of atmospheric CO₂ content in 2100 (in Gt C), accompanied by two sets of scenario probabilities.

Scenario <i>i</i>	Mean ($\hat{\mu}_i$)	SD ($\hat{\sigma}_i$)	Scenario Probability (p_i)	
			Case 1	Case 2
IS92a	1136.90	382.02	0.90	1/3
IS92c	848.32	186.56	0.05	1/3
IS92e	1422.30	579.17	0.05	1/3

Let y represent the atmospheric CO₂ content in 2100, x denote the means and standard deviations provided in Table 8, and $\hat{\sigma}_{ij}^2$ represent the predictive variance conditional on the scenario and model, assumed to be independent. In this case, the overall mean and variance equations are as follows:

$$\hat{\mu} = E_S[\hat{E}_M\{\hat{E}(y|x, M, S)\}] = \sum_{i=1}^S p_i \hat{\mu}_i \quad (5)$$

and

$$\begin{aligned} \hat{\sigma}^2 &= V_S[\hat{E}_M\{\hat{E}(y|x, M, S)\}] + E_S[\hat{V}_M\{\hat{E}(y|x, M, S)\}] + E_S[\hat{E}_M\{\hat{V}(y|x, M, S)\}] \\ &= \sum_{i=1}^S p_i (\hat{\mu}_i - \hat{\mu})^2 + \sum_{i=1}^S p_i \hat{\sigma}_i^2 + \sum_{i=1}^S \sum_{j=1}^m p_i w_j \hat{\sigma}_{ij}^2 = \hat{\sigma}_{BS}^2 + \hat{\sigma}_{BMWS}^2 + \hat{\sigma}_{BPWMS}^2 \end{aligned} \quad (6)$$

respectively, where S represents scenario, M represents model, BS denotes ‘between scenarios’, $BMWS$ indicates ‘between models within scenarios’, and $BPWMS$ signifies ‘between predictions within models and scenarios’.

As indicated by the results in Table 9, in both cases where different probabilities are assigned to the three scenarios, the primary determinant of overall uncertainty appears to be the input factors within each model. Specifically, input factor uncertainty accounts for approximately 72% in Case 1 and 64% in Case 2 of the overall uncertainty. Conversely, the contribution of scenarios to the overall uncertainty is minimal, comprising less than 2% in Case 1 and about 9% in Case 2. When models are assigned equal probabilities, the impact of model uncertainty on overall prediction uncertainty is moderate, contributing slightly over 26% in Case 1 and approximately 27% in Case 2.

These findings indicate that regardless of the scenario probabilities chosen, when equal weights are assigned to the three models, the uncertainty arising from input factors within each model is the predominant source of uncertainty in the predictions. Although model uncertainty significantly contributes to the overall uncertainty, the influence of scenario uncertainty on the overall prediction uncertainty remains relatively low.

Table 9. Results from partitioning the total uncertainty in predicted atmospheric CO₂ content in 2100 into three components: ‘between scenarios (BS)’, ‘between models within scenarios ($BMWS$)’, and ‘between predictions within models and scenarios ($BPWMS$)’, as a function of scenario probabilities.

Summary of the Results	Results with Scenario Probabilities	
	Case 1	Case 2
Overall mean ($\hat{\mu}$)	1136.74	1135.84
Overall variance ($\hat{\sigma}^2$)	571,549.17	636,087.42
Between scenario variance ($\hat{\sigma}_{BS}^2$)	8236.55	54,909.41
Between models within-scenario variance ($\hat{\sigma}_{BMWS}^2$)	149,854.78	172,057.81
Between predictions within models and scenario variance ($\hat{\sigma}_{BPWMS}^2$)	413,457.84	409,120.20
% of variance between scenarios	1.44	8.63
% of variance between models within scenarios	26.22	27.05
% of variance between predictions within models & scenarios	72.34	64.32

6. Discussion

The uncertainty inherent in model predictions can stem from various sources, including the imperfect representation of real-world systems by the model structure, diverse scenarios depicting alternative future perspectives, and uncertainties surrounding model input factors. In this study, model uncertainty, scenario uncertainty, and input factor uncertainty within the frameworks of three compartmental models of the global carbon cycle (GCC) are systematically examined.

Building upon the prior research (see [2]), which extensively explored the impact of input factor variability on prediction uncertainty, this study supplements the analysis with graphical representations (see Figure 2), illustrating the efficacy of optimizing influential input factors in reducing prediction uncertainty. Furthermore, a temporal trend of increasing uncertainty in predictions is observed, aligning with the recognized accumulation of uncertainty in such models.

Assessing scenario uncertainty involves evaluating the impacts of varying fossil fuel and land-use emissions on each model compartment. As demonstrated in Figures 4 and 5, when considering input factor uncertainty, discrimination between scenarios is feasible for most output variables in the 8-compartment models (Models I and II). However, in the 25-compartment model (Model III), except for the atmosphere, surface ocean, and deep ocean—layer5 compartments, it fails to differentiate between scenarios. This may be due to the slower processes and longer time required for carbon to be transferred to the deeper layers of the ocean and terrestrial ecosystem compartments.

The findings discussed in Section 4.1.3 emphasize a significant increase in uncertainty in predictions made by Models I and II. This heightened uncertainty is partly due to the simplified and linear mathematical structures employed in these models. Specifically, Models I and II utilize linear compartmental modeling formulations outlined in Section 2, simplifying the representation of complex processes within the Earth's system. While these models capture essential aspects of carbon dynamics, their linear nature may oversimplify certain nonlinear interactions or feedback mechanisms inherent in the carbon cycle. Consequently, this oversimplification could result in discrepancies between model predictions and the observed data. Such limitations highlight the importance of comprehending the primary sources of uncertainty in model predictions. This understanding can guide future research priorities, inform model enhancements, and drive development efforts aimed at improving predictive capabilities and informing mitigation strategies.

As presented in Section 5, partitioning the uncertainty in $y_{Atm}(t = 2100)$ between scenario and input factor uncertainties within a specific model yields additional insights. The analysis, incorporating two scenario probability vectors, corroborates the previous findings (see Section 4.1.2), emphasizing the prevalence of input factor uncertainty in Model III. In contrast, for Models I and II, the impact of scenario uncertainty on prediction uncertainty fluctuates with scenario probabilities, aligning with the prior observations in the scenario uncertainty section.

An additional endeavor entailed partitioning the overall uncertainty into three components: between scenarios, between models within scenarios, and between predictions within models and scenarios. The results of this investigation unveiled that for the specific models and scenarios analyzed, when assigning equal weights to the three models and considering the two chosen sets of scenario probabilities, input factor uncertainty significantly outweighs prediction uncertainties, with model uncertainty contributing moderately and scenario uncertainty having minimal impact. These findings underscore the critical role of input factors in shaping overall uncertainty and emphasize the need for targeted strategies to address them in future model development endeavors.

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