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SCCM – the Simple Carbon-Climate Model: Technical Documentation

Ian N. Harman, Cathy M. Trudinger and Michael R. Raupach

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Enquiries should be addressed to:

Dr. Ian Harman,
CSIRO Marine and Atmospheric Research,
FC Pye Laboratory,
GPO Box 3023,
Canberra, ACT, 2601
AUSTRALIA
email: ian.harman@csiro.au

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Contents

Executive summary 1

1. Introduction 2

2. The Simple Carbon-Climate Model (SCCM) 3

2.1 Carbon Dioxide and the Carbon Cycle 4

2.1.1 Ocean carbon cycle 4

2.1.2 Terrestrial Carbon Cycle 7

2.1.3 Land-Use and Land-Use Change (LULUC) 9

2.1.4 Atmospheric CO_2 Concentration 10

2.2. Methane 11

2.2.1. Oxidation of Methane to Carbon Dioxide 13

2.3. Nitrous Oxide 13

2.4. Chlorofluorocarbons 14

2.5. Radiative Forcing 15

2.6. Aerosols 16

2.7. Temperature 17

2.8. Separation of Components 19

2.9. Initialisation of SCCM 19

3. Projections of future climate 22

3.1 Sensitivity to Carbon Cycle Options 27

4. Model structure and use 31

4.1 Science Development Version 31

4.2 GIAM Version 33

4.3 Run Configuration 33

5. Summary 35

References 36

Appendix A – Tables of SCCM variables and parameters 40

Appendix B – Step response function for the CSIRO Mk3L GCM 45

Results 46

Appendix C – Emulation of Full Ocean CO2 Chemistry (CO2Sys) 47

The Ocean CO_2 System 47

CO_2Sys in SCCM 48

The Pade-Approximant Fit 49

The Power-Law Fit 50

List of Figures

Fig. 1 Schematic of the general structure of SCCM (specifically the version used within GIAM). Boxes indicate the state variables; solid lines are fluxes of material and dashed lines influences. Further details are given in the text. Not all components are required for every application. Additional components ($\delta^{13}CO_2$, PFCs, SF_6, HFCs) are available or in development. 3

Fig. 2 Schematic of the two box terrestrial carbon cycle model. 7

Fig. 3 Initialisation of the carbon pools in SCCM when $s_{CH42CO2}$=1 and F_{VOLC}=0. Arrows indicate the direction of a positive net flux of carbon between the SCCM carbon pools, assuming all rate terms *k* are positive. The endogenously determined terrestrial pools are given by Eq. (49) and the net fluxes from the atmosphere to the terrestrial pools are given by $F_{Cb10} = \gamma\ NPP_0 - (k_{1A} + k_{12} + k_{bs})\ C_{b10} - F_{CO2\_CH4}$ and, noting this term will be zero or negative as indicated by the arrow, $F_{Cb20} = (1-\gamma)\ NPP_0 - k_{2A}\ C_{b20} + k_{12}\ C_{b10}$. 20

Fig. 4 Emission time series used to drive SCCM. a) Fossil fuel emissions, b) LULUC emissions, c) CH_4 emissions, d) N_2O emissions. In each panel the black line gives the estimate of historical emissions (see text for further details) and the coloured lines the SRES marker scenarios (Red – A1FI, yellow – A1B, orange – A1T, blue – A2, green – B1, magenta – A2) used to force SCCM. The vertical dotted line marks the transition from historical estimates to SRES marker scenario projected emissions. 22

Fig. 5 Simulations (lines) and observations (from MacFarling Meure et al. (2006) - markers) of the atmospheric concentration of a) [CH_4] (in ppb) and b) [N_2O] (in ppb). Coloured lines refer to the SRES marker scenario. CH_4 and N_2O parameters and model choices given in the text. 23

Fig. 6 Simulations (lines) and observations (markers) of [CO_2] (in ppm) and change in global mean temperature (in K) from the period 1971-2000 (shaded). Coloured lines give the simulation using the GFDL (green), Mk3L (blue) and HadCM3 (red) temperature response functions. CO_2 observations are introduced further in the text; temperature observations from Jones et al. (2009) 23

Fig. 7 Simulation of [CO_2] (left) and ΔT (right) for the six SRES marker scenarios. Colours of lines as Fig. 6. Solid/dashed lines differentiate aerosol forcing option - see text for further details. 24

Fig. 8 Simulated evolution of the remaining terms in the carbon-cycle for each of the SRES marker scenarios. a) Change in the terrestrial carbon pool, $C_{b1}+C_{b2}$, b) change in the mixed layer carbon pool, ΣC_{si}, c) air-land flux, F_{AB}, and d) air-sea flux, F_{AS}. The change in the terrestrial carbon pool is the net result of F_{AB} and LUC. A positive value of either flux indicates transport from the atmosphere. Results using the Mk3L temperature response function shown only. Scenarios (Red – A1FI, yellow – A1B, orange – A1T, blue – A2, green – B1, magenta – A2). 26

Fig. 9 Simulations (lines) and observations (markers) of [CO_2] (a) and ΔT (b) when alternate model configurations are used. a) The increment to [CO_2] due to the oxidation of methane is included. b) Dashed lines have zero radiative forcing due to aerosols, solid lines as Fig. 6. b). Coloured lines give the simulation using the GFDL (green), Mk3L (blue) and HadCM3 (red) temperature response functions. 26

Fig. 10 Projections for the components of the carbon cycle and temperature change under different choices for the 2-box terrestrial carbon cycle model and carbon cycle fertilisation parameterisation schemes within SCCM. Solid and dashed lines show simulations using the ‘raupach’ and ‘trudinger’ 2 box model respectively. Black, blue and red lines show simulations using the ‘log’, ‘hyp’ and ‘hypm’ fertilisation options respectively. In a), b) and d) the ‘hypm’ and ‘log’ options are indistinguishable. The ‘trudinger’ 2-box model is calibrated to use different LULUC allocation and ocean options by default so these results are not truly reflective of the performance of this carbon cycle model. 28

Fig. 11 Projections for the components of the carbon cycle and temperature change under different choices for LULUC allocation within SCCM. All simulations use the ‘raupach’ 2-box terrestrial carbon cycle mode with the ‘log’ option for carbon fertilisation. Solid line shows the simulation using the ‘cb2’ choice for LULUC emissions allocation, dash-dotted line the simulation using the ‘gross’ option and dashed lines the simulation using the ‘added’ option…………………….. 29

Fig. 12 Projections for the components of the carbon cycle and temperature change under different choices for the *p*CO2 parameterisation scheme within SCCM. The black line gives the response with the ‘joos’ option, the magenta line that with the ‘enting’ option and the green line that with the ‘co2syspower’ option. The ‘co2syspade’ option is also plotted as a grey line but overlies the ‘co2syspower’ option. 29

Fig. 13 Projections for the components of the carbon cycle and temperature change under different choices for the ocean carbon cycle response functions within SCCM. The black line gives the response with the ‘raupach’ option, the blue line that with the ‘3d’ option, the red line that with the ‘hilda’ option and the green line that with ‘bdm’ option...................... 30

Fig. 14 Mk3L simulated (blue) and deduced SRF (black) representation of the change in globally-averaged near-surface air temperature after an instantaneous doubling of CO_2 in the long (left) and shorter (right) run. In the right panel the dashed line shows the corresponding 3-component SRF for the Mk3L which is indistinguishable from the 2-component PRF after *t*=40 years... 46

Fig. 15 The Pade-Approximant and Power-Law fits to the CO_2Sys model for a range of temperatures. Left panel: DIC(*x*CO2,*T*). Right panel: *x*CO2(DIC,*T*). Colours mark the variation of the fitted functions at temperatures 0°C (magenta), 10°C (blue), 15°C (green), 20°C (yellow) and 30°C (red). Solid line gives the Power-Law fit; dashed line the Pade-Approximant fit. Markers give the output from the full CO_2Sys model. Dotted lines mark estimates of preindustrial conditions.. 50

List of Tables

Table 1 Ocean mixed layer pulse response function coefficients in SCCM. Taken from Joos et al. (1996) and Raupach et al. (2011). 5

Table 2 Parameters describing the two-box terrestrial carbon cycle model in its 'trudinger' and 'raupach' configurations. For these preset options k_{bs}=0 and k_m is determined endogenously. 8

Table 3 Preconfigured options for 'aeromodelchoice' for the aerosol radiative forcing within SCCM. 17

Table 4 Temperature response functions and climate sensitivity values for the climate component options in SCCM. Note that the reciprocal of α_{TEMPi} is given in each case. Run refers to length of GCM simulation used to establish the response function. 18

Table 5 Example control file (*.ctl) for use with the science development version of SCCM. 31

Table 6 Example CO_2 component driver file (*.cmpt) for use with the science development version of SCCM. 32

Table 7 Example control file (*.gctl) for use with the GIAM version. 34

Table 8 Calculated time-varying quantities in SCCM. 40

Table 9 Fixed constants in SCCM. 40

Table 10 SCCM components. 41

Table 11 SCCM choices. 41

Table 12 SCCM parameters. 42

Table 13 SCCM time series inputs. 43

Table 14 SCCM outputs. 44

Table 15 2-component SRFs and climate sensitivity, $\Delta T_{2\times}$, for the Mk3L and 4 other GCMs. 46

EXECUTIVE SUMMARY

SCCM – the Simple Carbon-Climate Model – is a deterministic model for the globally averaged carbon cycle and climate system. It comprises representations of the carbon, methane, nitrous oxide, chlorofluorocarbon (CFC) mass balances of the Earth system and for the evolution of the global mean near-surface air temperature. The model is designed to provide broad scale information about the carbon cycle and climate systems within other applications, for example climate change policy analysis. A fundamental feature of SCCM is that each constituent component is calibrated against more complex models available in the literature and, where possible, against observations. Many of the components of SCCM have multiple options available; this includes some structural options and checks for internal consistency. This report documents the underlying scientific rationale of SCCM, its mathematical formulation, guidelines for the operation of the computer code including that within the CSIRO integrated assessment model (GIAM) and presents some initial, broad scale, results.

1. INTRODUCTION

The issues surrounding climate change, and in more generality Earth System Science or Human-Earth System Science, are many and complex. To aid in the understanding of these issues a wide range of models of the Earth System of varying complexities have been developed ranging from highly simplified 1-dimensional energy balance models for the Earth to highly complex coupled carbon-climate models in the natural sciences and integrated assessment models in the human-Earth sciences.

The Simple Carbon-Climate Model (SCCM) is a member of this suite of models. It seeks to capture the robust long-term dynamics of the coupled carbon cycle and climate system at a globally integrated level and in a simple form. The carbon cycle is typically resolved into 9 pools of carbon (one atmospheric, two terrestrial and 6 oceanic) and the fluxes between them. The climate system is typically represented by three pools of energy – all oceanic. As carbon (in multiple forms) is not the only driver of the global climate system, additional components such as atmospheric methane, nitrous oxide and aerosols are also included. By maintaining the simplicity of formulation of the model, the unavoidable uncertainties associated with complex systems can more easily be analysed and quantified.

SCCM aims to address questions in two, almost distinct, areas of science. First are questions concerning the historical and projected future development of the coupled carbon cycle and climate systems at the global level (e.g. Trudinger 2000; Le Quere et al. 2009). Through the combined use of high quality observations and SCCM, aspects of the natural and perturbed carbon cycle can be analysed and our understanding of the system improved.

Second are questions concerning the attribution of, and policy development to, climate change, including the balance between mitigation and adaptation actions (e.g. Trudinger and Enting 2005; Raupach et al. 2011; van Vuuren et al. 2011). The unavoidably contingent nature of the political process means that it is inappropriate to analyse the consequences of different human development trajectories and policy options with highly sophisticated and complex models of the carbon cycle and climate system – at least if the analyses are needed in a timely fashion. For these questions an understanding of the robust aspects of the carbon-climate problem and quantification of the uncertainty is critical. In order to aid timely analysis for these kinds of questions SCCM is now incorporated as the climate component of the Global Integrated Assessment Model (GIAM – Gunasekera et al. 2008; Harman et al. 2008).

This report concentrates on the scientific basis and performance of SCCM independent of GIAM. The report is structured as follows: In Section 2 we outline the scientific basis and mathematical formulation of SCCM. In Section 3 we document SCCM projections of future climate for some standard emissions scenarios. Section 4 describes how the model is written and structured, the different configurations available and how it is used. Finally, we provide a brief summary and Tables of the key terminology and variables used.

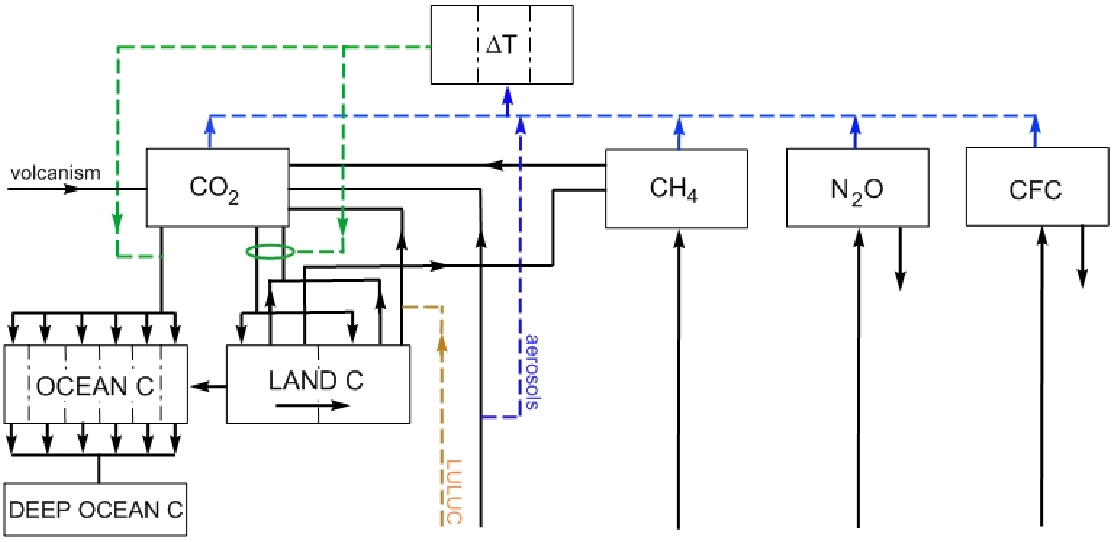

Fig. 1 Schematic of the general structure of SCCM (specifically the version used within GIAM). Boxes indicate the state variables; solid lines are fluxes of material and dashed lines influences. Further details are given in the text. Not all components are required for every application. Additional components ($\delta^{13}CO_2$, PFCs, SF_6, HFCs) are available or in development.

2. THE SIMPLE CARBON-CLIMATE MODEL (SCCM)

The Simple Carbon-Climate Model (SCCM) is a quantitative model for the globally-averaged carbon cycle and climate system. Its primary aim is to convert time series of estimates of emissions (either anthropogenic or total) of greenhouse gases (GHGs) to calculate the globally-averaged concentration of these gases, and the resulting increase in global radiative forcing and near-surface air temperature. This model is of a type which sits at the simpler end of the climate model spectrum with its focus being on ease of use and uncertainty estimation. Other models in this general category include MAGIC-C (Wigley 1991; 1993; Meinhausen et al. 2011a; 2011b) and the Bern-CC model (Joos et al. 2001).

SCCM calculates the change over time of various state variables in the state vector, $\mathbf{x}$. Typical state variables include the atmospheric concentration of CO_2 or other greenhouse gases (GHGs). At the global scale the near-surface air temperature is closely tied to the ocean surface temperature and as the ocean heat capacity is many times greater than that of the atmosphere it is the ocean then that provides the control and predictability. Model equations for the evolution of the state vector over time are written as differential equations ($\mathrm{d}\mathbf{x}/\mathrm{d}t = \ldots$) and solved using a 5th order adaptive time-step Runge-Kutta method.

The model can consider a number of different GHGs (CO_2, CH_4, N_2O, CFCs). These can be modelled at the same time or subsets can be chosen if the application demands this. Figure 1 shows a general linkage diagram for a standard (GIAM) configuration of SCCM, with boxes indicating state variables, solid lines fluxes and dashed lines influences. For many of the state variables there are different options that can be selected for the model equations. Throughout this report the subscript *pre* indicates the preindustrial (~1750) value of the variable concerned, with the correct units; in many cases these take the form of input parameters and need to be supplied (see Section 4).

2.1 Carbon Dioxide and the Carbon Cycle

There are three primary active stores of carbon in the Earth system – the atmosphere, the mixed layer of the ocean (including the marine biosphere) and the terrestrial biosphere. SCCM employs simple parameterisations of the exchange between these three stores to determine gross features of future projections of the carbon cycle.

2.1.1 Ocean carbon cycle

Carbon in the oceanic mixed layer is mixed into the rest of the ocean through a set of complex, spatially and temporally varying, physical and biological processes. Direct inclusion of these processes would be overly sophisticated for the purposes of SCCM. Instead SCCM takes the common approach of modelling the net effect of these processes through the use of Response Functions calibrated against more complex models of the ocean carbon cycle (e.g. Joos et al. 1996). Specifically the change in the global stock of carbon in the ocean mixed layer, Cs, is modelled as a number of separate 'pools', Cs_i, each with its own turn-over time scale. The evolution of each of the carbon pools is then modelled as

$$\frac{\mathrm{dCs}_i}{\mathrm{d}t} = a_{\mathrm{ML}i}\left(F_{\mathrm{CO2\_AS}}(t)+F_{\mathrm{CO2\_BS}}(t)\right)-\alpha_{\mathrm{ML}i}\mathrm{Cs}_i \tag{1}$$

where $F_{\mathrm{CO2\_AS}}$ is the air-sea flux of CO_2 in GtC yr^{-1} with a positive value indicating a flux from the air into the ocean and $F_{\mathrm{CO2\_BS}} = k_{bs}\mathrm{Cb}_1$ is the land-sea flux of carbon in GtC yr^{-1} with a positive value indicating a flux from the land into the ocean (where Cb_1 is amount of carbon in pool 1 of the terrestrial carbon model, discussed in more detail in Section 2.1.2). $\alpha_{\mathrm{ML}i}$ provide the temporal response of each of the carbon pools and $a_{\mathrm{ML}i}$ provide the partitioning of the air-sea flux between the different pools with $\sum_i a_{\mathrm{ML}i} = 1$. The total change in ocean mixed layer carbon, $\mathrm{Cs}{=}\sum_i \mathrm{Cs}_{\mathrm{ML}i}$.

Formally Eq. (1) is the implementation of the convolution form for the ocean mixed layer response function in AR1 form (Wigley 1991; Enting 2007), i.e. the implementation of

$$\mathrm{Cs} = \int_{t_0}^{t}\left(F_{\mathrm{CO2\_AS}}(t')+F_{\mathrm{CO2\_LS}}(t')\right)R_{\mathrm{ML}}(t-t')\,\mathrm{d}t' \tag{2}$$

where R_{ML} is the mixed layer response function. Conversion to Eq. (1) requires the assumption that R_{ML} can be well-approximated by a series of exponentials. This is the only approximation that removes the dependence of t' from the dynamical systems representation of the convolution.

The coefficients $\alpha_{\mathrm{ML}i}$ and $a_{\mathrm{ML}i}$ are obtained by calibration against more complete ocean carbon cycle models. Joos et al. (1996) provides two expressions for the response functions for four such ocean models – for the short and long run. As we are primarily interested in the long (multi-year) time scales we employ the long run expressions however, in order to strictly conserve carbon we include a fast response pool, with the same characteristics as the short run expressions, which carries any unallocated carbon. Table 1 gives the resultant coefficients for the three ocean models included in SCCM (Joos et al. 1996) together with the four-pool approximation to the BDM and HILDA models as used by Raupach et al. (2011).

Table 1 Ocean mixed layer pulse response function coefficients in SCCM. Taken from Joos et al. (1996) and Raupach et al. (2011).

	Fast pool	Mixed layer response function						
BDM								
$a_{\mathrm{ML}i}$	0.52444	0.16851	0.11803	0.076817	0.050469	0.010469	0.031528	0.019737
$\alpha_{\mathrm{ML}i}$	4.78389	1/1.6388	1/4.8702	1/14.172	1/43.506	1/148.77	1/215.71	0.0
HILDA								
$a_{\mathrm{ML}i}$	0.431967	0.24278	0.13963	0.089318	0.037820	0.035549	0.022936	
$\alpha_{\mathrm{ML}i}$	6.78378	1/1.26798	1/5.2528	1/18.601	1/68.736	1/232.30	0.0	
3D-Princeton								
$a_{\mathrm{ML}i}$	0.0	0.70367	0.24966	0.066485	0.038344	0.019439	0.014819	
$\alpha_{\mathrm{ML}i}$	0.0	1/0.70177	1/2.3488	1/15.281	1/65.359	1/347.55	0.0	
Raupach								
$a_{\mathrm{ML}i}$	0.0	0.512934	0.320278	0.142183	0.024605			
$\alpha_{\mathrm{ML}i}$	0.0	5.22893	0.356532	0.0194692	0.0			

The sink term in Eq. (1) represents the loss of carbon from the ocean mixed layer into the deep ocean either through mixing or the fall of detritus. SCCM tracks the resultant change in deep ocean carbon content, $\mathrm{Cs}_{\mathrm{deep}}$, where

$$\frac{\mathrm{dCs}_{\mathrm{deep}}}{\mathrm{d}t} = \sum_i \alpha_{\mathrm{ML}i} \mathrm{Cs}_i \qquad (3)$$

For numerical reasons the ocean carbon cycle therefore consists of ten state variables – 8 carbon pools as given by the mixed layer response function, a fast response pool and the deep ocean carbon pool. In cases where the original response function has less than 8 pools then the unused pools have zero content.

The air-sea flux $F_{\mathrm{CO2\_AS}}$ is determined by the difference in the partial pressure of CO_2 in the atmosphere and ocean mixed layer and parameterised as

$$F_{\mathrm{CO2\_AS}} = k_g \left(\mathrm{CO2}_{\mathrm{ppm}} - p\mathrm{CO2}_{\mathrm{ML}} \right) \big/ \mathrm{r}_{\mathrm{CO2\_ppmGtC^{-1}}} \qquad (4)$$

where $\mathrm{CO2}_{\mathrm{ppm}}$ is the atmospheric concentration of CO_2 in ppm, $p\mathrm{CO2}_{\mathrm{ML}}$ is the partial pressure of oceanic mixed layer CO_2 in ppm, $\mathrm{r}_{\mathrm{CO2\_ppmGtC^{-1}}} = 0.4695$ (in ppm GtC^{-1}) is a conversion factor for CO_2 between Gt of carbon and ppm, and k_g is the gas exchange coefficient and is an input parameter (see Section 4). $p\mathrm{CO2}_{\mathrm{ML}}$ is related to the change in the ocean mixed layer carbon through a two step process. First, the change in ocean mixed layer carbon is related to the change in dissolved inorganic carbon δDIC, in moles m^{-3}, as

$$\delta \mathrm{DIC} = \frac{\mathrm{Cs}}{12 \times \mathrm{OA} \times \mathrm{MLD}} = \frac{\mathrm{Cs}}{321.21} \qquad (5)$$

where OA is the Ocean surface area in multiples of 10^{15} m^2 and MLD is the depth of the oceanic mixed layer. The value for MLD and the mixed layer response function are not independent.

Second, δDIC is related to $p\mathrm{CO2}_{\mathrm{ML}}$ through one of four options. The pco2choice='enting' option follows Bacastow (1981) and Enting and Lassey (1993) by parameterising this relationship as

$$p\mathrm{CO2}_{\mathrm{ML}} = p\mathrm{CO2}_{\mathrm{ref}}[1 + y\xi(y)] \tag{6}$$

where $p\mathrm{CO2}_{\mathrm{ref}} = \mathrm{CO2}_{\mathrm{pre}}$ in ppm is a reference partial pressure and

$$y = \delta\mathrm{DIC}/\mathrm{DIC}_{\mathrm{pre}} \tag{7}$$

with $\mathrm{DIC}_{\mathrm{pre}}$ = 2.089 moles m^{-3} is the preindustrial value for dissolved inorganic carbon. The buffer, or Revelle, factor ξ is parameterised as a quadratic function of y namely

$$\xi(y) = 9.36 + 59.56y + 4558y^3 \tag{8}$$

The second option for $p\mathrm{CO2}_{\mathrm{ML}}$, pco2choice='joos', is taken from Sarmiento et al. (1992) and utilised by Joos et al. (1996) as

$$p\mathrm{CO2}_{\mathrm{ML}} = p\mathrm{CO2}_{\mathrm{ref}} + \frac{1000\, z_0(T)\, \delta\mathrm{DIC}}{1 - 1000\, z_1(T)\, \delta\mathrm{DIC}} \tag{9}$$

with

$$\begin{aligned} z_0 &= 1.7561 - 0.031618T + 0.000444T^2 \\ z_1 &= 0.004096 - 7.7086\times10^{-5}T + 6.10\times10^{-7}T^2 \end{aligned} \tag{10}$$

where T is the temperature of the ocean mixed layer in °C. Note that the factor of 1000 difference between Eq. (9) and the equivalent expression in Joos et al. (1996) arises from the use of different units for δDIC. Note that under the 'joos' option for pco2choice, increasing the temperature decreases the value of $p\mathrm{CO2}_{\mathrm{ML}}$ which is counter to the conventional understanding of the oceanic carbon cycle (e.g. Skirrow 1975).

The third and fourth options, pco2choice='co2syspade' and pco2choice='co2syspower', invoke Pade-Approximant and Power-Law parameterisations of the $\mathrm{CO_2Sys}$ model for ocean carbon chemistry (Lewis and Wallace 1998). The $\mathrm{CO_2Sys}$ model quantifies the complex carbonate chemistry that occurs in seawater drawing on ~50 years of research in the field. Both 'CO2SysPade' and 'CO2Syspower' operate in both forward and backward modes i.e.

$$p\mathrm{CO2}_{\mathrm{ML}} = f\left(\mathrm{DIC}, T\right) \quad \text{and} \quad \mathrm{DIC} = f\left(p\mathrm{CO2}_{\mathrm{ML}}, T\right) \tag{11}$$

are given. While entirely self-contained, the use of $\mathrm{CO_2Sys}$ within SCCM does depend on one exogenous parameter, namely $\mathrm{DIC}_{\mathrm{pre}}$. Further details of the $\mathrm{CO_2Sys}$ parameterisations are given in Appendix C. With the 'joos' and CO2Sys forms for $p\mathrm{CO2}$, if the temperature component is not active then $T = T_{pre}$ throughout, where T_{pre} is a parameter giving the preindustrial global mean temperature (in °C).

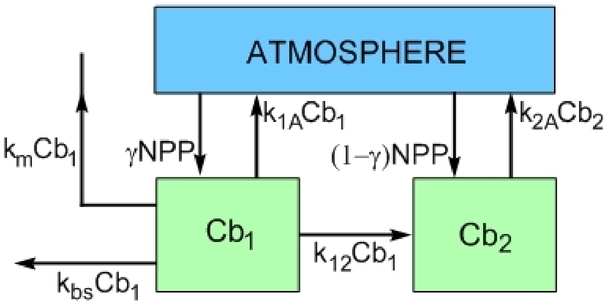

Fig. 2 Schematic of the two box terrestrial carbon cycle model.

2.1.2 Terrestrial Carbon Cycle

The terrestrial carbon cycle, in an analogous manner to the oceanic carbon cycle, is the net result of a range of biological processes which are too many and too complex to capture explicitly in a model of the simplicity of SCCM. SCCM instead employs a two-box model of the terrestrial carbon cycle as shown schematically in Fig. 2 The model has two pools of carbon (in GtC) and can take three different configurations dependent on parameter choices. The net flux between the atmosphere and the terrestrial biosphere is comprised of the flux to the biosphere, the net primary productivity, NPP (principally the balance between the assimilation of carbon associated with photosynthesis and the release of carbon through autotrophic respiration), and the flux from the biosphere, heterotrophic respiration. The heterotrophic respiration is assumed proportional to the carbon stock in each pool.

In all three options the time evolution of the terrestrial carbon cycle is described by

$$\begin{aligned}\frac{\mathrm{dCb}_1}{\mathrm{d}t} &= \gamma\mathrm{NPP} - \left(k_{1A} + k_{12} + k_{bs} + k_m\right)\mathrm{Cb}_1 \\ \frac{\mathrm{dCb}_2}{\mathrm{d}t} &= \left(1-\gamma\right)\mathrm{NPP} + k_{12}\mathrm{Cb}_1 - k_{2A}\mathrm{Cb}_2\end{aligned} \tag{12}$$

where k_{ij} are the rate constants describing the fluxes from/between the pools and γ determines the partitioning of the NPP between the two pools. A flux directly between the land and sea is allowed through the $k_{bs}\mathrm{Cb}_1$ term; similarly a loss of terrestrial carbon to atmospheric methane is incorporated through the $k_m\mathrm{Cb}_1$ term. Arguments can easily be made for equivalent fluxes to be incorporated from the Cb_2 pool, however for simplicity this is not done.

The first option, twoboxchoice=‘trudinger’, employs the two-box carbon cycle model from the CSIRO Box Diffusion Model (Enting and Lassey 1993; Trudinger et al. 1999; Trudinger 2000). The interpretation is that one box, Cb_1, represents the short-lived component of the terrestrial biosphere and the second box, Cb_2, the long-lived component which includes dead organic matter in the soil. All NPP is assigned to the short-lived box (γ=1) and there is a flux between the two boxes. The default parameters for the configuration were chosen to give the same isotopic pulse response as that obtained by Emanuel et al. (1981) (Trudinger et al. 1999).

The second option, twoboxchoice=‘raupach’, employs the two-box carbon cycle model from Raupach et al. (2011). The interpretation is that Cb_1 represents fast-response systems such as grasslands and grassy components of savannah systems, and Cb_2 represents slower-response woody systems. In each case, biotic and soil carbon are lumped together. The majority of NPP (γ = 0.8) is assigned to fast response systems but there is no internal flux between the systems. With these two options the rate constants are prescribed as shown in Table 2.

Table 2 Parameters describing the two-box terrestrial carbon cycle model in its ‘trudinger’ and ‘raupach’ configurations. For these preset options k_{bs}=0 and k_m is determined endogenously.

parameter	**NPP$_{\mathrm{pre}}$**	γ	k_{1A}^{-1}	k_{12}^{-1}	k_{2A}^{-1}	**Cb$_{1\mathrm{pre}}$**	**Cb$_{2\mathrm{pre}}$**
units	(GtC yr^{-1})		(yr)	(yr)	(yr)	(GtC)	(GtC)
‘trudinger’	84.3	1.0	6.3	20.3	54.5	405.3	1089
‘raupach’	40	0.8	3	∞	300	96	2400

The final option, twoboxchoice=‘userdef’, places the responsibility for the parameter values and interpretation onto the user. The preindustrial values for the two pools, Cb$_{1\mathrm{pre}}$ and Cb$_{2\mathrm{pre}}$, are calculated to ensure initial equilibrium.

NPP is prescribed to be constant unless affected by increasing atmospheric CO$_2$ – the so-called CO$_2$ fertilisation effect - or increasing temperature. SCCM includes three, albeit very simple, parameterisations for the CO$_2$ fertilisation effect.

The first option, fertchoice=‘log’, parameterises the effect using a logarithmic function (Raupach et al. 2011) i.e.

$$\mathrm{NPP(CO2)} = \mathrm{NPP}_{\mathrm{pre}}\left[1+\beta\ln\left(\frac{\mathrm{CO2}}{\mathrm{CO2}_{\mathrm{pre}}}\right)\right] \tag{13}$$

where β is an input parameter (typically between 0.4 and 0.8) and NPP$_{\mathrm{pre}}$ is the preindustrial value of NPP (an input parameter with a typical value of 40-60 GtC yr^{-1} (Prentice et al. 2001)). Note that the CO$_2$ fertilisation effect influences current day observations of NPP.

The second option, fertchoice=‘hyp’, uses the functional form proposed by Allen et al. (1987)

$$\mathrm{NPP} = \mathrm{NPP}_{\mathrm{pre}}\left[1+\mathrm{f}_{\mathrm{NPP}}\left(G(\mathrm{CO2}_{\mathrm{ppm}})-1\right)\right] \tag{14}$$

with

$$G(\mathrm{CO2}_{\mathrm{ppm}}) = G_{\infty}\frac{\mathrm{CO2}_{\mathrm{ppm}}-C_c}{\mathrm{CO2}_{\mathrm{ppm}}+d} \tag{15}$$

where f$_{\mathrm{NPP}}$ is the fraction of NPP to which the enhancement applies, C_c is the compensation concentration below which photosynthesis ceases, G_{∞} is the limiting growth factor and $d=(G_{\infty}-1)C_0-G_{\infty}C_c$ ensures that NPP = NPP$_{\mathrm{pre}}$ at CO2=CO2$_{\mathrm{pre}}$. Calculations by Trudinger et al. (1999) used f$_{\mathrm{NPP}}$ =0.81, C_c=80ppm, G_{∞}=2.4.

The third option, fertchoice=‘hypm’, is the hyperbolic function used in MAGICC6 (Meinshausen et al. 2011a; 2011b).

$$\mathrm{NPP} = \mathrm{NPP}_{\mathrm{pre}}\frac{\left[1+b(\mathrm{CO2}_{\mathrm{pre}}-\mathrm{C}_c)\right]\left[\mathrm{CO2}-\mathrm{C}_c\right]}{\left[\mathrm{CO2}_{\mathrm{pre}}-\mathrm{C}_c\right]\left[1+b(\mathrm{CO2}-\mathrm{C}_c)\right]} = \mathrm{NPP}_{\mathrm{pre}}\frac{b+1/(\mathrm{CO2}_{\mathrm{pre}}-\mathrm{C}_c)}{b+1/(\mathrm{CO2}-\mathrm{C}_c)} \tag{16}$$

where CO2 is in ppm, C$_c$ is the compensation concentration below which photosynthesis ceases and b is an adjustable parameter. By choosing b as

$$b = \frac{(680-\mathrm{C}_c)-r(340-\mathrm{C}_c)}{(r-1)(680-\mathrm{C}_c)(340-\mathrm{C}_c)} \tag{17}$$

where r is the ratio

$$r = \frac{1+\beta \ln\left(680/\mathrm{CO2}_{\mathrm{pre}}\right)}{1+\beta \ln\left(340/\mathrm{CO2}_{\mathrm{pre}}\right)} \tag{18}$$

the NPP enhancement due to a CO_2 increase from 340 to 680 ppm matches that of the logarithmic method. This option is similar to the ‘hyp’ option but with one fewer adjustable parameter. Meinshausen et al. (2011a; 2011b) used C_c=31 ppm.

Both NPP and R_H are known to vary with temperature. This variation is included through the use of Q_{10}-factors independently of the parameter values used in the two box model or the choice of CO_2 fertilisation parameterisation. Any flux into or out of either terrestrial carbon pool $F(T)$ is given by

$$F(T) = F(T_{\mathrm{pre}}) \times Q_{10}^{\frac{T-T_{\mathrm{pre}}}{10}} \tag{19}$$

where T is the temperature in °C and T_{pre} is the mean temperature in preindustrial times. Separate Q_{10}-factors are possible for NPP ($Q_{10\mathrm{NPP}}$) and for respiration ($Q_{10\mathrm{resp}}$) the flux between the boxes Cb_1 and Cb_2 is also set to depend on $Q_{10\mathrm{resp}}$. The Q_{10}-factors are implemented by adjusting the rate constants k_{ij} with temperature i.e.

$$\ln\left(k_{ij}(T)\right) = \ln\left(k_{ij}(T_{\mathrm{pre}})\right) + \frac{T-T_{\mathrm{pre}}}{10}\ln(Q_{10}) \tag{20}$$

If the temperature component of SCCM is not active and temperature is not supplied as an input (see Section 2.8), a constant temperature of $T=T_{\mathrm{pre}}$ is assumed.

Finally the net flux of carbon from the atmosphere to the terrestrial biosphere, $F_{\mathrm{CO2\_AB}}$, in the absence of a flux due to Land-use and Land-use change (LULUC), is given by

$$F_{\mathrm{CO2\_AB}} = \mathrm{NPP}\left(\mathrm{NPP}_{\mathrm{pre}}, \mathrm{CO2}, T\right) - k_{1A}(T)\mathrm{Cb}_1 - k_{2A}(T)\mathrm{Cb}_2 \tag{21}$$

2.1.3 Land-Use and Land-Use Change (LULUC)

Anthropogenic activities impact the terrestrial carbon stores both indirectly, by perturbing the climate within which the natural ecosystems operate, but also directly. The resulting net fluxes of carbon between the terrestrial and atmospheric stores are also known as the emissions due to Land use and Land use change (LULUC) and are particularly difficult to quantify, predict or model. Despite this difficulty most estimates of LULUC indicate that these have been over the recent history the second largest source of emissions of GHGs, after fossil fuel emissions, into the atmosphere and so cannot be neglected (e.g. Le Quere et al. 2009).

The net flux of carbon from the terrestrial store to the atmosphere is included in SCCM via one of three options. The first option, lucchoice=‘added’, simply adds the exogenous estimate of the LULUC flux to the atmosphere as $F_{\mathrm{CO2\_LUC}}$ in Eq. (23) but with no corresponding sink term applied to the terrestrial carbon pools. This option does not conserve carbon between the terrestrial and atmospheric stores.

The second option, lucchoice=‘cb2’, similarly applies the LULUC flux as a source in Eq. (23) but, in order to conserve carbon, treats the LULUC flux as a sink of carbon from box 2 (Cb_2) of the terrestrial carbon cycle model (Eq. (12)). With this option, the LULUC flux estimates are interpreted as quantifying the long term (permanent) loss of carbon from the terrestrial biosphere that is associated with the conversion of land between being dominated by woody vegetation to being dominated by grassy vegetation (e.g. the transition from forested land to cropped land due to the expansion of agriculture).

The final option, lucchoice='gross', recognises and corrects for a model characteristic when using LULUC estimates generated through carbon accounting methods that account for not only the initial removal and oxidation of the carbon in the vegetation, but also subsequent regrowth and changes in soil carbon (e.g. Houghton 2008). This is a net effect of both anthropogenic activities and the natural responses to these activities. If we apply this kind of LULUC estimate directly as a sink to Cb_2 we also decrease the respiration from the pool, $k_{2A}Cb_2$ – i.e. there is an additional impact on the modelled respiration. Yet this effect is already included in the LULUC estimates. There is a double counting occurring and the net impact on the atmospheric CO_2 content is different from that intended by the LULUC estimates.

To compensate for this 'double counting' Enting and Lassey (1993) propose converting the net LULUC flux estimate, *B*, into a gross LULUC flux estimate, *D*, using

$$D(t) = B(t) + k_{2A} \int_{t_0}^{t} B(t')\mathrm{d}t' \qquad (22)$$

where t_0 is the start time of the time series of the net LULUC flux estimates, and use $F_{\mathrm{CO2\_LUC}} = D$. In effect, the net LULUC flux is converted into a model-dependent gross flux before being added to the atmosphere and subtracted from box 2 of the terrestrial carbon cycle model (Cb_2) as in the case of the 'cb2' option.

Finally, the optimisation of the parameters in the carbon cycle model implicitly depends on the source of, and methodology used to implement the LULUC flux estimate. The 'trudinger' and 'raupach' terrestrial carbon cycle options for twoboxchoice both utilise the Houghton (2008) LULUC flux estimates for calibration purposes. However the parameters for the 'trudinger' option are found employing the 'gross' option for the LULUC flux whereas the parameters for the 'raupach' carbon cycle option are found using the 'cb2' option for the LULUC flux. Ideally, if we are to change the methodology of implementing the LULUC flux estimates, then we would also reoptimise for the parameter values in the carbon cycle model.

2.1.4 Atmospheric CO_2 Concentration

The third active store of active carbon in the Earth system is that carbon contained as CO_2 in the atmosphere. In SCCM the total amount of CO_2 in the atmosphere (in GtC) is given by

$$\frac{\mathrm{dCO2}}{\mathrm{d}t} = F_{\mathrm{CO2\_FOSS}}(t) + F_{\mathrm{CO2\_LUC}}(t) - F_{\mathrm{CO2\_AS}}(t) - F_{\mathrm{CO2\_AB}}(t) + F_{\mathrm{CO2\_CH4}}(t) + F_{\mathrm{VOLC}}(t) \qquad (23)$$

where *t* is time in years, $F_{\mathrm{CO2\_FOSS}}$(t) are CO_2 emissions due to fossil fuel burning and other industrial sources (including cement production), $F_{\mathrm{CO2\_LUC}}$(t) are net CO_2 emissions due to land use and land use change (LULUC - Section 2.1.3), $F_{\mathrm{CO2\_AS}}$(t) is the calculated net air-sea flux (Section 2.1.1), $F_{\mathrm{CO2\_AB}}$(t) is the calculated net air-land flux (Section 2.1.2), $F_{\mathrm{CO2\_CH4}}$(t) is the calculated flux of CO_2 resulting from the oxidation of methane (Section 2.2.1) and F_{VOLC}(t) are any sources of CO_2 from volcanism and other exogenous sources. Positive values of $F_{\mathrm{CO2\_AS}}$ and $F_{\mathrm{CO2\_AB}}$ represent a flux from the atmosphere into the ocean or terrestrial store so act as a sink on the atmospheric store. All these fluxes are expressed in GtC yr^{-1}. Estimates of historical CO_2 emissions due to fossil fuel emissions and LULUC are given by Boden et al. (2009) and

Houghton (2008) respectively although other estimates are available. The F_{VOLC} term must be prescribed exogenously.

SCCM uses units of GtC to quantify the amount of CO_2 in the atmosphere however some relationships, Eq. (4) and (15) in particular, require the amount of CO_2 expressed as a concentration in ppm. These two measures of atmospheric CO_2 are related by

$$\mathrm{CO2}_{\mathrm{ppm}} = \mathrm{CO2} \times \mathrm{r}_{\mathrm{CO2\_ppmGtC^{-1}}} \tag{24}$$

where $\mathrm{r}_{\mathrm{CO2\_ppmGtC^{-1}}} = 0.4695$ (in ppm $\mathrm{GtC^{-1}}$).

The preindustrial value of atmospheric CO_2 content is added back onto the state variable before output, given in ppm.

A number of recent studies have demonstrated the usefulness of the cumulative anthropogenic emissions of carbon dioxide, q, within climate change policy analyses (e.g. Allen et al. 2009; Matthews et al. 2009; Meinhausen et al. 2009; Zickfeld et al. 2009; Raupach et al. 2011). q is carried endogenously in SCCM and given by

$$\frac{\mathrm{d}q}{\mathrm{d}t} = F_{\mathrm{CO2\_FOSS}} + F_{\mathrm{CO2\_LUC}} \tag{25}$$

where q is given in GtC and takes a value of 0 at the start of the simulation.

2.2. Methane

Increasing attention is being paid to the role methane plays in the natural and perturbed climate system. Methane is a more powerful GHG than CO_2 but has a shorter residence time in the atmosphere. There are also multiple sources of anthropogenic methane making efforts to reduce emissions of methane appear promising as a form of climate change mitigation.

The methane cycle, however, presents a number of key problems when attempting to model it. First there are a large number of both natural and anthropogenic sources of methane and there is no clear dominance between the two. A large effort is then needed to track both the anthropogenic emissions and the natural sources, including perturbations to these natural sources as a result of climate or other factors. Second, the principal sink of methane is oxidation to, eventually, CO_2 in the atmosphere. (There are smaller sinks at wet surfaces including the soil e.g. Boucher et al. 2009). This sink is the result of a complex chain of chemical reactions some of which, particularly those involving the hydroxyl radical OH, are susceptible to competition from other chemical reactions including those which only occur in the presence of other anthropogenically emitted species. Finally, the relatively short residence time of methane also implies that emissions are not fully mixed in the atmosphere and there can be a noticeable dissimilarity between the methane concentration in the two hemispheres of the Earth and consequent impacts on climate and chemistry. All three of these features present challenges to a simple model such as SCCM.

SCCM quantifies methane in the atmosphere, in Tg-CH_4, as a single globally integrated quantity. The globally integrated sink of methane, $\mathrm{S}_{\mathrm{CH4}}$, is assumed proportional to the amount of CH_4 present in the atmosphere, via a lifetime for methane, τ_{CH4}, i.e.

$$S_{\mathrm{CH4}} = \frac{\mathrm{CH4} + \mathrm{CH4}_{\mathrm{pre}}}{\tau_{\mathrm{CH4}}} \tag{26}$$

where $\mathrm{CH4}_{\mathrm{pre}}$ is the preindustrial quantity of atmospheric methane and CH4 the perturbation from that value (again in units of Tg-CH_4). As described above, τ_{CH4} is dependent on a range of factors including other chemical species. Unlike MAGIC-C (Wigley 1991), SCCM makes no attempt to model the variation of τ_{CH4} or its dependencies over time, instead two options for the time variation of τ_{CH4} are available.

The first option, ch4tauchoice='const', uses a constant, specifiable, value for τ_{CH4}. A range of methodologies (e.g. inversion, chemical modelling) indicate that a suitable value for τ_{CH4} in preindustrial times (i.e. the inferred value for the lifetime of methane in the absence of anthropogenic emission of species which interact with the methane cycle) was approximately 8-9 yr (Forster et al. 2007). Estimates for more recent times indicate that the lifetime of methane has increased (to approximately 10 years according to Boucher et al. (2009)) indicating a slower rate of methane oxidation in the atmosphere.

The second option, ch4tauchoice='power', is taken from Raupach et al. (2011). Here inferred estimates for the variation of τ_{CH4} over time have been simply parameterised using a power-law dependence. Specifically τ_{CH4} is found to depend on the atmospheric concentration of methane as

$$\tau_{\mathrm{CH4}} = \tau_{\mathrm{CH4pre}} \left(\frac{\mathrm{CH4}_{\mathrm{pre}}}{\mathrm{CH4} + \mathrm{CH4}_{\mathrm{pre}}} \right)^{\alpha} ; \quad \alpha = -0.12 \tag{27}$$

where τ_{CH4pre} is the (specifiable) value for τ_{CH4} in preindustrial times.

The (globally integrated) amount of methane in the atmosphere is hence modelled as

$$\frac{\mathrm{dCH4}_{\mathrm{pre}}}{\mathrm{d}t} + \frac{\mathrm{dCH4}}{\mathrm{d}t} = \frac{\mathrm{dCH}_4}{\mathrm{d}t} = F_{\mathrm{CH4}} - \frac{\mathrm{CH4} + \mathrm{CH4}_{\mathrm{pre}}}{\tau_{\mathrm{CH4}}} \tag{28}$$

where F_{CH4} is the total source of methane from anthropogenic and natural sources. The model itself can be implemented in three ways, depending on the character of the source information.

The first option, ch4forchoice='total', is the appropriate form to use when the source information (in Tg-CH_4 yr^{-1}) includes all sources, including natural sources, of methane e.g. those determined through model inversion. The time dependence of CH4 is determined through Eq. (28) directly.

The second option, ch4forchoice='anthro', invokes the 2-box terrestrial carbon cycle model in order to determine the perturbations to the natural release of methane. The total source of methane, F_{CH4}, is given by

$$F_{\mathrm{CH4}} = AF_{\mathrm{CH4}} + k_m \mathrm{Cb}_1 \tag{29}$$

and the anthropogenic forcing, AF_{CH4}, is exogenously provided.

The final option, ch4forchoice='perturbation', assumes that in preindustrial times the natural sources and sinks of methane were in long term equilibrium. Eq. (28) can then be rewritten as

$$\frac{\mathrm{dCH4}_{\mathrm{preind}}}{\mathrm{d}t}+\frac{\mathrm{dCH4}}{\mathrm{d}t}=\frac{\mathrm{dCH4}}{\mathrm{d}t}=\Delta F_{\mathrm{CH4}}-\frac{\mathrm{CH4{+}CH4}_{\mathrm{pre}}}{\tau_{\mathrm{CH4}}}+\frac{\mathrm{CH4}_{\mathrm{pre}}}{\tau_{\mathrm{CH4pre}}} \qquad (30)$$

where ΔF_{CH4} is now the perturbation to the methane sources and *includes* any induced perturbations to the natural sources of methane from preindustrial times. Options 'anthro' and 'perturbation' are better suited when the forcing data time series used are obtained through "bottom-up" inventory studies (e.g. Stern and Kaufmann 1998) or from the output of integrated assessment models such as GIAM.

All options for ch4choice can accommodate either option for the methane lifetime. The preindustrial value of atmospheric CH_4 content is added back onto the state variable before output, given in ppb.

2.2.1. Oxidation of Methane to Carbon Dioxide

The oxidation of methane acts as both the primary sink of atmospheric methane but also as a small source in the atmospheric CO_2 budget (Eq. (23)) and (smaller) other sources elsewhere (Boucher et al. 2009). In SCCM the only pathway represented for the CO_2 produced by oxidation of methane is into the atmosphere as the flux $F_{\mathrm{CH4\_CO2}}$ where

$$F_{\mathrm{CH4\_CO2}}=\frac{s_{\mathrm{CH42CO2}}}{1000}\frac{r_{\mathrm{MC}}}{r_{\mathrm{MCH4}}}\frac{\mathrm{CH4{+}CH4}_{\mathrm{pre}}}{\tau_{\mathrm{CH4}}} \qquad (31)$$

with s_{CH42CO2} a parameter (taking a value between 0 and 1) quantifying the amount of the CO_2 which remains in the atmosphere. The ratio $r_{\mathrm{MC}}/r_{\mathrm{MCH4}}=0.75$ provides the conversion between Pg-CH_4 and Gt-C as CO_2 and the factor of 1000 converts between Tg-CH_4 and Pg-CH_4. If the methane component is not active then either an 'observed' time series of methane concentrations (see Section 2.8) or a default value of 700ppb is used in Eq. (31). Finally note that the optimal parameter values for neither the 'trudinger' nor 'raupach' options in the terrestrial carbon cycle were obtained with this oxidation of methane included.

2.3. Nitrous Oxide

Nitrous oxide, N_2O, presents many of the same challenges to SCCM as methane, particularly in that its sources are both natural and anthropogenic in nature. However the chemical sink of N_2O is less complicated than that of methane. The globally integrated amount of N_2O in the atmosphere, measured in Mt-N as N_2O, is modelled as

$$\frac{\mathrm{dN2O}_{\mathrm{pre}}}{\mathrm{d}t}+\frac{\mathrm{dN2O}}{\mathrm{d}t}=\frac{\mathrm{dN2O}}{\mathrm{d}t}=F_{\mathrm{N2O}}-\frac{\mathrm{N2O}+\mathrm{N2O}_{\mathrm{pre}}}{\tau_{\mathrm{N2O}}} \qquad (32)$$

where τ_{N2O} is the, assumed constant, lifetime of N_2O, F_{N2O} is the total sources of N_2O, $\mathrm{N2O}_{\mathrm{pre}}$ the preindustrial amount of N_2O in the atmosphere and N2O the perturbation from that value. Analogously to the methane cycle the N2O model can be implemented in three ways depending on the character of the source information.

The first option, n2oforchoice='total', is the appropriate form to use when the source information (in Mt-N yr^{-1} as N_2O) includes all sources, including natural sources, of nitrous oxide e.g. those determined through model inversion. The time dependence of N_2O is determined through Eq. (32) directly.

The second choice, n2oforchoice='anthro', explicitly partitions the globally integrated source of N_2O into an (invariant) natural component and an anthropogenic forcing ie.

$$F_{\mathrm{N2O}} = AF_{\mathrm{N2O}} + \frac{\mathrm{N2O}_{\mathrm{pre}}}{\tau_{\mathrm{N2O}}} \tag{33}$$

The final option, n2oforchoice='perturbation', explicitly considers the perturbation balance for N_2O. The preindustrial sources and sinks of N_2O are assumed to have been in equilibrium allowing Eq. (32) to be rewritten as

$$\frac{\mathrm{dN2O}}{\mathrm{d}t} = \Delta F_{\mathrm{N2O}} - \frac{\mathrm{N2O} + \mathrm{N2O}_{\mathrm{pre}}}{\tau_{\mathrm{N2O}}} + \frac{\mathrm{N2O}_{\mathrm{pre}}}{\tau_{\mathrm{N2O}}} = \Delta F_{\mathrm{N2O}} - \frac{\mathrm{N2O}}{\tau_{\mathrm{N2O}}} \tag{34}$$

where ΔF_{N2O} is now the perturbation to the N_2O sources and *includes* any induced perturbations to the natural sources of N_2O from preindustrial times. The latter two options are better suited when the source information comes from inventory estimates or from integrated assessment models such as GIAM. Note that, because the N_2O balance is entirely linear, these three options are equivalent provided the emissions files are appropriately offset.

The preindustrial value of atmospheric N_2O content is added back onto the state variable before output, given in ppb.

2.4. Chlorofluorocarbons

Two species of chlorofluorocarbon (CFC), specifically CFC-11 and CFC-12, are currently included in SCCM. The globally integrated amount of these species, measured in Tg of gas, is modelled analogously to the atmospheric CH_4 and N_2O balances, i.e.

$$\begin{aligned} \frac{\mathrm{dCFC11}}{\mathrm{d}t} &= \Delta F_{\mathrm{CFC11}} - \frac{\mathrm{CFC11}}{\tau_{\mathrm{CFC11}}} \\ \frac{\mathrm{dCFC12}}{\mathrm{d}t} &= \Delta F_{\mathrm{CFC12}} - \frac{\mathrm{CFC12}}{\tau_{\mathrm{CFC12}}} \end{aligned} \tag{35}$$

where $\Delta F_{\mathrm{CFC11}}$ and $\Delta F_{\mathrm{CFC12}}$ are the global emissions of CFC-11 and CFC-12 in Tg yr^{-1} respectively and τ_{CFC11} and τ_{CFC12} are the respective lifetimes of CFC-11 and CFC-12 in the atmosphere. Typical values for these lifetimes are $\tau_{\mathrm{CFC11}} = 45$ yr and $\tau_{\mathrm{CFC12}} = 100$ yr (Forster et al. 2007). Only two options – cfcforchoice='total' or 'perturbation' – are implemented for these gases. As there are no known natural sources of these gases an 'anthro' option is unnecessary. Furthermore as the preindustrial values for CFC11 and CFC12 were 0 these two options are identical in practice. Output is given in ppt.

2.5. Radiative Forcing

The perturbations to the chemical composition of the atmosphere due to anthropogenic activities is one of the fundamental causes of recent changes in the Earth's climate (others include solar output variation and volcanic eruptions). Multiple changes in composition can be quantified by a single metric, namely the globally integrated radiative forcing, by considering the net impact on the radiation balance of the troposphere (Forster et al. 2007). Simple 1- or 2-equation parameterisations of the complex radiative exchanges induced by increasing the atmospheric content of various GHGs have existed for some time (e.g. IPCC 2001; Gohar and Shine 2007; Forster et al. 2007 and references therein). SCCM employs the IPCC (2001) recommended parameterisations whereby the radiative forcing resulting from increased atmospheric CO_2, RF_{CO2}, is given by

$$\mathrm{RF}_{\mathrm{CO2}} = f_{\mathrm{CO2}} \ln\left(\frac{\mathrm{CO2}}{\mathrm{CO2}_{\mathrm{pre}}}\right) \tag{36}$$

where f_{CO2} (in Wm^{-2}) is parameter with a default value of f_{CO2}=5.35 Wm^{-2} (IPCC 2007).

The radiative forcing due to increased CH_4 and N_2O in the atmosphere is more complicated as the radiatively active wavelengths of the two gases are similar. The radiative forcing is calculated by (e.g. Gohar and Shine 2007)

$$\begin{aligned}\mathrm{RF}_{\mathrm{CH4}} = 0.036\Big[&\sqrt{\mathrm{CH4{+}CH4}_{\mathrm{pre}}} - \sqrt{\mathrm{CH4}_{\mathrm{pre}}}\Big] \\ &- f_{\mathrm{overlap}}\left(\mathrm{CH4}_{\mathrm{pre}} + \mathrm{CH4,N2O}_{\mathrm{pre}}\right) + f_{\mathrm{overlap}}\left(\mathrm{CH4}_{\mathrm{pre}},\mathrm{N2O}_{\mathrm{pre}}\right)\end{aligned} \tag{37}$$

and

$$\begin{aligned}\mathrm{RF}_{\mathrm{N2O}} = 0.036\Big[&\sqrt{\mathrm{N2O} + \mathrm{N2O}_{\mathrm{pre}}} - \sqrt{\mathrm{N2O}_{\mathrm{pre}}}\Big] \\ &- f_{\mathrm{overlap}}\left(\mathrm{CH4}_{\mathrm{pre}},\mathrm{N2O} + \mathrm{N2O}_{\mathrm{pre}}\right) + f_{\mathrm{overlap}}\left(\mathrm{CH4}_{\mathrm{pre}},\mathrm{N2O}_{\mathrm{pre}}\right)\end{aligned} \tag{38}$$

where

$$f_{\mathrm{overlap}}\left(\mathrm{C,N}\right) = 0.47\ln\left[1 + 2.01\times10^{-5}\left(\mathrm{CN}\right)^{0.75} + 5.31\times10^{-15}\mathrm{C}\left(\mathrm{CN}\right)^{1.52}\right] \tag{39}$$

quantifies the interaction between CH_4 and N_2O on the wavelength-by-wavelength radiation balance.

Finally, the radiative forcing for CFC-11 and CFC-12 is given by

$$\begin{aligned}\mathrm{RF}_{\mathrm{CFC11}} &= 0.25\,\mathrm{CFC11} \\ \mathrm{RF}_{\mathrm{CFC12}} &= 0.32\,\mathrm{CFC12}\end{aligned} \tag{40}$$

In Eqs. (36)-(40) concentrations of the gases are used (ppm, ppb, ppt as appropriate) not masses of gas.

SCCM allows for the independent inclusion of different radiative forcings even if all components are active e.g. in order to analyse the impacts of increasing temperatures on the terrestrial carbon cycle. The total radiative forcing applied to the temperature component is given by

$$\mathrm{RF} = \sum_{i=\left\{\substack{\mathrm{CO2,CH4,N20} \\ \mathrm{CFC11,CFC12}}\right\}} \mathrm{s}_{fi} \mathrm{RF}_{\mathrm{i}} + \mathrm{RF}_{\mathrm{aero}} \qquad (41)$$

where s_{fi} are a set of parameters (with value between 0 and 1). $\mathrm{RF}_{\mathrm{aero}}$ is the radiative forcing due to perturbations to the aerosol loading of the atmosphere as discussed next.

2.6. Aerosols

Aerosols interact with climate through a series of complex physical processes. The IPCC-AR4 estimate for the perturbation aerosol radiative forcing in 2000 is approximately equal in magnitude to the estimate of forcing due to the non-CO_2 GHG gases (Fig SPM2; Forster et al. 2007), i.e. approximately -1 Wm^{-2}. However, the confidence interval around this value is large reflecting a low level of scientific understanding (Forster et al. 2007). This low level of understanding presents significant difficulties if we wish to capture the effects of aerosols in a simple model such as SCCM.

First, there is a large range of aerosol species, each with their own route to impact. Second, many of these impacts are conditional or contingent on other aspects of climate (e.g. location in the atmosphere or the presence of clouds) implying that the covariance terms in the global average are significant. Finally, many species of aerosol are themselves the result of chemical or physical processes in the atmosphere (which are often uncertain or contingent) and the underlying sources for the aerosols (or their precursors) are poorly constrained. Aerosol-climate interaction science is still developing and hence a simple (e.g. 1-equation) formulation is problematic.

In many IAMs and EMICs the issue of aerosol radiative forcing is addressed by assuming that anthropogenic aerosol emissions, and the resultant forcing, is directly related to other anthropogenic emissions (often of carbon monoxide). Both the emissions and the forcing can be linked in this way because the residency time of most aerosols is short (<1 year). Unfortunately time series estimates of the global emissions of aerosol precursors or correlates such as CO are hard to determine from bottom-up estimates or (especially) through inversion techniques because of the short time and length scales of the sink processes involved in these cycles. Additionally GIAM (one of the principal users of SCCM) does not provide emissions of CO, or indeed other precursors, into the future as one of its outputs.

SCCM employs a simple parameterisation for the radiative forcing of the climate due to perturbations to the aerosol loading of the atmosphere. This functional form is consistent with the assumptions that aerosols are short lived in the atmosphere and originate through processes coincident with anthropogenic energy use and hence correlated with the anthropogenic emissions of carbon dioxide[1]. The aerosol radiative forcing, $\mathrm{RF}_{\mathrm{aero}}$, is parameterised by

$$\mathrm{RF}_{\mathrm{aero}} = f_{\mathrm{aero}}\left(F_{\mathrm{CO2}}, t, \ldots\right) = a_{val} + a_{prop} F_{\mathrm{CO2}}(t) \min\left[1, \exp\left\{-(t-2000)/a_{tau}\right\}\right] \qquad (42)$$

---

[1] The majority of options for aerosol radiative forcing in SCCM depend only on fossil fuel emissions of CO_2. Raupach et al. (2011) parameterizes the forcing in a similar manner but in terms of the fossil fuel plus LULUC emissions. Arguments could also be formulated to include emissions of methane associated with power generation.

Table 3 Preconfigured options for 'aeromodelchoice' for the aerosol radiative forcing within SCCM.

Option	a_{val}	a_{prop}	a_{tau}	F_{CO2}
'none'	0	0	–	–
'const'	Input*	0	–	–
'prop'	0	Input	–	$F_{CO2}=F_{CO2\_FOSS}$
'cleanup'	0	Input	Input (>0)	$F_{CO2}=F_{CO2\_FOSS}$
'all'	Input	Input	Input (>0)	$F_{CO2}=F_{CO2\_FOSS}$
'allluc'	Input	Input	Input (>0)	$F_{CO2}=F_{CO2\_FOSS}+F_{CO2\_LUC}$

* Values indicated as Input are supplied to SCCM through the control files – see Section 4.

In this three (four) parameter functional form, a_{val} represents a constant value of forcing irrespective of human activity. From first principals we would expect this parameter to be zero or otherwise very small. a_{prop} provides the quantification of the link between radiative forcing due to anthropogenic generated aerosols and the anthropogenic emissions of CO_2, F_{CO2}. Finally, the min[] function captures the notion that with time human activities will become more efficient and generally cleaner implying a reduction in the precursor emissions for aerosols, such as CO and sulphate aerosol, per unit of emitted CO_2. This 'cleanup' process is parameterised to occur after the year 2000 and over a time scale given by a_{tau}. All three parameters and the precise meaning of F_{CO2} can be set independently within SCCM.

There are six preset options available for the aerosol radiative forcing, controlled by the model choice 'aeromodelchoice' described further in Table 3. As current estimates (Forster et al. 2007) indicate that the aerosol radiative forcing approximately cancels the radiative forcing arising from the non-CO_2 GHGs (in 2000) and we expect a_{val} to be small, we can estimate the value of a_{prop} to be -0.1 $Wm^{-2}(PgC)^{-1}$ (-0.15 – -0.08), depending on the exact value of F_{CO2_FOSS}.

2.7. Temperature

Change in the globally averaged near surface air temperature remains the primary metric for analysing climate change. In common with nearly all aspects of the climate system, the net impact on temperature is the result of many competing and complimentary physical processes. SCCM parameterises these multiple processes through the use of response functions for the global climate system which are functions of the global mean radiative forcing. This is analogous to the methodology behind the oceanic carbon cycle in SCCM. Specifically the change in the global mean near surface air temperature, ΔT, is modelled as a number of separate 'pools', T_i, each with its own turn-over time scale. The evolution of each of the temperature pools is then modelled as

$$\frac{\mathrm{d}T_i}{\mathrm{d}t} = C_{sens} a_{\mathrm{TEMP}i} \alpha_{\mathrm{TEMP}i} \mathrm{RF}(t) - \alpha_{\mathrm{TEMP}i} T_i \tag{43}$$

where C_{sens} (in K $W^{-1}m^2$) is a measure of the heat capacity of the climate system, $\alpha_{\mathrm{TEMP}i}$ quantify the temporal response of each of the pools and $a_{\mathrm{TEMP}i}$ the partitioning of the radiative forcing between the different pools. Conservation of energy requires that $\sum_i a_{\mathrm{TEMP}i} = 1$.

Table 4 Temperature response functions and climate sensitivity values for the climate component options in SCCM. Note that the reciprocal of $\alpha_{\mathrm{TEMP}i}$ is given in each case. Run refers to length of GCM simulation used to establish the response function.

GCM	$\Delta T_{2\times}$	a_{TEMP1}	$\alpha_{\mathrm{TEMP1}}^{-1}$	a_{TEMP2}	$\alpha_{\mathrm{TEMP2}}^{-1}$	a_{TEMP3}	$\alpha_{\mathrm{TEMP3}}^{-1}$	Run
IMAGE	2.37	0.585	1.6	0.415	58.0			~200 yr
ECHAM	1.58	0.686	2.86	0.314	41.67			~200 yr
GFDL	1.85	0.473	1.2	0.527	23.5			~200 yr
Mk3L	3.64	0.446	4.48	0.554	369.09			1000 yr
ACCC	2.78	0.596	8.4	0.404	409.54			1000 yr
OSU	2.78	0.355	1.1	0.240	18.0	0.405	220.0	
HadCM3	3.74	0.43	4.51	0.18	140.3	0.39	1476.0	1000 yr

The IMAGE 2.1, ECHAM and GFDL response functions are obtained from Table 3.4. of den Elzen (1999); originally from Hasselmann et al. (1993). The CSIRO Mk3L (Phipps 2006) response function is documented in Appendix B of this report. ACCC and HadCM3 denote the two- and three-pool response functions for the Hadley Centre HadCM3 model (Trudinger and Enting 2005; Li and Jarvis 2009). Finally OSU is obtained from Schlesinger and Jiang (1990).

As in the case of the ocean carbon cycle, Eq. (43) is the implementation of the convolution form for the climate response function in AR1 form i.e. the implementation of

$$\Delta T(t) = C_{sens}\int_{t_0}^{t} \mathrm{RF}(t')R_{\mathrm{TEMP}}(t-t')\mathrm{d}t' \tag{44}$$

where R_{TEMP} is the temperature response function which we have assumed can be well approximated by a series of exponentials.

The temperature response function is obtained by calibrating against more complex GCMs by analysing specific simulations (see Li and Jarvis 2009, Appendix B). Seven options for the temperature response function are included in SCCM and described in Table 4. The traditional climate sensitivity of a climate model, $\Delta T_{2\times}$, is given by (from Eqs (36) and (43))

$$\Delta T_{2\times} = f_{\mathrm{CO2}}C_{sens}\ln 2\ . \tag{45}$$

Note that $\Delta T_{2\times}$, C_{sens} and the temperature response functions are not independent of each other nor, truly, from f_{CO2} when we determine these from GCM output. Hence, within SCCM, a default value of the climate sensitivity, $\Delta T_{2\times 0}$ is specified in conjunction with each temperature response function. Then, given a value for f_{CO2}, the value for C_{sens} is then inferred from Eq (45) (varying f_{CO2} is then equivalent to varying the relative weighting between the radiative forcing due to increased atmospheric content $\mathrm{CO_2}$ and that due to other changes in atmospheric composition). It is also possible to vary $\Delta T_{2\times}$, and therefore C_{sens}, through an exogenous surrogate parameter c_{lsens} with a default value of 1, where

$$\Delta T_{2\times 0}c_{lsens} = \Delta T_{2\times} = f_{\mathrm{CO2}}C_{sens}\ln 2 \tag{46}$$

Finally the total temperature change and projected global mean temperature are given by

$$T(t) = T_{\mathrm{pre}} + \Delta T = T_{\mathrm{pre}} + \sum_i T_i(t) \tag{47}$$

where the preindustrial temperature T_{pre} is a parameter specified through the SCCM configuration files, taking a typical value of 15°C.

It is noticeable, from Table 4, that those temperature response functions calibrated against ‘short run’ simulations tend to produce pools with shorter time scales. This is not overly surprising as any long time scale response is less likely to appear from the background variability, as simulated by the GCMs, over the simulation if this is of short length.

2.8. Separation of Components

There are a number of critical co-dependencies between the components of SCCM, specifically the carbon cycle can depend on temperature and the methane concentration and the evolution of the temperature depends on all the other components. To aid in the calibration of SCCM a set of model choices has been included whereby SCCM can be directed to either use its endogenous variables or externally provided (i.e. observed) variables for this forcing. Specifically, the co2 component includes choices co2tempchoice and co2ch4choice, which can take values ‘observed’ or ‘modelled’, directing the co2 component to use either modelled or observed time series of the global mean temperature and atmospheric concentration of methane when required. The co2 component also includes the choice ‘oceantempchoice’, which can take a value of ‘varying’ or ‘preind’, and directs the ‘joos’ and CO_2Sys p_{CO2} parameterisation schemes to use either varying (modelled or observed) or preindustrial temperatures. Within the temperature component, five equivalent choices (‘tempco2choice’, ‘tempch4choice’, ‘tempn2ochoice’, ‘tempcfc11choice’ and ‘tempcfc12choice’) exist so that the temperature can either be forced by modelled or observed time series of the GHGs included in SCCM. SCCM can be run with external forcing at the same time as endogenous calculations are made, however unless the ‘choice’ options are set to ‘modelled’ SCCM uses the external forcing. ‘tempco2choice’ can also take the value ‘co2e’; this option indicates that the time series of CO2 used should be interpreted to be CO_2-equivalent and hence all other forcing is set to zero.

When SCCM is directed to use ‘observed’ time series for these variables it is also necessary to provide those data files (in the correct format) through the driver files (see Section 4). The corresponding inputs names are ‘co2tempdata’ and ‘co2ch4data’ for the temperature and CH_4 concentration data to be used in the co2 component and ‘tempco2data’, ‘tempch4data’, ‘tempn2odata’, ‘tempcfc11data’ and tempcfc12data’ for the concentration data to be used in the temperature component.

2.9. Initialisation of SCCM

The majority of the state variables in SCCM can be directly initialised as described in Section 4. In contrast, initialisation of the carbon cycle is handled endogenously. The carbon cycle is multiply connected to the other components of SCCM and is the primary control of its dynamic response. Hence a poor initialisation of the carbon cycle can result in unrealistic behaviour of the entire model.

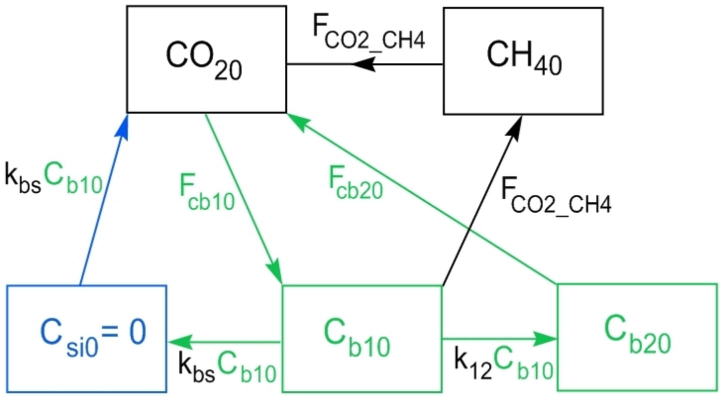

Fig. 3 Initialisation of the carbon pools in SCCM when s_{CH42CO2}=1 and F_{VOLC}=0. Arrows indicate the direction of a positive net flux of carbon between the SCCM carbon pools, assuming all rate terms *k* are positive. The endogenously determined terrestrial pools are given by Eq. (49) and the net fluxes from the atmosphere to the terrestrial pools are given by $F_{\mathrm{Cb10}} = \gamma\,\mathrm{NPP}_0 - (k_{1A} + k_{12} + k_{bs})\,C_{b10} - F_{\mathrm{CO2\_CH4}}$ and, noting this term will be zero or negative as indicated by the arrow, $F_{\mathrm{Cb20}} = (1-\gamma)\,\mathrm{NPP}_0 - k_{2A}\,C_{b20} + k_{12}\,C_{b10}$.

The initial state for the carbon cycle is *defined* to be the steady-state of SCCM in the absence of any anthropogenic forcing (fossil fuel emissions, LULUC emissions) and volcanic forcing, given initial values for the atmospheric concentration of carbon dioxide and methane. This definition is therefore appropriate for simulations which commence in preindustrial times. A more general method for initialisation of the carbon cycle will be the subject of future development.

The requirement for a steady-state initial condition has three immediate consequences:

1. All d/dt terms are zero and the system reverts to a set of linear equations in the *fluxes* of carbon.

2. $\mathrm{Cs}_{\mathrm{deep}} = \mathrm{Cs}_i = 0$ for all oceanic pools[2]. This implies that $F_{\mathrm{CO2\_AS}}(0) = -k_{ls}\mathrm{Cb}_{10}$.

3. The steady-state methane cycle implies that the natural source of methane (from Cb_1) balances exactly the sink of methane by oxidation (if included) i.e.

$$k_m\mathrm{Cb}_{10} = F_{\mathrm{CH4\_CO2}} = s_{\mathrm{CH42CO2}}\frac{r_{\mathrm{MC}}}{r_{\mathrm{MCH4}}}\frac{\mathrm{CH4}_{\mathrm{pre}}}{\tau_{\mathrm{CH4pre}}} \tag{48}$$

Together these three conditions combine to give the initial state, $\left\{\mathrm{Cb}_{10},\mathrm{Cb}_{20}\right\}$ of the carbon stores in the 2-box terrestrial carbon cycle model as

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[2] $d\mathrm{Cs}_{\mathrm{deep}}/dt = 0$ implies that a positive value for Cs_i must be balanced by a negative value for at least one Cs_j. The equations for $d\mathrm{Cs}_i/dt$ and $d\mathrm{Cs}_j/dt$ then imply that the self-induced tendency of the two terms are of opposite sense and so must be balanced by sources of opposing signs. However, the sources for these variables are positive, $a_{\mathrm{ML}i}>0$, multiples of $F_{\mathrm{CO2\_AS}} + F_{\mathrm{CO2\_LS}}$. The only viable steady-state solution is therefore $\mathrm{Cs}_{\mathrm{deep}} = \mathrm{Cs}_i = 0$.

$$\begin{aligned}\left(k_{1A}+k_{12}+k_{ls}\right)\mathrm{Cb}_{10} &= \gamma\mathrm{NPP}-s_{\mathrm{CH42CO2}}\left(r_{\mathrm{MC}}/r_{\mathrm{MCH4}}\right)\left(\mathrm{CH4}_{\mathrm{pre}}/\tau_{\mathrm{CH4pre}}\right)\\ k_{2A}\mathrm{Cb}_{20} &= \left(1-\gamma\right)\mathrm{NPP}+k_{12}\mathrm{Cb}_{10}\end{aligned} \tag{49}$$

with associated conditions

$$\begin{aligned}k_m &= s_{\mathrm{CH42CO2}}\left(r_{\mathrm{MC}}/r_{\mathrm{MCH4}}\right)\left(\mathrm{CH4}_{\mathrm{pre}}/\tau_{\mathrm{CH4pre}}\right)\left(\mathrm{Cb}_{10}\right)^{-1}\\ p\mathrm{CO2}_0 &= \mathrm{CO2}_0-k_{ls}\mathrm{Cb}_{10}/k_g\end{aligned} \tag{50}$$

the second of which sets the value of the free parameter ($p\mathrm{CO2}_{\mathrm{ref}}$ or DIC_0) in the parameterisation of pCO2.

Figure 3 shows the net fluxes between the carbon pools in SCCM at initialisation for the case where s_{CH42CO2}=1 and F_{VOLC}=0. Terms coloured black are those supplied exogenously or derived by the steady-state requirement for $\mathrm{CH_4}$. Terms coloured green are derived by requiring a steady-state of the terrestrial biosphere and terms coloured blue are derived by requiring a steady-state in the ocean carbon cycle. The net fluxes from the atmosphere to/from the biosphere are complicated functions of the other terms.

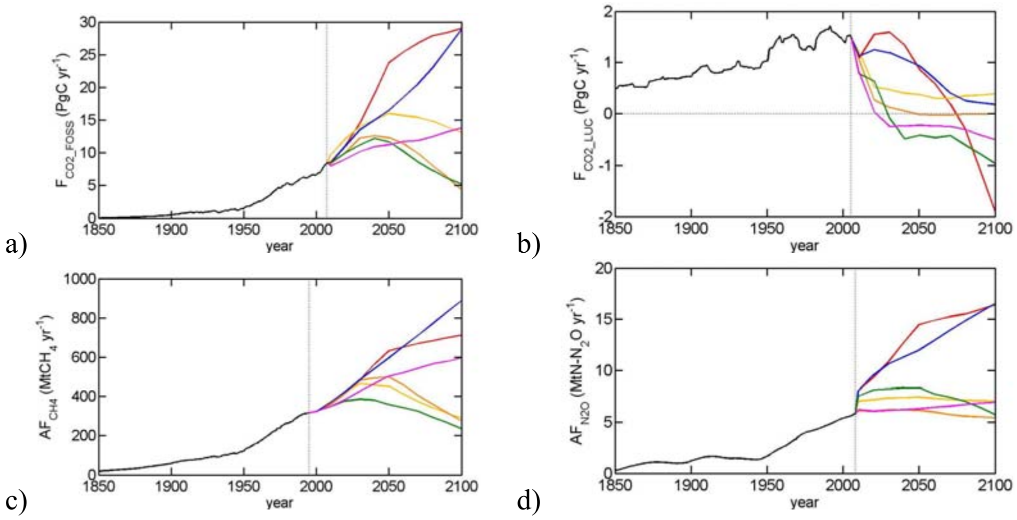
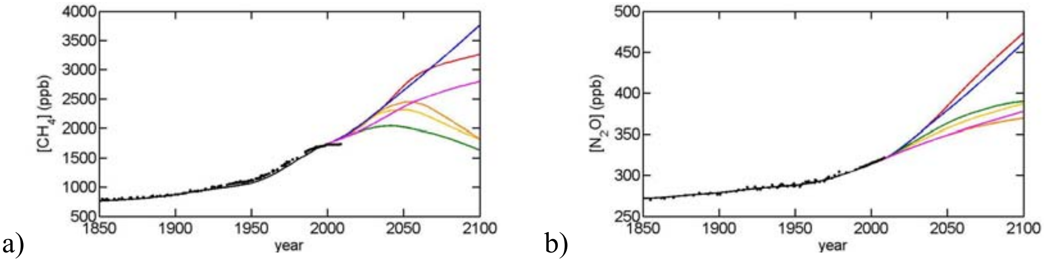


Fig. 4 Emission time series used to drive SCCM. a) Fossil fuel emissions, b) LULUC emissions, c) CH_4 emissions, d) N_2O emissions. In each panel the black line gives the estimate of historical emissions (see text for further details) and the coloured lines the SRES marker scenarios (Red – A1FI, yellow – A1B, orange – A1T, blue – A2, green – B1, magenta – A2) used to force SCCM. The vertical dotted line marks the transition from historical estimates to SRES marker scenario projected emissions.

3. PROJECTIONS OF FUTURE CLIMATE

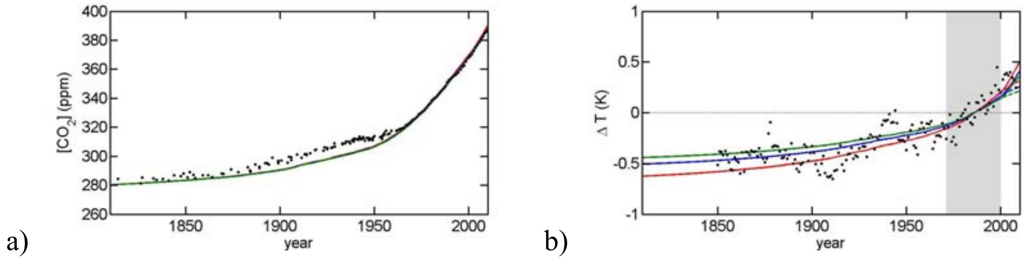
SCCM can be run in many configurations and for a range of purposes. To illustrate the performance of SCCM the following results show simulations against recent observations and projections of future climate under the 6 SRES marker scenarios (Nakicenovic et al. 2000). Purely deterministic results will be presented as a formal analysis of uncertainty forms part of ongoing research. For these results SCCM is configured as follows (based on the configuration used by Raupach et al. (2011) with some minor differences).

- Only the CO_2, CH_4, N_2O and temperature modules are active.
- The ‘raupach’ forms for the terrestrial carbon cycle and ocean mixed layer response function are used with LUC emissions taken from the Cb_2 pool. The ‘joos’ option for $pCO2$ is used. The preindustrial (1752) value for the CO_2 concentration is 278ppm.
- The CH_4 and N_2O modules are in ‘perturbation’ mode; the methane lifetime takes the ‘power’ law form (τ_{CH4}=8.2 yr, $CH4_0$=710 ppm, τ_{N2O}=122 yr, $N2O_0$=210 ppb).
- Aerosol forcing is active (unless stated otherwise) and depends on fossil fuel emissions only (a_{val}=0 Wm^{-2}, a_{prop}=-0.1 Wm^{-2} PgC^{-1} yr, a_{tau}=10 yr, corresponding to ‘aeromodelchoice’=‘cleanup’).
- CO_2 resulting from methane oxidation is not included in the atmospheric CO_2 budget (in order facilitate comparison with earlier results where this flux was not included).
- The emissions files required are taken from observed estimates for the early years of the simulation, either from bottom up inventories (fossil fuels, LULUC and CH_4) or inverted from atmospheric concentrations (N_2O) – see later for further details. Emissions for later years of the simulations are taken from the SRES marker scenarios (see Fig. 4). The exact year of the transition between the two emissions estimates depends on the availability of the historical estimates. For the LULUC and N_2O emissions there is a noticeable discontinuity between the historical estimates and projected emissions.



a) b)

Fig. 5 Simulations (lines) and observations (from MacFarling Meure et al. (2006) - markers) of the atmospheric concentration of a) [CH_4] (in ppb) and b) [N_2O] (in ppb). Coloured lines refer to the SRES marker scenario. CH_4 and N_2O parameters and model choices given in the text.



a) b)

Fig. 6 Simulations (lines) and observations (markers) of [CO_2] (in ppm) and change in global mean temperature (in K) from the period 1971-2000 (shaded). Coloured lines give the simulation using the GFDL (green), Mk3L (blue) and HadCM3 (red) temperature response functions. CO_2 observations are introduced further in the text; temperature observations from Jones et al. (2009)

In this configuration of SCCM the simulations of CH_4 and N_2O are independent from all other components. SCCM is able to reproduce the historical observations of both CH_4 and N_2O, shown in Fig. 5. The estimate of the historical emissions of N_2O were obtained through inference from the growth rate of [N_2O] (observations from MacFarling Meure et al. (2006) using a 50 year spline). Consequently the agreement between the observations and the SCCM simulations for N_2O is unsurprising as the emissions and observations are not independent. The historical emissions of CH_4 are taken from the bottom-up inventory estimates of Stern and Kaufmann (1998) and, so, are independent of SCCM. The subsequent agreement of the SCCM simulations with the observations is then less exact. SCCM under predicts the atmospheric CH_4 concentration through much of the 20th century with the exception of the period after the mid-1990's. The physical cause(s) of the "flattening" of the observed [CH_4] time series between the mid 1990's and 2007 is still the topic of research (e.g. Dlugokencky et al. 2011). The projected concentrations of both CH_4 and N_2O into the 21st century is largely determined by the emissions scenario although the shorter life time of CH_4 is evident by the greater variation in growth rates and concentrations between scenarios when compared with that for N_2O.

In contrast to the CH_4 and N_2O components, the CO_2 and temperature components of SCCM are dependent on the other modules. Consequently SCCM simulations of these components of the climate are dependent on multiple model choices and parameter values as well as the emissions scenario considered. The historical estimates of fossil fuel emissions of CO_2 are taken from CDIAC (Marland et al. 2008) while those for LULUC are taken from Houghton (2008). Aerosol radiative forcing during the pre-2000 period is assumed to be proportional to fossil fuel emissions. The resulting simulations of [CO_2] and change in global mean temperature (ΔT) for the historical period are given in Fig. 6, those for the 21st century are given in Fig. 7 for each SRES marker scenario separately. In each panel 6 simulations are shown; the different colours refer to different temperature response functions (GFDL, Mk3L or HadCM3) and the dashed and solid lines indicate cases where aerosol radiative forcing is maintained ($a_{tau} = \infty$ yr) or reduced ($a_{tau} = 10$ yr) after 2000 respectively.

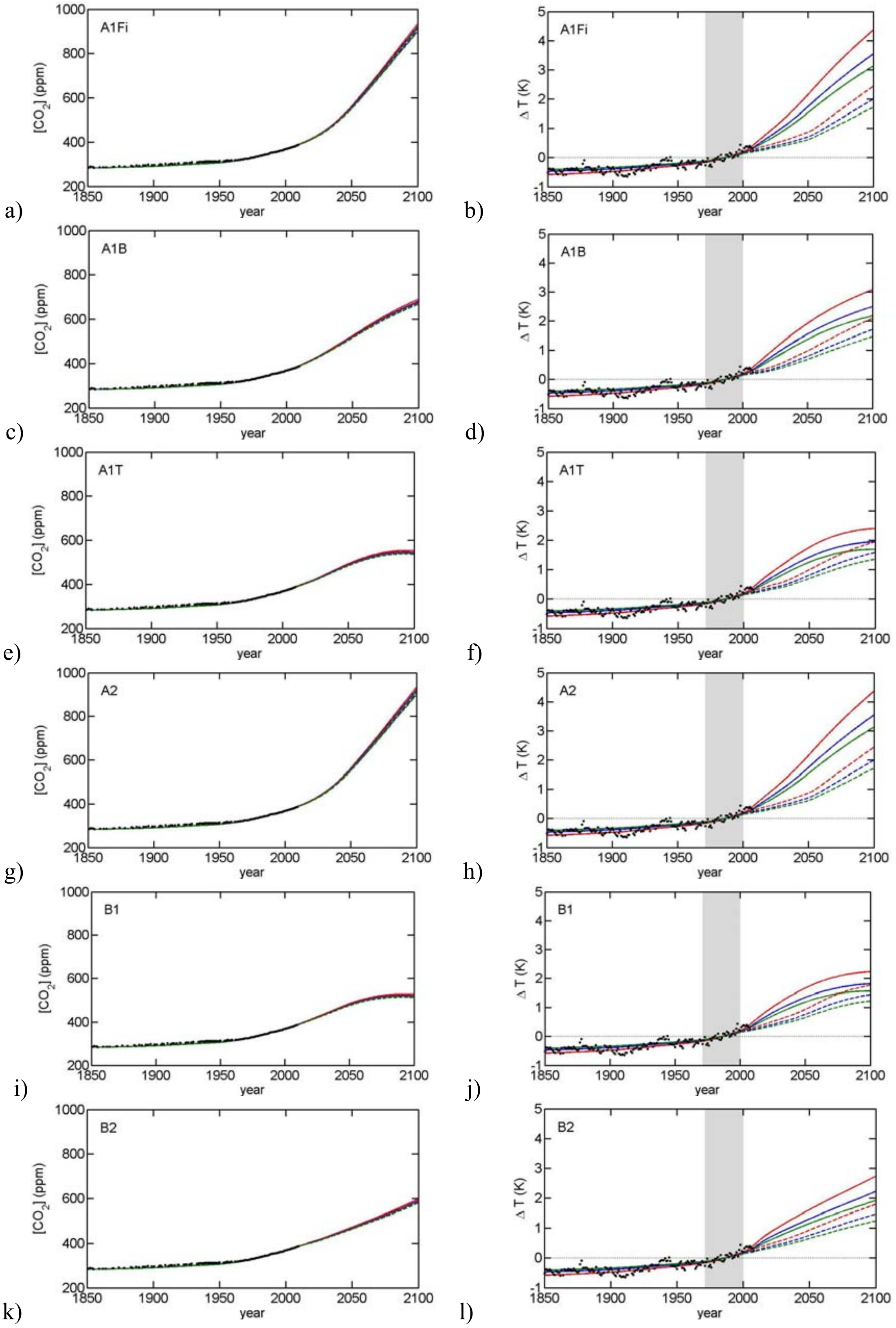


Fig. 7 Simulation of [CO_2] (left) and ΔT (right) for the six SRES marker scenarios. Colours of lines as Fig. 6. Solid/dashed lines differentiate aerosol forcing option - see text for further details.

Fig. 6 demonstrates that SCCM is able to broadly reproduce the historical time series of [CO_2] given these estimates of emissions. The observations of [CO_2] shown are a composite time series using Law Dome ice and firn data (MacFarling Meure et al. 2006) prior to 1960, Mauna Loa and South Pole data (weighted 3:1) between 1960 and 1980, and the ESRL (2009) globally averaged data after 1980. The MacFarling Meure et al. (2006) data are also corrected for the systematic difference between the globally averaged and Antarctic values as determined by comparing the two data sets post 1980 and extrapolating that back to zero preindustrially. The SCCM simulation has a consistent but small over prediction of approximately 3ppm in [CO_2] over the later half of the 20th century and a more serious under prediction between 1900 and 1950. The disagreement in the mid 20th century is likely to be related to natural processes that cause variability in terrestrial and oceanic CO_2 exchange on interannual to decadal timescales, including changes in ocean circulation and terrestrial responses to regional climate variations, which are not included in SCCM (e.g. Trudinger et al. 2003). As the temperature dependence of the carbon cycle model in this configuration of SCCM is modest, the six simulations of [CO_2] shown in Figs 6 and 7 are largely coincident through the entire simulation and across all SRES scenarios. The choice of emissions scenario then largely determines the evolution of [CO_2] into the future, for this single choice of carbon cycle model.

In contrast the choice of the temperature response function is important for the simulations of temperature change. The three response functions shown span the full range of default climate sensitivities available in SCCM (green – GFDL, $\Delta T_{2\times} = 1.85$ K; blue - Mk3L, $\Delta T_{2\times} = 3.6$ K; red – HadCM3 $\Delta T_{2\times} = 4.62$ K; note that, in comparison to other GCMs, while the Mk3L has a mid-high value for the climate sensitivity the transient climate response of the Mk3L is more modest). The agreement between the simulations of past temperature change and the observations is acceptable for all simulations shown given the variability in the observations (Fig. 6b). As expected the differences between simulations with different response functions become greater over time especially for those scenarios with larger anthropogenic emissions (Figs 7b,d,f,h,j and m). The choice for aerosol forcing (here we consider cases where no efforts to clean up emissions are undertaken – dashed lines, and where clean-up efforts realise a rapid decrease in aerosol forcing - $a_{tau} = 10$ yr) is also important in determining the projections of future temperature change. The choice of emissions scenario, temperature pulse response function and aerosol forcing are then seen to be of comparable importance in determining the magnitude and nature of the projected temperature change.

Fig. 8 shows the evolution of the terrestrial and marine pools of carbon and the associated exchanges between these pools and the atmosphere for each of the six SRES marker scenarios. As the carbon cycle evolution is similar under all six simulations, as shown in Figs 6 and 7, only results using the ‘mk3l’ response function with aerosol clean-up simulation are shown. Until very recently (~1990) the evolution of the combined terrestrial carbon pool is simulated to have been dominated by the reduction in carbon arising from LULUC. More recently, and projected into the future for all marker scenarios, the combined terrestrial carbon pool increases in magnitude due to decreases in LULUC and increases in NPP due to the carbon fertilisation effect. The ocean mixed layer is simulated to have been, more modestly, monotonically increasing in magnitude and is projected to continue doing so under all marker scenarios. Only for the two lowest emissions scenarios (A1T and B1) does the mixed layer carbon content approach stabilisation through the 21st century. Associated with this increase are substantial increases in the deep ocean content over time (not shown), indeed the majority of the increases in carbon content in the Earth system are projected to (eventually) reside in the deep ocean. In 2000 fossil fuel and LULUC CO_2 emissions totalled 8.16 PgC. After allowing for internal adjustment over the year SCCM allocated this carbon as follows: 2.81 PgC resided in the ocean mixed layer (34.4%), 2.15 PgC in the terrestrial biosphere (26.3%) and 3.19 PgC remained in the atmosphere. The 20th century airborne fraction predicted by SCCM is then close to 40% and in agreement with other, more complex, analyses of the carbon cycle (e.g. Le Quere et al. 2009).

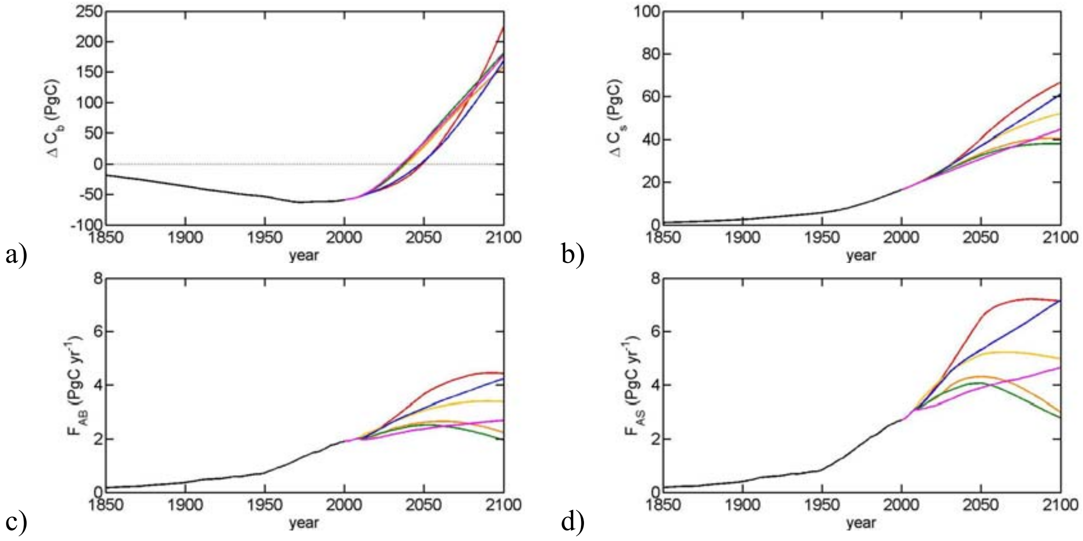


Fig. 8 Simulated evolution of the remaining terms in the carbon-cycle for each of the SRES marker scenarios. a) Change in the terrestrial carbon pool, $C_{b1}+C_{b2}$, b) change in the mixed layer carbon pool, ΣC_{si}, c) air-land flux, F_{AB}, and d) air-sea flux, F_{AS}. The change in the terrestrial carbon pool is the net result of F_{AB} and LUC. A positive value of either flux indicates transport from the atmosphere. Results using the Mk3L temperature response function shown only. Scenarios (Red – A1FI, yellow – A1B, orange – A1T, blue – A2, green – B1, magenta – A2).

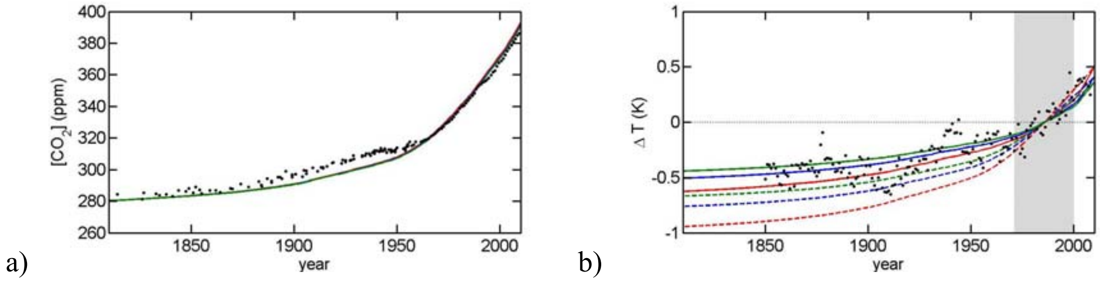


Fig. 9 Simulations (lines) and observations (markers) of $[CO_2]$ (a) and ΔT (b) when alternate model configurations are used. a) The increment to $[CO_2]$ due to the oxidation of methane is included. b) Dashed lines have zero radiative forcing due to aerosols, solid lines as Fig. 6. b). Coloured lines give the simulation using the GFDL (green), Mk3L (blue) and HadCM3 (red) temperature response functions.

Finally, we briefly touch on two important aspects of SCCM. First, Fig. 9a) shows the same six simulations of the evolution of $[CO_2]$ but now with the CO_2 that results from the oxidation of atmospheric methane included in the mass budget for atmospheric CO_2 ($s_{CH42CO2}$=1). In comparison to Fig. 6a) the differences between the simulations and the observations remain small, however the bias between observations and simulations after 1950 is increased, with the differences now generally greater than 7ppm (from 3ppm) and the gradient of the $[CO_2]$ increase over this period is higher. The methane oxidation parameterisation included in SCCM predicts that, in pre-industrial times with $[CH_4]$=710ppb and τ_{CH4}=8.2 yr^{-1}, an additional 0.18GtC yr^{-1} should be included in the mass budget for $[CO_2]$. The oxidation of atmospheric methane could then be expected to have resulted in an additional 37ppm in $[CO_2]$ (approximately and contingent on issues around the lifetime of atmospheric methane) over the period 1750 and 2000. Only a fraction of this additional CO_2 remains in the atmosphere as this CO_2 is also shared between the other carbon pools. Importantly, the inclusion of the oxidation of methane also results in a systematic change in the initial conditions (Cb_1 is reduced by approximately 1GtC), with consequent changes in the simulated respiration over long periods, and the net impact on the simulation of [CO_2] is much smaller.

More critically, this figure illustrates a key aspect of SCCM. The underlying reason for this change in performance is that the carbon cycle model parameters specified under the 'raupach' option were determined through calibration when the oxidation of atmospheric methane was neglected. As demonstrated in Section 3.1 the terrestrial carbon cycle model in SCCM is flexible enough that, through recalibration of this component of SCCM alone, we could retrieve the agreement with the observations of [CO_2] post 1950 – this issue will the subject of forthcoming research. The disagreement with the observations in the mid 20th century, however, is unlikely to be resolved through recalibration because SCCM does not include a number of natural processes that can cause variability in land and ocean CO_2 exchange on interannual to decadal timescales, such as changes in ocean circulation or terrestrial responses to regional climate variations.

Second, Fig. 9b) shows simulations of ΔT using the same three pulse response functions as Fig. 6b) only now where different values of the aerosol radiative forcing are used (solid lines, a_{prop}=-0.1 Wm^{-2} PgC^{-1} as Fig. 6b; dashed lines, a_{prop}= 0 Wm^{-2} PgC^{-1} i.e. there is no radiative forcing due to aerosols). The three temperature response functions used span a wide range of climate sensitivity and climate transient response. Nevertheless Fig. 9b) shows that the (variable) observations cannot be used to definitively decide on either a choice of pulse response function or value for a_{prop} – though a value of a_{prop}= 0 Wm^{-2} PgC^{-1} would seem implausible. A low value for the climate sensitivity can be largely compensated for by a low value for a_{prop} and vice-versa – the climate component of SCCM demonstrates equifinality, i.e. multiple combinations of model parameters and model choices give equally good agreement with the available observations. It follows that, at best, these choices can be co-constrained and the resulting uncertainty analysed through ensemble runs of SCCM. Future improvements in the understanding of the climate system through the development of GCMs and in aerosol-radiation science, particularly by using spatial information of radiative forcing and aerosol loading as a further constraint on a_{prop}, will hopefully assist in this issue.

3.1 Sensitivity to Carbon Cycle Options

The analysis in the previous section demonstrates that i) SCCM is able to reproduce the recent trajectories in global temperature and atmospheric concentrations of the main greenhouse gases, and ii) the projections of future temperature change are dependent the emissions scenario, including that of aerosols, and the underlying model for the temperature response. There is, however, a third important component determining the uncertainty in the projections of future climate from SCCM, namely the precise configuration of the carbon cycle model and its constituent parameterisation schemes. Figures 10-13 show how choices of carbon cycle components impact the projections of the carbon cycle and climate away from one particular configuration (base case) of the carbon and climate components of SCCM, given the A1B emission scenario. The base case considered is that shown in Figs 6 and 7c) and d) using the 'hadcm3' temperature response function (Table 4 and Eq (43)) and with the aerosol parameters taking the values a_{prop}=-0.1 Wm^{-2} PgC^{-1} as a_{tau} = 10 yr (i.e. the red solid lines in those figures). In each of Figs 10-13 this base case is given by the solid black line, while the other lines will show the simulations where components of the carbon cycle (2-box model configuration, carbon cycle fertilisation, LULUC allocation, p_{CO2} and ocean PRF) are varied away from the base case.

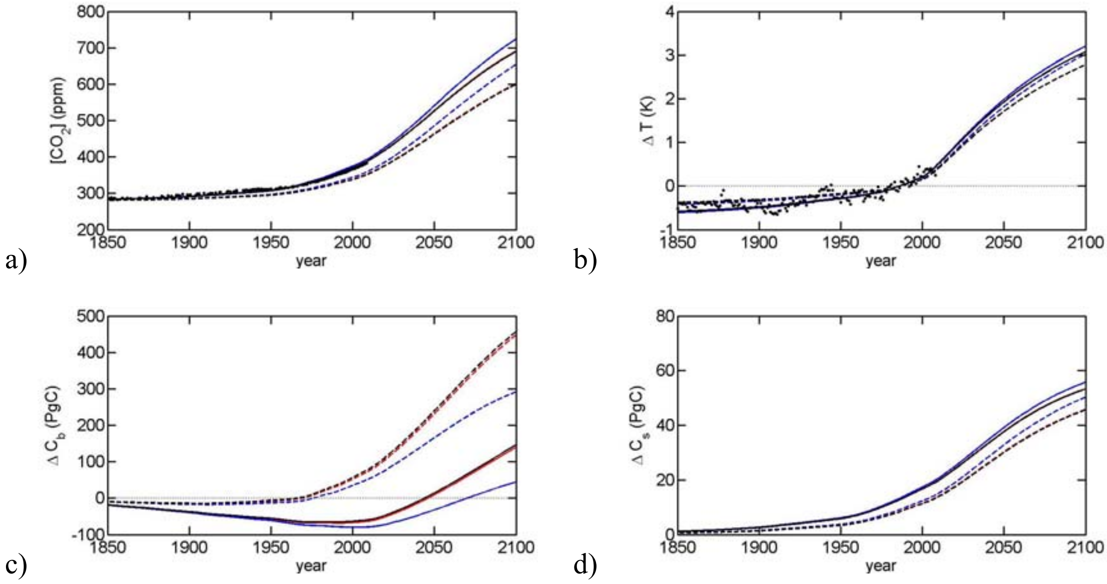


Fig. 10 Projections for the components of the carbon cycle and temperature change under different choices for the 2-box terrestrial carbon cycle model and carbon cycle fertilisation parameterisation schemes within SCCM. Solid and dashed lines show simulations using the 'raupach' and 'trudinger' 2 box model respectively. Black, blue and red lines show simulations using the 'log', 'hyp' and 'hypm' fertilisation options respectively. In a), b) and d) the 'hypm' and 'log' options are indistinguishable. The 'trudinger' 2-box model is calibrated to use different LULUC allocation and ocean options by default so these results are not truly reflective of the performance of this carbon cycle model.

Figures 10 and 11 show the response of SCCM to different choices for the terrestrial carbon cycle model configuration, carbon cycle fertilisation and LULUC allocation options. The close agreement between the simulations with different fertilisation options and with the observations indicates that the observations of global [CO_2] and temperature will not be able to discriminate between the model configurations. Equally, it is important to recognise that the carbon cycle exhibits equifinality in a similar manner to the climate system, i.e. multiple parameter values and model options can lead to equivalent agreement with the observations. In particular the 'trudinger' choice for the terrestrial carbon cycle was calibrated using alternative options for the LULUC allocation and ocean mixed layer response function. Hence the variation shown in Figs 10 and 11 a) and c) actually overestimates the true variation between these model configurations given that proper calibration has yet to be undertaken (including of the turn over timescales k_{1a}, k_{2a} and k_{12} and the partitioning coefficient γ) for many of these configurations.

Figures 10 and 11 illustrate the critical role of the terrestrial biosphere within SCCM. The variation shown in the projections of future atmospheric CO_2 concentration is comparable to the differences to that resulting from different SRES emissions scenarios (Fig. 7). For the LULUC options this is expected as the different options do imply different net emissions. However the magnitude of the variation and the different nature and timing of the impacts seen when applied to the 'raupach' or 'trudinger' 2-box terrestrial carbon cycle models suggest that this component is not well constrained by the observations of global [CO_2] and temperature and/or the embedded process-based knowledge. Such a large variation of response is not specific to SCCM but is also seen between more complex carbon cycle models (e.g. Friedlingstein et al. 2006). This suggests that the equifinality issue for carbon cycle models is common and could be addressed through the careful use of (independent) observations of the terrestrial and oceanic carbon pools.

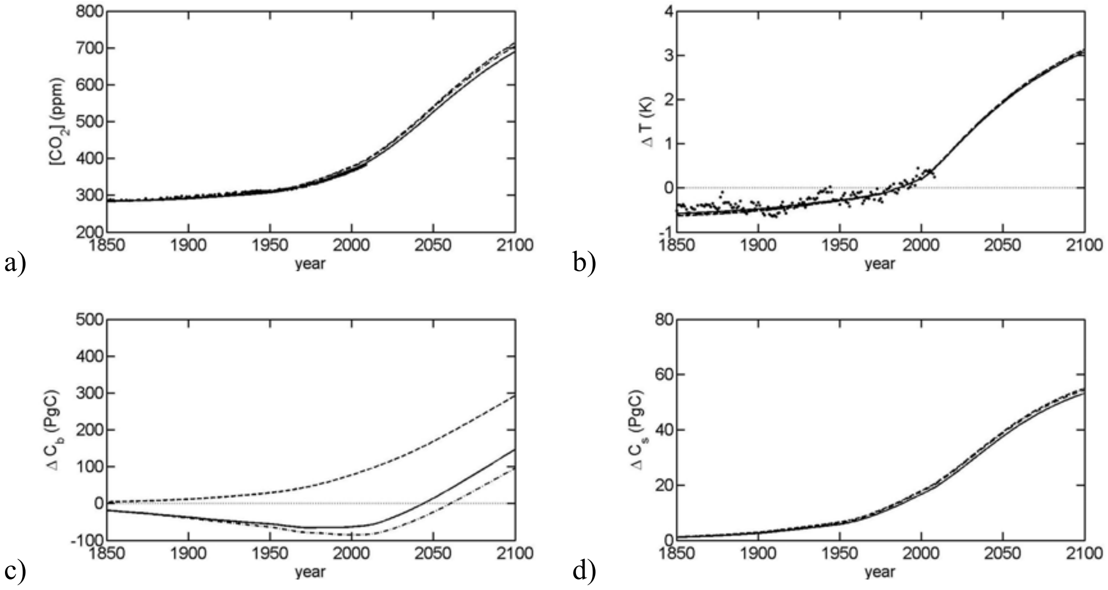


Fig. 11 Projections for the components of the carbon cycle and temperature change under different choices for LULUC allocation within SCCM. All simulations use the ‘raupach’ 2-box terrestrial carbon cycle mode with the ‘log’ option for carbon fertilisation. Solid line shows the simulation using the ‘cb2’ choice for LULUC emissions allocation, dash-dotted line the simulation using the ‘gross’ option and dashed lines the simulation using the ‘added’ option.

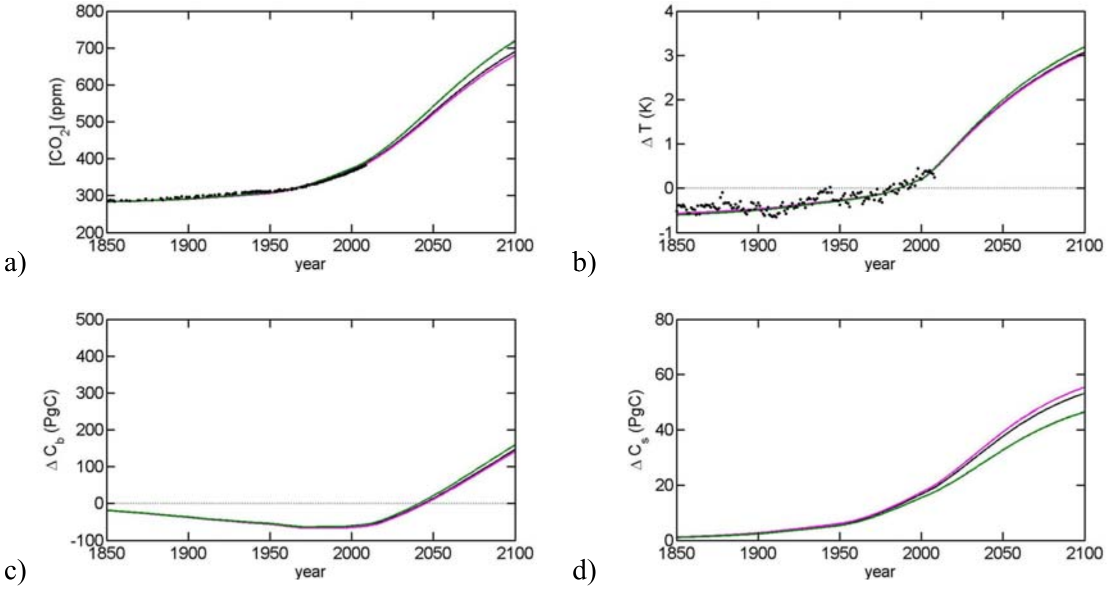


Fig. 12 Projections for the components of the carbon cycle and temperature change under different choices for the *p*CO2 parameterisation scheme within SCCM. The black line gives the response with the ‘joos’ option, the magenta line that with the ‘enting’ option and the green line that with the ‘co2syspower’ option. The ‘co2syspade’ option is also plotted as a grey line but overlies the ‘co2syspower’ option.

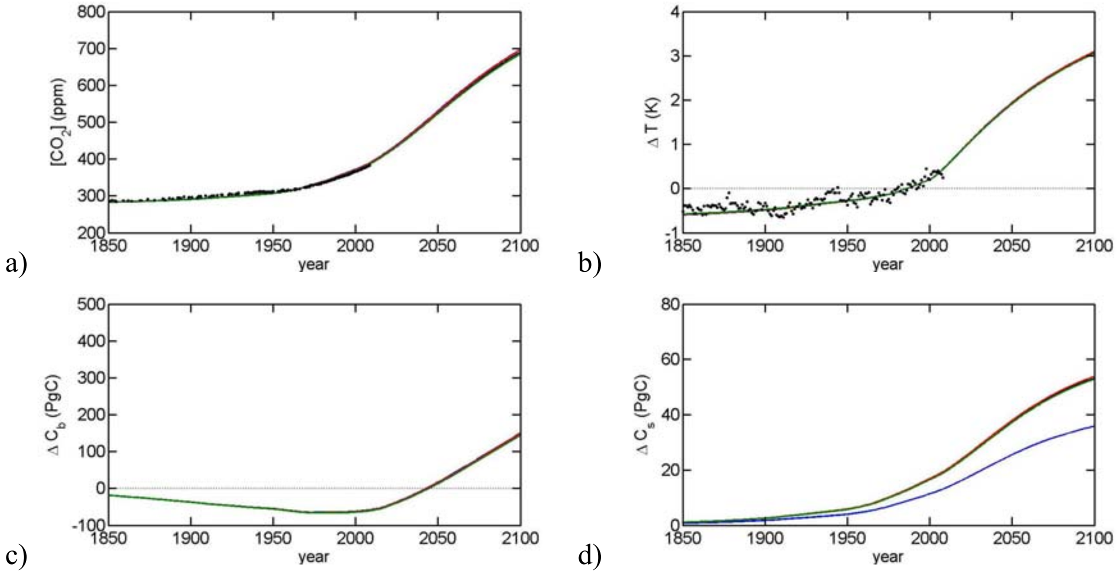


Fig. 13 Projections for the components of the carbon cycle and temperature change under different choices for the ocean carbon cycle response functions within SCCM. The black line gives the response with the 'raupach' option, the blue line that with the '3d' option, the red line that with the 'hilda' option and the green line that with 'bdm' option.

In contrast, Figs 12 and 13 show the variation in the SCCM projections when the ocean carbon cycle options for p_{CO2} and the pulse response function are varied. The resulting variation, in all components of the carbon cycle and temperature, is much smaller than shown in Figs 10 and 11. This suggests either that the ocean carbon cycle is better constrained by the observations and embedded knowledge than the terrestrial carbon cycle *or* that the current options for the ocean carbon cycle in SCCM do not span the true uncertainty of this component.

Two features in Figs 12 and 13 are worth noting. First the p_{CO2} choices that incorporate the most complete description of ocean carbon chemistry (namely the two parameterisations based around the CO_2Sys model – Appendix C) are also those which lead to a reduced ocean carbon uptake, increased atmospheric CO_2 content and increased surface temperatures. However this change is modest in comparison to the variation shown across the emissions scenarios and terrestrial carbon cycle options. Second, the projection of the change in mixed-layer ocean carbon content given by the '3d' choice for the ocean carbon cycle response function would appear to be an outlier. However this is not the case as this simply reflects the difference in values for the mixed-layer depth embedded into the different response functions (50m in contrast to 75m). Once normalised to account for the different mixed layer depths, i.e. by considering the concentration of DIC, the projections of $\Delta C_s / \mathrm{MLD}$ are almost indistinguishable. This further reinforces the earlier comment concerning the embedded confidence around the ocean mixed layer carbon cycle in SCCM.

Figures 10-13 show how the options for the carbon cycle within SCCM impact the simulations independently of each other. Considering all possible combinations of model choices would lead to an increased spread in the final projections of the carbon cycle and, consequently the climate system. However much of the increase in the spread in the simulations is the result of simulations those whose performance against past observations would be considered poor by almost any metric. The additional implied uncertainty from these configurations cannot be considered realistic unless recalibration to the new configuration is also undertaken. Hence for simplicity we do not show the co-varying simulations and accept that each configuration of SCCM will require individual parameter calibration.

4. MODEL STRUCTURE AND USE

SCCM has been developed to operate in two distinct versions – a science development version and as the climate component within GIAM. Both versions are written in modularised Fortran90. The science development version has a greater flexibility in terms of possible options and consequently a greater demand on the i/o. In the GIAM version many of the available options and parameter values are hardwired and the i/o structure is simpler. Switching between the versions is achieved through the logical variable GIAMflag and recompiling.

The core structure of both versions is identical and is comprised of three main groups of modules, namely definitions and utilities, initialisation and output, the dynamical system and time integration. Once initialised, the integration modules determine the time-evolution of each of the state variables as defined by the dynamical system. The numerical integration is performed using double precision floating point format through a 5th order Runge-Kutta scheme with an adaptive time step to ensure numerical accuracy and stability.

4.1 Science Development Version

In the science development version a two-layer input structure is employed. The upper layer control file, named *.ctl and input at a prompt, provides information about the run including description, run length and composition. A typical composition includes CO_2 (atmospheric, oceanic and terrestrial), temperature, CH_4, N_2O and CFCs components. Additional components exist or are in development for $\delta^{13}CO_2$, SF_6, PFCs and other non-CO_2 GHGs. Most components can be run in isolation or together with other components and consist of a number of state variables (see Tables 8 and 10). An example control file is given in Table 5 (where '!' indicates a comment that is ignored by SCCM).

Table 5 Example control file (*.ctl) for use with the science development version of SCCM.

```
! Control file for SCCM
! GIAM CO2, CH4, N2O temperature run
! RUN DESCRIPTION
t1a                  ! run identifier
'GIAM test run'      ! run description ( <= 20 char )
'Case 1'             ! case description
'output.dat'         ! output file name
!
! TIME INFORMATION
1752.0               ! Initial time
2100.0               ! Final time
1.0                  ! dt
!
! COMPONENT INFORMATION
5                    ! Number of model components
'co2', 'co2.cmpt'        ! CO2 (includes atmosphere, biosphere, ocean)
'ch4', 'ch4.cmpt'        ! CH4
'n2o', 'n2o.cmpt'        ! N2O
'cfcs', 'cfcs.cmpt'      ! CFC11 and CFC12
'temp', 'temperature.cmpt'  ! Temperature
!
! RUN TYPE (single, multiple, GA)
'single'             ! 'single', 'multiple' or 'GA'
```

Table 6 Example CO_2 component driver file (*.cmpt) for use with the science development version of SCCM.

```
'co2'          ! Component name
! STATE VARIABLES
14             ! No. state variables to represent component
'co2'           ! Atmospheric CO2 (GtC)
'cb1'          ! Short-lived biospheric CO2 (GtC)
'cb2'          ! Long-lived biospheric CO2 (GtC)
'cs0'          ! Ocean mixed-layer component 0 (fast response)
'cs1'          ! Ocean mixed-layer component 1 (mixed layer pulse resp fns)
'cs2'          ! Ocean mixed-layer component 2 (mixed layer pulse resp fns)
'cs3'          ! Ocean mixed-layer component 3 (mixed layer pulse resp fns)
'cs4'          ! Ocean mixed-layer component 4 (mixed layer pulse resp fns)
'cs5'          ! Ocean mixed-layer component 5 (mixed layer pulse resp fns)
'cs6'          ! Ocean mixed-layer component 6 (mixed layer pulse resp fns)
'cs7'          ! Ocean mixed-layer component 7 (mixed layer pulse resp fns)
'cs8'          ! Ocean mixed-layer component 8 (mixed layer pulse resp fns)
'cs9'          ! deep ocean
‘q’            ! cumulative carbon emissions
!
! OTHER MODEL COMPONENTS ASSUMED PRESENT FOR THIS RUN
0              ! No. other model components assumed present
!
! MODEL PARAMETERS (value, parameter name in code)
9              ! No. model parameters for this component
280.0,  'co2preind'  ! Preindustrial CO2 level
40.0,   'npppreind'   ! Preindustrial NPP (GtC)
0.8,   'gamma'     ! Fraction of NPP into bio box 1 (1-gamma into box 2)
0.8,   'beta'       ! beta for fertilisation (Gt y-1)
2.0,   'q10resp'     ! Q10 factor for temperature dependence of respiration
1.0,   'q10npp'     ! Q10 factor for temperature dependence of NPP
2.089,  'dic0'       ! Preindustrial C in mixed layer (mol m-3)
0.0,   ‘volc’       ! constant source of C into atm from volcanism and other exogenous forcing
1.0,   ‘sch42co2’   ! include oxidised methane in the co2 budget – values 0-1
!
! MODEL CHOICES (value, variable name in code)
7                    ! No. model choices for this component
'log',    'fertchoice'      ! fertilisation type: choices = 'log', 'hyp' or ‘hypm’
'raupach', 'twoboxbiochoice  ! 2-box biosphere model: 'trudinger', 'raupach', or 'userdef'
'cb2',    'lucchoice'      ! Implementation of LUC: choices = 'added', 'cb2', 'gross'
'joos',  'pco2choice'      ! pco2: choices = 'enting', 'joos', ‘co2syspade’, or ‘co2syspower’
'3d', 'oceanmodelchoice'   ! Ocean-C PRF: 'bdm', 'hilda', '3d', or ‘raupach’
'modelled', ‘co2tempchoice'  !use observed or modelled temperature: choices = 'modelled', 'observed'
'modelled', ‘co2ch4choice'   !use observed or modelled methane: choices = 'modelled', 'observed'
!
! INPUT DATA FILES (file name, array name in code)
2                                  ! No. input data files required
'EmissFossil_CO2_CDIAC_A2marker.dat', 'fossdata'  ! Fossil fuel emissions
'EmissLUC_CO2_CDIAC.dat',          'lucdata'   ! Land-use change emissions
!
! OUTPUT QUANTITIES
4
'co2'   1, 'Atm CO2 (ppm)'       ! Atmospheric CO2 (ppm)
'cb'    1, 'total bio (GtC)'        ! total biospheric CO2 (GtC)
'cs'    1, 'mixed layer change (GtC)' ! total mixed layer change
'csd'   1, 'deep ocean pool'      ! deep ocean
!
! OBSERVATIONS TO PLOT WITH OUTPUT
0
```

The second layer of control, the component driver files, provides further information as required for each component specified in the control file. This additional information includes the number and names of the state variables, parameter values, forcing data and output requirements. The names of the component driver files (*.cmpt) are given in the *.ctl file. The exact composition of each *.cmpt file depends on the case being considered and the configuration of SCCM; as a consequence there is no set list for those parameters or model choices that are required. Error messages are provided if configuration specific values are not provided. Note that all names of model choices, parameters, inputs and outputs and the valid options for the choices are cases sensitive, and should all be lower case. Case doesn't matter for the names of input data files. An example *.cmpt (for the CO_2 component) is given in Table 6.

The science development version of SCCM has been developed in Visual Fortran. Through the use of two libraries (DFLIB and DFPORT) it can be complied, run and output in different directories. However these libraries are not available with all compilers. Minor modifications to the Init subroutine (specifically commenting out the USE, FULLPATHQQ, SPLITPATHQQ calls in Init and all uses of chdir) produces a version which bypasses these library issues but which compiles and runs in the same directory.

4.2 GIAM Version

In contrast the GIAM version operates with a single control file (*.gctl). The name of the file is hardwired within SCCM (to enable user independent running) within the InitGIAM subroutine. The *gctl file (see Table 7 for an example) provides information concerning the run description and length together with a limited number of parameter values and the necessary forcing. The GIAM version is configured to run with the co2, ch4, n2o, cfc and temperature components active. The large majority of the required parameter values and options are hardwired however most of the options of the scientific development version can still be accessed. The GIAM version compiles and runs in the same directory.

The science development version can be operated in GIAM development mode by changing the GIAMflag. However, as a result of the library issue highlighted above, the GIAM version does not include the standard initialisation routine (and other facilities see Section 4.3) so cannot be operated in science development mode.

4.3 Run Configuration

The science development version of SCCM can operate in three distinct run configurations – single, multi and GA. These different configurations allow for different uses of SCCM within a single executable.

The single run configuration performs one run of the model from tstart to tfinish, with one set of model parameters, choices and input files, as described in the *.ctl and *.cmpt files.

The multi configuration involves more than one run of the model, where each run operates with different model parameters, choices or input files. A first run is done from tstart to tfinish with the parameters, choices and input files, as described in the *.cmpt files. This is followed by Nmulti further model runs from tstart to tfinish with the same parameters, choices and input files as the first run apart from one or more differences as given in the *.ctl file.

Table 7 Example control file (*.gctl) for use with the GIAM version.

```
! Control file for SCCM
! GIAM CO2, CH4, N2O temperature run
! RUN DESCRIPTION
t1a                  ! run identifier
'GIAM test run'          ! run description ( <= 20 char )
'Case 1'              ! case description
'output.dat'            ! output file name
!
! TIME INFORMATION
1752.0              ! Initial time
2100.0              ! Final time
1.0              ! dt
!
! additional PARAMETER VALUES
280.0,  'co2preind'    ! Preindustrial CO2 level
40.0,   'npppreind'    ! Preindustrial NPP (Gt)
679.0,  'cspreind'     ! Preindustrial C in mixed layer (GtC)
0.8,    'beta'         ! beta for fertilisation (Gt y-1)
700,    'ch4preind'    ! preindustrial CH4 level
270,    'n2opreind'    ! preindustrial N2O level
1.0,    'clsens'       ! climate gain(=1.0) else varying climate sensitvity from AOGCM value
5.35,   'fco2'         !RF forcing per change in atm co2 RF=fco2 ln(co2/co2init)
0.0,    'aeroval'      !constant value for aerosol forcing (-ve values are cooling)
-0.1,   'aeroprop'     !constant of proportionality for aerosol forcing (typically -0.1)
40.0,   'aerotau'      !time scale for aerosol forcing (must be positive, ~40)
!
!additional MODEL CHOICES
'power', 'ch4tauchoice'      ! lifetime: choices = 'const', 'linear', or 'power'
!
!time series for FORCING DATA FILES
'EmissFossil_CO2_CDIAC_A2marker.dat', 'fossdata'       ! Fossil fuel emissions
'EmissLUC_CO2_CDIAC.dat',          'lucdata'        ! Land-use change emissions
'EmissAnthrop_CH4.dat',            'ch4emissdata'   ! perturbation CH4 emissions
‘EmissAnthrop_N2O.dat',            'n2oemissdata    ! perturbation n2o emissions
'EmissAnthrop_CFC11.dat',          'cfc11emissdata'    ! CFC11 emissions
'EmissAnthrop_CFC12.dat',          'cfc12emissdata'    ! CFC12 emissions
```

Finally SCCM includes the genetic algorithm code from Haupt and Haupt (2004). When configured to run in GA mode the model is run repeatedly with the output from different model runs compared to specified observations. By minimising a measure of the mismatch between the model runs and the observations a range of model parameters can be tuned. The *.ctl file lists which of the model parameters are to be tuned, their prior ranges and the source of observations for comparison against.

Within the GIAM development version only the single run configuration is facilitated. Multiple or ensemble runs, if desired, are to be configured through an outer scripting environment. The location of the *.gctl driver file can be specified within the InitGIAM subroutine with recompilation.

5. SUMMARY

SCCM – the Simple Carbon-Climate Model – is a deterministic model for the globally averaged carbon cycle and climate system. It comprises representations of the carbon, methane, nitrous oxide, CFC mass balances of the Earth system and for the evolution of the global mean near-surface air temperature. Each component of SCCM is derived and calibrated against more complex models and, where possible, compared to independent observations. Many of the components of SCCM have multiple configurations. The primary role of SCCM is to provide aggregate level information about the carbon-climate system and its potential future evolution when needed in other studies, or for use in interpreting global-scale measurements such as those from ice cores. SCCM can be configured to investigate measures of uncertainty (including some measures of structural uncertainty) through the use of multi-member ensemble runs in a timely fashion.

SCCM is able to reproduce with reasonable accuracy the recent (post 1850) evolution of the atmospheric concentration of the main GHGs in addition to that of the global mean temperature. The agreement between model simulations and independent observations is dependent on the forcing provided (e.g. emissions) but also model configuration. There is considerable evidence that SCCM exhibits equifinality i.e. multiple combinations of parameter values and model choices can lead to similar performance compared to past observations. Projections into the future lie within the broad bands for the atmospheric concentration of CO_2 and for global mean temperature given by the IPCC (2007) 4th Assessment Report. Estimates of the relative sources of uncertainty can be provided through analysis of SCCM output. According to SCCM, approximately 50% of the uncertainty in future temperature changes over the next century stems from the precise emissions trajectory followed. The large majority of the remaining 50% of uncertainty stems from the uncertainty in the climate response including that due to uncertainty in the coupling between the carbon cycle and climate systems. Under one specific configuration of SCCM, the variation in emissions across the range of the SRES marker scenarios (Nakicenovic et al. 2000) is shown to lead to temperature increases over the 21st century of between 1.8-3.3ºC (see Fig. 7). For comparison, different choices for the representation of the climate system response lead to a temperature range of 3.1-4.4ºC around the upper limit of 3.3ºC. Of particular importance in determining both sources of uncertainty are assumptions concerning the emissions trajectory of and climate impacts of aerosols which could easily double the range of projected temperature change. Over longer periods of time uncertainty arising from the response of carbon cycle, especially the terrestrial component, becomes appreciable.

SCCM remains a modelling tool in active development. Additional components considering the isotopes of carbon and the other GHGs covered by the Kyoto-protocol are under development. The Genetic Algorithm functionality will enable better calibration of SCCM parameters by comparing SCCM output against not only observations but also output from more complex models such as Earth System models that contain feedbacks and mutual constraints that might be difficult to characterise from observations alone. This last objective is expected to lead to a much better analysis of uncertainty and its various sources, including structural, in models of this generic type, which will be an important aspect of the use of SCCM within GIAM.

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APPENDIX A – TABLES OF SCCM VARIABLES AND PARAMETERS

Table 8 Calculated time-varying quantities in SCCM.

Symbol	Units	Description
CO2	GtC	CO_2 content in the atmosphere
$CO2_{ppm}$	ppm	CO_2 concentration in the atmosphere
Cb_1, Cb_2	GtC	Carbon content in the two terrestrial pools
$Cs = \sum Cs_i$	GtC	Carbon content in the ocean mixed layer
Cs_{deep}	GtC	Perturbation to carbon content in the deep ocean
q	GtC	Cumulative emissions of carbon dioxide
$pCO2_{ML}$	ppm	Partial pressure of CO_2 in the ocean mixed layer
δDIC	moles m^{-3}	Perturbation in dissolved inorganic carbon in the ocean mixed layer
F_{CO2_AS}	GtC yr^{-1}	Net air-sea flux of CO_2
F_{CO2_AB}	GtC yr^{-1}	Net air-land flux of CO_2
CH4	Tg-CH4	Perturbation to the CH_4 content in the atmosphere from preindustrial times
N2O	Tg-N	Perturbation to the N_2O content in the atmosphere from preindustrial times
CFC11	Tg CFC-11	CFC-11 content in the atmosphere
CFC12	Tg CFC-12	CFC-12 content in the atmosphere
$\Delta T = \Sigma T_i$	^oC	Change in the globally averaged near-surface air temperature form preindustrial times
RF	W m^{-2}	Radiative forcing above preindustrial levels

The first column gives the symbol in the document, the second the units used and the third column gives a description.

Table 9 Fixed constants in SCCM.

Symbol	Value	Units	Description
$r_{CO2\_ppmGtC}{}^{-1}$	0.4695	ppm GtC^{-1}	Converts CO_2 atmospheric mass in GtC to concentration in ppm.
$r_{CH4\_ppbTg}{}^{-1}$	0.3515	ppb Tg^{-1}	Converts CH_4 atmospheric mass in Tg to concentration in ppb.
$r_{N20\_ppbTgN}{}^{-1}$	0.2013	ppb $Tg\text{-}N^{-1}$	Converts N_2O atmospheric mass in Tg-N to concentration in ppb.
$r_{CFC11\_pptTg}{}^{-1}$	0.04104	ppb Tg^{-1}	Converts CFC-11 atmospheric mass in Tg to concentration in ppb.
$r_{CFC12\_pptTg}{}^{-1}$	0.04664	ppb Tg^{-1}	Converts CFC-12 atmospheric mass in Tg to concentration in ppb
k_g	1/9.16256	yr^{-1}	Gas exchange coefficient **
MLD	75 or 50	m	Depth of the ocean mixed layer
OA	0.3569	10^{15} m^2	Area of the ocean
$pCO2_{MLpre}$		ppm	Preindustrial $pCO2_{ML}$

The first column gives the symbol used in this document, the second the fixed value, the third the units used and the fourth column gives a description. ** It is anticipated that k_g will be converted into a co2 component parameter in a future version of SCCM.

Table 10 SCCM components.

Comp	Other comps required	State variables
co2	none (uses temp and ch4 if directed to)	co2, cb1, cb2, cs0, cs1, cs2, cs3, cs4, cs5, cs6, cs7, cs8, cs9, q
ch4	none	ch4
n2o	none	n2o
cfcs	none	cfc11, cfc12
temp	none (uses ch4, n2o, cfcs if directed to)	temp1, temp2, temp3

The first column gives each component name, the second lists other components that must also be chosen and the third column lists the state variables for each component.

Table 11 SCCM choices.

Comp	Name in code	Defined options
co2	fertchoice	‘log’, ‘hyp’ or ‘hypm’
co2	twoboxbiochoice	‘trudinger’, ‘raupach’, or ‘userdef’
co2	lucchoice	‘added’, ‘cb2’, or ‘gross’
co2	pco2choice	‘enting’, ‘joos’ or ‘co2syspade’ or ‘co2syspower’
co2	oceanmodelchoice	‘bdm’, ‘hilda’, ‘3d’ or ‘raupach’
co2	oceantempchoice	‘varying’ or ‘preind’
co2	co2tempchoice	‘modelled’ or ‘observed’
co2	co2ch4choice	‘modelled’ or ‘observed’
ch4	ch4tauchoice	‘const’ or ‘power’
ch4	ch4forchoice	‘total’, ‘anthro’ or ‘perturbation’
n2o	n2otauchoice	‘const’
n2o	n2oforchoice	‘total’, ‘anthro’ or ‘perturbation’
cfcs	cfcforchoice	‘total’, or ‘perturbation’
temp	tempmodelchoice	‘accc’, ‘image’, ‘echam’, ‘gfdl’, ‘mk3l’, ‘hadcm3’ or ‘osu’
temp	aeromodelchoice	‘none’, ‘const’, ‘prop’, ‘cleanup’, ‘all’ or ‘allluc’
temp	tempco2choice	‘modelled’, ‘observed’ or ‘co2e’
temp	tempch4choice	‘modelled’ or ‘observed’
temp	tempn2ochoice	‘modelled’ or ‘observed’
temp	tempcfc11choice	‘modelled’ or ‘observed’
temp	tempcfc12choice	‘modelled’ or ‘observed’

The first column gives the relevant component name, the second the choice name in the model code and the third column the options available. See text for further information.

Table 12 SCCM parameters.

Comp	Name in code	Symbol	Typical value	Description
co2	co2preind	$CO2_{pre}$	280	Preindustrial CO_2 concentration (ppm)
co2	npppreind	NPP_{pre}	84.3 or 40	Preindustrial NPP (GtC yr^{-1})
co2	gamma	γ	1.0 or 0.8	Fraction of NPP into Cb_1[†]
co2	temppreind	T_{pre}	15	Preindustrial temperature (in °C)
co2	k1ainv	k_{1A}^{-1}	6.3 or 3	Turnover time for exchange from Cb_1 to atm[†]
co2	k12inv	k_{12}^{-1}	20.3 or ∞	Turnover time for exchange from Cb_1 to Cb_2[†]
co2	k2ainv	k_{2A}^{-1}	54.5 or 300	Turnover time for exchange from Cb_2 to atm[†]
co2	kbsinv	k_{bs}^{-1}	300	Turnover time for exchange from Cb_1 to the ocean mixed layer.
co2	beta	β	0.4	Beta in CO_2 fertilisation equation
co2	q10resp	Q_{10resp}	1.0 or 2.0	Q_{10} factor for T dependence of respiration
co2	q10npp	Q_{10NPP}	1.0 or 1.4	Q_{10} factor for T dependence of NPP
co2	kg	k_g	0.1091	Gas exchange coefficient **
co2	cspreind	Cs_{pre}	679	Preindustrial C in mixed layer (GtC)[@]
co2	dic0	DIC_{pre}	2.089	Preindustrial C in mixed layer (moles m^{-3})[@]
co2	volc	F_{VOLC}	0-0.3	Fixed value for other non-anthropogenic exogenous sources of atmospheric CO_2 (GtC yr^{-1})
ch4	ch4preind	$CH4_{pre}$	710	Preindustrial CH_4 concentration (ppb)
ch4	ch4tauconst	τ_{CH4}	8.4	Constant methane lifetime (yr)
n2o	n2opreind	$N2O_{pre}$	271	Preindustrial N_2O concentration (ppb)
n2o	n2otauconst	τ_{N2O}	114	Constant N_2O lifetime (yr)
cfc	cfc11preind	$CFC11_{pre}$	0	Preindustrial CFC-11 conc. (ppt)
cfc	cfc12preind	$CFC12_{pre}$	0	Preindustrial CFC-12 conc. (ppt)
cfc	cfc11tauconst	τ_{CFC11}	45	CFC-11 lifetime (yr)
cfc	cfc12tauconst	τ_{CFC12}	100	CFC-12 lifetime (yr)
temp	t2x	ΔT_{2x}	~3	default climate sensitivity (K)[‡]
temp	clsens	c_{lsens}	1	multiplier of default climate sensitivity
temp	fco2	f_{co2}	5.35-5.7	RF conversion factor for atmospheric carbon dioxide (Wm^{-2})
temp	aeroval	a_{val}	0	constant value for aerosol RF
temp	aeroprop	a_{prop}	-0.1	constant of proportionality in RF parameterisation (Wm^{-2} $(PgC)^{-1}$)
temp	aerotau	a_{tau}	~40	aerosol emission ‘clean up’ time scale (yr)
temp	sfco2	s_{fco2}	0 or 1	switch to apply the radiative forcing due to changed atmospheric CO_2 on temperature.
temp	sfch4	s_{fch4}	0 or 1	as s_{fco2} but for atmospheric methane
temp	sfn2o	s_{fn2o}	0 or 1	as s_{fco2} but for atmospheric nitrous oxide
temp	sfcfcs	s_{fcfc}	0 or 1	as s_{fco2} but for the cfcs
co2, ch4	sfch42co2	$s_{ch42co2}$	0 or 1	switch to include the oxidation of CH_4 to the atmospheric CO_2 balance

The first column gives the component name, the second the parameter name in the model code and in this document, the third column gives typical values, the fourth the units used and the fifth column gives a description.

Further notes on Table 12

†Parameters $\gamma_{\cdot 2}$ k_{1A}^{-1} , k_{12}^{-1} , k_{2A}^{-1} , k_{bs}^{-1} are only required to be specified when twoboxmodelchoice = 'userdef'.

‡ ΔT_{2x} is set through tempmodelchoice; to vary the climate sensitivity use c_{lsens}

** k_g is currently a fixed constant in SCCM. It is anticipated that k_g will be converted into a co2 component parameter in a future version of SCCM.

@ For most configurations of SCCM dic0 is the required parameter. cspreind is included here for completeness and correspondence with earlier versions.

Table 13 SCCM time series inputs.

Comp	Symbol	Name in code	Description
co2	$F_{CO2\ FOSS}$	co2fossdata	CO_2 emissions due to fossil fuel (GtC/yr)
co2	$F_{CO2\ LUC}$	co2lucdata	CO_2 emissions due to land use change (GtC/yr)
co2		co2tempdata	temperature data to be used in co2 component.
co2		co2ch4data	CH_4 data to be used in co2 component.
ch4	F_{CH4}	ch4emissdata	CH_4 emissions (Tg CH4/yr)
n2o	F_{N2O}	n2oemissdata	N_2O emissions (Tg N/yr)
cfcs	F_{CFC11}	cfc11emissdata	CFC-11 emissions
cfcs	F_{CFC12}	cfc12emissdata	CFC-12 emissions
temp		tempco2data	CO_2 data to be used in temperature component
temp		tempch4data	as above for CH_4 data
temp		tempn2odata	as above for N_2O data
temp		tempcfc11data	as above for CFC_{11} data
temp		tempcfc12data	as above for CFC_{12} data

The first column gives the relevant component name and the second the symbol used in the equations. The third column gives the name used in the model code and the fourth column gives a description.

Table 14 SCCM outputs.

Comp	Output	Description
co2	co2	CO_2 concentration (ppt)
co2	cb	Carbon content of biosphere (GtC)**
co2	cs	Carbon content of ocean mixed layer (GtC)**
co2	csd	Carbon content of deep ocean (GtC)
co2	foss	Fossil fuel emissions (GtC yr^{-1})
co2	luc	Land-use change emissions (GtC yr^{-1})
co2	fas	Air-sea flux of CO_2 (GtC yr^{-1})
co2	fab	Air-land flux of CO_2 (GtC yr^{-1})
co2	q	Cumulative carbon dioxide emissions (GtC)
co2	co2temp	Temperature used in the co2 module (^oC)
ch4	co2meth	CH_4 concentration used in the co2 module (ppb)
ch4	ch4	CH_4 concentration (ppb)
ch4	ch4emiss	CH_4 emissions (Tg yr^{-1})
ch4	ch4tau	CH_4 atmospheric lifetime (yr)
n2o	n2o	N_2O concentration (ppb)
n2o	n2oemiss	N_2O emissions (Tg yr^{-1})
n2o	n2otau	N_2O atmospheric lifetime (yr)
cfcs	cfc11	CFC-11 concentration (ppt)
cfcs	cfc12	CFC-12 concentration (ppt)
cfcs	cfc11emiss	CFC-11 emissions (Tg yr^{-1})
cfcs	cfc12emiss	CFC-12 emissions (Tg yr^{-1})
temp	rf	Total radiative forcing (Wm^{-2})
temp	rfco2	Radiative forcing due to CO_2 (Wm^{-2})
temp	rfch4	Radiative forcing due to CH_4 (Wm^{-2})
temp	rfn2o	Radiative forcing due to N_2O (Wm^{-2})
temp	rfcfc11	Radiative forcing due to CFC-11 (Wm^{-2})
temp	rfcfc12	Radiative forcing due to CFC-12 (Wm^{-2})
temp	rfaero	Radiative forcing due to aerosols (Wm^{-2})
temp	temp	Global temperature (^oC)**

The first column gives the relevant component name, the second the name of the output quantity in the model code and the third column gives a description.

** It is possible within SCCM to output the component terms of Cb, Cs and temp in addition to the summations above.

APPENDIX B – STEP RESPONSE FUNCTION FOR THE CSIRO MK3L GCM

The original Global Integrated Assessment Model (GIAM) (Gunasekera et al. 2008; Harman et al. 2008) used the CSIRO Mk3L GCM (Phipps 2006) as its climate module. To facilitate the comparison with previous results it is therefore useful to have the Step Response Function (SRF), the basis of the temperature component in SCCM, corresponding to the Mk3L (see Appendix B of Raupach et al. (2011) for a description of Step and Pulse Response Functions).

To this end the Mk3L was run in a paired simulation configuration with one simulation subjected to an instantaneous doubling of atmospheric CO_2 once initial transients had settled[3]. The time series of the difference in global mean temperature between the pair of simulations provides the information needed to estimate the SRF as follows. Employing a SRF with *i* terms for the change in global mean temperature implies using a model where

$$\frac{\mathrm{d}T_i}{\mathrm{d}t} = c_{sens}\alpha_i a_i RF(t) - \alpha_i T_i \tag{51}$$

with the total change in near-surface air temperature $\Delta T = \sum_i T_i$ and $\sum_i a_i$. In Eq. (51) RF is the time series of radiative forcing of the climate system, c_{sens} a measure of the sensitivity of the climate system (taking the value $\Delta T_{2\times} / RF_{2\times}$ where $2\times$ indicates the equilibrium values on a doubling of atmospheric CO_2), α_i provide the time scale of the response of each of components and a_i the partitioning of the radiative forcing between the components.

Most General Circulation Models exhibit a thermal behaviour which can be well approximated using a SRF with 2 or 3 components. For the case of a 2 component SRF the temperature response predicted by Eq. (51) after a step change in radiative forcing of RF at $t = 0$ is

$$\Delta T(t) = c_{sens} RF \left[a_1 \left(1 - \mathrm{e}^{-\alpha_1 t}\right) + \left(1 - a_1\right)\left(1 - \mathrm{e}^{-\alpha_2 t}\right)\right] \tag{52}$$

which is a 4 parameter, non-linear analytical expression for the change in temperature.

Determining the SRF therefore amounts to a parameter estimation problem. An appropriate metric in these circumstances (though not the only one) is the least-squares difference between the time series of analytical (Eq. (52)) and simulated temperature change. Specifically we seek the vector of parameters $\mathbf{P} = (a_1, \alpha_1, \alpha_2, c_{sens} RF)$ such that the cost function *J* is minimised, where

$$J\left(\mathbf{P}\right) = \int_0^\infty \left(\Delta T(\mathbf{P}, t) - \Delta\hat{T}(t)\right)^2 \mathrm{d}t \tag{53}$$

and $\Delta\hat{T}$ is the difference in globally-averaged near-surface air temperatures from the two GCM simulations. In order to reduce the influence of the GCM simulated weather events on *J* Eq. (53)

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[3] In practice the transients in a GCM simulation will never settle due to the chaotic nature of the climate system and the long-responses of the oceanic circulations. On this issue we rely on expert opinion as to how long is long enough.

is approximated using annual averages over the (finite) period of the simulations (in this case N=1000 years), i.e.

$$J(\mathbf{P}) \approx \sum_{j=1}^{N} \left(\Delta T(\mathbf{P}, t = j\Delta t) - \overline{\Delta T}(t = j\Delta t) \right)^2 \tag{54}$$

with $\overline{\Delta T}$ the annual average of $\Delta \hat{T}$. The minimisation of J is achieved through a down-gradient search method.

Results

The SRF for the CSIRO Mk3L obtained using the above methodology is given below in Table 15 alongside the SRFs for other GCMs included in SCCM. No error estimates are possible at this time as only single GCM ensemble members are available.

Table 15 2-component SRFs and climate sensitivity, $\Delta T_{2\times}$, for the Mk3L and 4 other GCMs.

	Mk3L	**HadCM3(2)**	**IMAGE**	**ECHAM**	**GFDL**
a_1	0.446	0.60	0.585	0.686	0.473
α_1	1/4.48	1/8.40	1/1.6	1/2.86	1/1.2
α_2	1/369.09	1/409.54	1/58.0	1/41.67	1/23.5
$c_{sens} RF$	4.09				
$\Delta T_{2\times}$	3.64	3.06	2.37	1.58	1.85

Assuming that the Mk3L applies a radiative forcing of $RF = 5.35\ln(2) = 3.7\,\text{Wm}^{-2}$ upon a doubling of atmospheric CO_2 the value of $c_{sens} RF$ implies a value of $c_{sens} = 0.90\,\text{KW}^{-1}\text{m}^2$. This is somewhat higher than the conventional value of $c_{sens} = 0.75\,\text{KW}^{-1}\text{m}^2$ but close to recent results using a long-run simulation of the HadCM3 model (Li and Jarvis 2009). It is interesting to note that those SRFs obtained using relatively short simulations (IMAGE, ECHAM and GFDL) exhibit general faster response characteristics and low climate sensitivities. Indeed the best fit 3-component SRF for the Mk3L has components with time scales of 1.8, 20.5 and 407.5 years and does approximate the GCM simulations better during the period from 10-40 years after the doubling of CO_2 (see Fig. 14). This suggests that simulations of a suitable length (greater than 500 years) are required in order to establish the important long-term components of a climate model's behaviour.

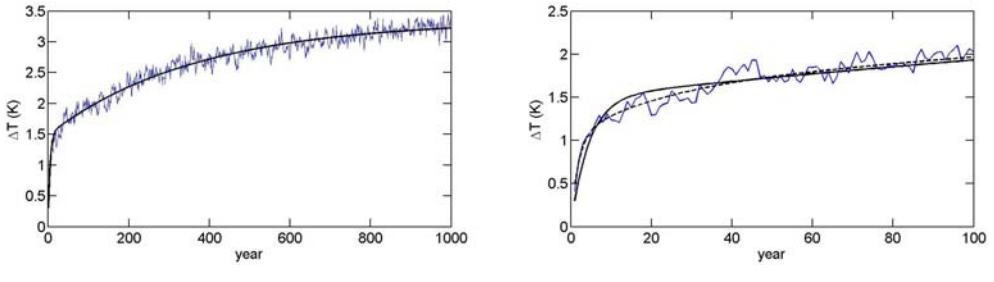

Fig. 14 Mk3L simulated (blue) and deduced SRF (black) representation of the change in globally-averaged near-surface air temperature after an instantaneous doubling of CO_2 in the long (left) and shorter (right) run. In the right panel the dashed line shows the corresponding 3-component SRF for the Mk3L which is indistinguishable from the 2-component PRF after t=40 years.

APPENDIX C – EMULATION OF FULL OCEAN CO2 CHEMISTRY (CO2SYS)

The Ocean CO_2 System

The ocean CO_2 system is characterised by four variables:

1. The Dissolved Inorganic Carbon or Total Carbonate (DIC measured in µmol/kgSW where kgSW is kg of seawater) given by

$$\begin{aligned} \text{DIC} &= \left[\text{CO}_2^*(\text{aq})\right] + \left[\text{HCO}_3^-\right] + \left[\text{CO}_3^{2-}\right] \\ &\quad \text{with } \left[\text{CO}_2^*(\text{aq})\right] = \left[\text{CO}_2(\text{aq})\right] + \left[\text{H}_2\text{CO}_3\right] \end{aligned} \tag{55}$$

2. The equilibrium CO_2 concentration in air, expressed as mole fraction in dry air (xCO2 in ppm), partial pressure of CO_2 (pCO2 in Pa or µatm) or fugacity of CO_2 (fCO_2 in Pa or µatm). Fugacity (fCO_2) is a modified partial pressure accounting for non-ideal gas behaviour and is a little lower than pCO_2 (for example fCO_2=348.9 µatm at pCO_2 = 350 µatm when T =15 °C).

3. pH (in pH units defined as $\log_{10}([H^+])$ where $[H^+]$ is measured in mol/kgSW or similar.

4. Total Alkalinity (TA measured in µmol/kgSW). This is defined as

$$\begin{aligned} \text{TA} &= \sum[+ \text{ charges for conservative ions}] - \sum[- \text{ charges for conservative ions}] \\ &= \sum[- \text{ charges for nonconservative ions}] \\ &\qquad - \sum[+ \text{ charges for nonconservative ions}] \end{aligned} \tag{56}$$

where conservative ions do not undergo acid-base reactions (proton exchange) in the pH range of interest, and non-conservative ions do not undergo acid-base reactions (Jacobson *et al.* 2000, p90). In seawater, Na^+ and Cl^- are typical conservative ions and HCO_3^-, CO_3^{2-}, $B(OH)_4^-$ (Borate ions), OH^- and H^+ are the main non-conservative ions. Therefore, TA is given by

$$\text{TA} = \left[\text{HCO}_3^-\right] + 2\left[\text{CO}_3^{2-}\right] + \left[\text{B(OH)}_4^-\right] + \left[\text{OH}^-\right] - \left[\text{H}^+\right] \tag{57}$$

The above four variables (DIC, xCO_2, pH, TA) are constrained by two equations, the carbon mass balance and the charge balance. Hence, specifying any two of the variables specifies the other two. Other (subsidiary) variables can then be determined given that

- Subsidiary species (B, Si, P, S, ...) are constrained by their own mass balances.
- The relationship between fCO_2 and $[CO_2^*(aq)]$ is given by a solubility or Henry's law constant, $K_0 = [CO_2^*(aq)]/fCO_2$.
- The partition of DIC among its constituent species ($[CO_2^*(aq)]$, $[HCO_3^-]$ and $[CO_3^{2-}]$) is determined by the first and second dissociation constants for CO_2 in water (usually denoted K_1 and K_2). Similar dissociation constants constrain the partition of minor species, for example between $[B(OH)_3]$ and $[B(OH)_4^-]$.

- Empirical quantities like K_0, K_1 and K_2 are dependent on temperature, pressure and salinity.

Many descriptions of this system are available (e.g. Jacobson *et al.* 2000, p288-289; Dickson 2010, Millero 1979, Millero 1995, Skirrow 1975). The simple chemistry of CO_2 in pure water (relating DIC, $x\mathrm{CO_2}$ and pH with TA = 0) is given in basic texts (e.g. Mahan 1965). The system is actually relatively simple and can be reduced to solving one cubic equation (Millero 1995). Unfortunately there are several real-world complications (Lewis and Wallace 1998) specifically

- There are two definitions of TA in use, which differ in their treatment of minor species.

- There are four different pH scales in use.

There are multiple specifications of empirical quantities (K_0, K_1 and K_2 and similar), in different (often unspecified) units, and sometimes suffering from typos in extant codes. Also these empirical quantities are poorly characterised by experiment at high (deep-ocean) pressures and over wide salinity ranges.

These complications mean that attempting to solve the ocean CO_2 system from first principles is unwise. Fortunately, there exists a user-friendly code (CO_2Sys, developed by Lewis and Wallace 1998) that allows calculations of the CO_2 system with options to specify definitions of TA and pH, and with "best available" resolution of the difficulties around empirical quantities. A huge added advantage is that units for all quantities are scrupulously specified. Given any two of (DIC, $x\mathrm{CO_2}$, pH, TA), the code finds the other two. The code also requires:

- Specification of 5 external variables namely temperature, salinity, pressure, total Si and total P;

- Specification of choices for empirical constants (8 options), treatment of $KHSO_4$ (2 options), and pH scale (4 options).

The code is freely available in Basic, MatLab and Excel versions.

CO_2Sys in SCCM

Rather than importing the full CO_2Sys program into SCCM, the approach used is to emulate the results of the CO_2Sys program in empirical functions for $x\mathrm{CO_2}(\mathrm{DIC}, T)$ (and $\xi(\mathrm{DIC}, T)$ - the Revelle factor used in the 'enting' formulation for pCO2) – namely Pade-approximant and Power-law fits to the original CO_2Sys output. The advantages of doing this are computational speed, elimination of redundant CO_2Sys features not needed in SCCM, reduction of the coding task, and compatibility with existing SCCM formulations for ocean CO_2. The disadvantages are that changes in CO_2Sys parameters (including TA, Si and P) and options (choices for empirical constants, treatment of $KHSO_4$, and pH scale) would require different new empirical fits.

In the results that follow the background conditions taken are that salinity = 35, TA = 2350 μmol/kgSW, Si = 0, P = 0 (zero values for Si and P are the CO_2Sys defaults). The CO_2Sys option used were the default (first) values in each of the menu option specifically (1) Set of constants = "K1, K2 from Mehrbach et al, 1973 refitted by Dickson and Millero, 1987", (2) KHSO4 = "Dickson", (3) pH scale = "Seawater scale (mol/kg-SW)". In Fig. 15 the markers show results from the original CO_2Sys program. No other background conditions and options have been tested at this stage.

The Pade-Approximant Fit

One advantage of both the Pade-Approximant and power-law functions is that they are analytically invertible. The Pade-Approximant function and its inverse are given by

$$f(x) = \frac{a_0 x}{1 + a_1 x + a_2 x^2}; \qquad x(f) = \frac{a_0 - a_1 f + \sqrt{(a_0 - a_1 f)^2 - 4a_2 f^2}}{2a_2 f} \tag{58}$$

For numerical reasons it is expedient to obtain fits for DIC(xCO2, T) and then invert analytically to determine (the desired) $x\mathrm{CO_2}$(DIC, T). Equation (58) was fitted to output from $\mathrm{CO_2}$Sys with

- $x = x\mathrm{CO_2}/x\mathrm{CO}_{2R}$, f = DIC with $x\mathrm{CO}_{2R}$ = 380 ppm.
- Units are DIC [μmolC/kgSW], $x\mathrm{CO_2}$ [ppm dry air].
- Temperature dependence was introduced by making the coefficients depend quadratically on temperature i.e.

  $$a_{Pi}(T) = a_{iR}\left(1 + a_{PiT1}(T - T_R) + a_{PiT2}(T - T_R)^2\right), \qquad i = 0,1,2 \tag{59}$$

  The reference temperature (at which $a_i = a_{iR}$) is fixed at T_R = 15°C. The functions $a_{Pi}(T)$ describe *proportional* dependencies of a_i on temperature (that is, a_i/a_{iR} is a quadratic in $(T - T_R)$ with a zeroth-order or constant coefficient of 1).
- The same temperature dependence applies to coefficients in the forward ($f(x)$) and inverse ($x(f)$) forms, because these are identical.

The resulting expression has 9 parameters (3 for each a_i). The fitting was done with a down-gradient (Levenberg-Marquardt) method in Mathematica. Care was needed to specify starting points. The process was:

1. Fit coefficients (a_i) at the individual temperatures 0, 10, 15, 20, 30°C;
2. Plot the resulting coefficients against temperature, to obtain prior estimates of the coefficients in the quadratics (59) (as required);
3. Using these priors as starting conditions, search for the 9 parameters in each expression.

In summary this process yielded the following empirical function for $x\mathrm{CO_2}$(DIC, T)

$$\frac{x\mathrm{CO_2}(\mathrm{DIC}, T)}{380\ \mathrm{ppm}} = \frac{a_{P0}(T) - a_{P1}(T)f + \sqrt{(a_{P0}(T) - a_{P1}(T)f)^2 - 4a_{P2}(T)f^2}}{2a_{P2}(T)f} \tag{60}$$

where f = DIC and

$$a_{\mathrm{0R}} = 30015.6, \quad a_{\mathrm{P0T1}} = -0.0226536, \quad a_{\mathrm{P0T2}} = 0.000167105,$$

$$a_{\mathrm{1R}} = 13.4574, \quad a_{\mathrm{P1T1}} = -0.019829, \quad a_{\mathrm{P1T2}} = 0.000113872,$$

$$a_{\mathrm{2R}} = -0.243121, \quad a_{\mathrm{P2T1}} = 0.000443511, \quad a_{\mathrm{P2T2}} = -0.000473227$$

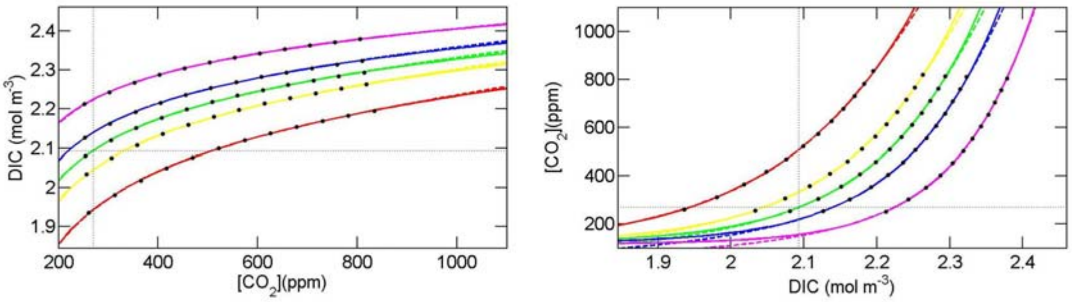

Fig. 15 The Pade-Approximant and Power-Law fits to the CO_2Sys model for a range of temperatures. Left panel: DIC(*x*CO2,*T*). Right panel: *x*CO2(DIC,*T*). Colours mark the variation of the fitted functions at temperatures 0°C (magenta), 10°C (blue), 15°C (green), 20°C (yellow) and 30°C (red). Solid line gives the Power-Law fit; dashed line the Pade-Approximant fit. Markers give the output from the full CO_2Sys model. Dotted lines mark estimates of preindustrial conditions.

The Power-Law Fit

The second empirical function used to parameterise the full CO_2Sys model is a power law i.e.

$$f(x) = p_0 (x - p_2)^{p_1}\ ; \qquad x(f) = (f/p_0)^{1/p_1} + p_2 \tag{61}$$

Similarly to the Pade-Approximant, the fit was obtained for DIC(*x*CO2, *T*) and then inverted analytically to determine *x*CO2(DIC, *T*). The same general procedure is used to determine the coefficients i.e.

$$p_{Pi}(T) = p_{iR}\left(1 + p_{PiT1}(T - T_R) + p_{PiT2}(T - T_R)^2\right), \quad i = 0,1,2 \tag{62}$$

In summary this process yields the following empirical function for *x*CO2(DIC, *T*)

$$\frac{x\mathrm{CO}_2(\mathrm{DIC}, T)}{380\ \mathrm{ppm}} = p_{P2}(T) + \left(f/p_{P0}(T)\right)^{1/p_{P1}(T)}, \quad \text{with } f = \mathrm{DIC} \tag{63}$$

where

$$p_{0\mathrm{R}} = 2160.156, \quad p_{\mathrm{P0T1}} = \text{-}0.00347063, \quad p_{\mathrm{P0T2}} = \text{-}0.0000250016,$$
$$p_{1\mathrm{R}} = 0.0595961, \quad p_{\mathrm{P1T1}} = 0.0200328, \quad p_{\mathrm{P1T2}} = 0.000192084,$$
$$p_{2\mathrm{R}} = 0.318665, \quad p_{\mathrm{P2T1}} = \text{-}0.00151292, \quad p_{\mathrm{P2T2}} = \text{-}0.000198978$$

Fig. 15 shows both parameterisations against output from the full CO_2Sys model for DIC(*x*CO2, *T*) (left) and $x\mathrm{CO}_2$(DIC, *T*) (right). Overall the agreement with CO_2Sys is good, particularly when we note that the usual operating range for SCCM covers global *T* from 15 to 20^{o}C (from the green to the yellow lines). Only for extremely low and high amounts of carbon content in the environment are the two fitted functions noticeably different. Given the functional requirements of the Pade-Approximant fit (it tends to zero at ±∞ for non-zero a_2) it is recommended that the Power-Law fit is used if a high concentration of CO_2 (>800 ppm) are anticipated.

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