Appendix A

Experimental design

A.1 Introduction

The experimental design employed throughout this project followed that specified by PMIP2 (*Paleoclimate Modelling Intercomparison Project*, 2005), enabling a direct comparison between Mk3L and other models. PMIP2 experimental design is summarised in Section A.2, while Sections A.3 and A.4 provide further details regarding spin-up procedures and the coupled model experiments respectively.

The procedures followed to generate the restart and auxiliary files required by Mk3L are described in detail by *Phipps* (2006).

A.2 PMIP2 experimental design

PMIP2 experimental design is summarised in Table A.1. For coupled model experiments, it is specified that a control run be conducted for pre-industrial conditions, which are taken as being those which existed around the year AD 1750. Pre-industrial values are specified for the atmospheric concentrations of the "greenhouse gases" carbon dioxide (CO_2), methane (CH_4) and nitrous oxide (N_2O); it is also specified that the atmospheric concentration of chlorofluorocarbons be set to zero. The specified epoch is 0 years Before Present, and the values for the Earth's orbital parameters therefore correspond to the year AD 1950. Otherwise, "modern" boundary conditions are specified, which can be interpreted as meaning that present-day values should be used.

While no specific spin-up procedure is prescribed for the coupled model, it is specified that the ocean model should be initialised using the World Ocean Atlas 1998 dataset (*National Oceanographic Data Center*, 2002, commonly referred to as the "Levitus 1998" dataset).

The boundary conditions for the mid-Holocene experiment differ only in the atmospheric methane concentration and the values of the Earth's orbital parameters. While the ocean model can again be initialised using the World Ocean Atlas 1998 dataset, it can also be initialised from year 100 of a control run.

Boundary condition	**Control run (~AD 1750)**	**Mid-Holocene (6ka BP)**
Vegetation	Fixed	As for control run
Ice sheets	Modern	As for control run
Topography/coastlines	Modern	As for control run
CO_2 concentration [ppm]	280	280
CH_4 concentration [ppb]	760	650
N_2O concentration [ppb]	270	270
Chlorofluorocarbons	None	None
O_3 concentration	Modern	As for control run
Solar constant [Wm^{-2}]	1365	1365
Epoch [years BP]	0	6,000
Eccentricity of Earth's orbit	0.016724	0.018682
Obliquity of Earth's axis [°]	23.446	24.105
Longitude of perihelion [°]	102.04	0.87
Initial ocean state	World Ocean Atlas 1998	World Ocean Atlas 1998 *or* year 100 of control run

Table A.1: PMIP2 experimental design for coupled model experiments: the pre-industrial control run, and the mid-Holocene experiment.

A.3 Spin-up procedures

The spin-up procedures for the atmosphere and ocean models are outlined in Sections 2.3.1 and 2.3.2 respectively. This section provides further information regarding the experimental design.

A.3.1 Ocean model

Configuration

The default configuration of the ocean model was employed, as described by *Phipps* (2006). Following PMIP2 experimental design, the bathymetry and coastlines were configured for the present day.

Initial state

The initial state of the ocean model was one in which the ocean is at rest. Following PMIP2 experimental design, the initial temperatures and salinities were set equal to the annual-mean World Ocean Atlas 1998 values.

Boundary conditions

The default surface boundary conditions on the stand-alone ocean model were derived from the World Ocean Atlas 1998, and from the NCEP-DOE Reanalysis 2 (*Kanamitsu et al.*, 2002).

As the upper layer of the Mk3L ocean model has a thickness of 25 m, the temperature and salinity of this layer simulate the average temperature and salinity of the upper 25 m of the water column, and not the sea surface temperature (SST) and sea surface salinity (SSS) *per se*. The temperature and salinity of this layer should be relaxed towards an equivalent observational quantity; the surface boundary conditions on the ocean model were *not* therefore the observed SST and SSS, but were instead the averages of the World Ocean Atlas 1998 temperatures and salinities over the upper 25 m of the water column.

The surface wind stresses were taken from the NCEP-DOE Reanalysis 2, and consisted of the climatological wind stresses for the period 1979–2003.

A.3.2 Atmosphere model

Configuration

The default configuration of the atmosphere model was employed, as described by *Phipps* (2006). Following PMIP2 experimental design, the topography, coastlines, ice sheets and vegetation were configured for the present day. The solar constant was set to 1365 Wm^{-2}, and AD 1950 values were used for the Earth's orbital parameters. The atmospheric carbon dioxide concentration was set to 280 ppm, and ozone concentrations were taken from the AMIP II recommended dataset (*Wang et al.*, 1995).

PMIP2 experimental design also specifies the atmospheric concentrations of methane, nitrous oxide and chlorofluorocarbons; however, the Mk3L atmosphere model does not allow for the radiative effects of these gases.

Initial state

The atmosphere model was initialised using the original restart file, as supplied with the model source code.

Boundary conditions

For consistency with the ocean model, the surface boundary conditions on the stand-alone atmosphere model consisted of the averages of the World Ocean Atlas 1998 temperature and salinity over the upper 25 m of the water column.

The currents required by the sea ice model were diagnosed from the final 100 years of ocean model spin-up runs, avoiding any need to apply "flux" adjustments to the currents within the coupled model.

A.4 Coupled model

A.4.1 Control runs

Configuration

For coupled model control runs, the atmosphere and ocean models were configured exactly as for the respective spin-up runs. Flux adjustments were derived using the surface fluxes, sea surface temperatures and sea surface salinities diagnosed from the spin-up runs, as described in Section 2.6.

Initial state

The atmospheric and oceanic components of the coupled model were initialised from the state of each model at the end of the appropriate spin-up run.

A.4.2 Mid-Holocene experiments

Configuration

For the mid-Holocene experiments, only two changes were made to the configuration of the coupled model, relative to the control runs. Following PMIP2 experimental design, the epoch was changed from 0 to 6,000 years BP. The atmospheric carbon dioxide concentration was also reduced to 277 ppm, in order to represent the radiative forcing arising from the specified reduction in the methane concentration (Table A.1).

This *effective* carbon dioxide concentration was calculated using the following expressions, which give the radiative forcings arising from changes in the atmospheric concentrations of carbon dioxide and methane (*Ramaswamy et al.*, 2001, Table 6.2):

$$\mathrm{CO_2}: \quad \Delta F = 5.35 \ln\left(\frac{C}{C_0}\right) \tag{A.1}$$

$$\mathrm{CH_4}: \quad \Delta F = 0.036(\sqrt{M} - \sqrt{M_0}) - (f(M, N_0) - f(M_0, N_0)) \tag{A.2}$$

In these expressions, ΔF is the radiative forcing ($\mathrm{Wm^{-2}}$), C_0 and C are the original and perturbed carbon dioxide concentrations respectively (ppm), M_0 and M are the original and perturbed methane concentrations respectively (ppb), N_0 is the nitrous oxide concentration (ppb), and $f(M, N)$ is given by

$$F(M, N) = 0.47 \ln\left[1 + 2.01 \times 10^{-5}(MN)^{0.75} + 5.31 \times 10^{-15} M (MN)^{1.52}\right] \tag{A.3}$$

Using $M_0 = 760$ ppb, $M = 650$ ppb and $N_0 = 270$ ppb, Equations A.2 and A.3 give a value of -0.066 $\mathrm{Wm^{-2}}$ for the radiative forcing arising from the reduction in the atmospheric methane concentration.

By re-arranging Equation A.1, the following expression is obtained, enabling an *effective* carbon dioxide concentration C to be derived, which gives rise to a radiative forcing ΔF ($\mathrm{Wm^{-2}}$) relative to the *actual* concentration C_0:

$$C = C_0\, e^{\Delta F / 5.35} \tag{A.4}$$

Using $C_0 = 280$ ppm and $\Delta F =$ -0.066 $\mathrm{Wm^{-2}}$, this expression gives a value for the effective carbon dioxide concentration of 277 ppm.

Initial state

Following PMIP2 experimental design, the coupled model was initialised from the end of year 100 of the appropriate control run.

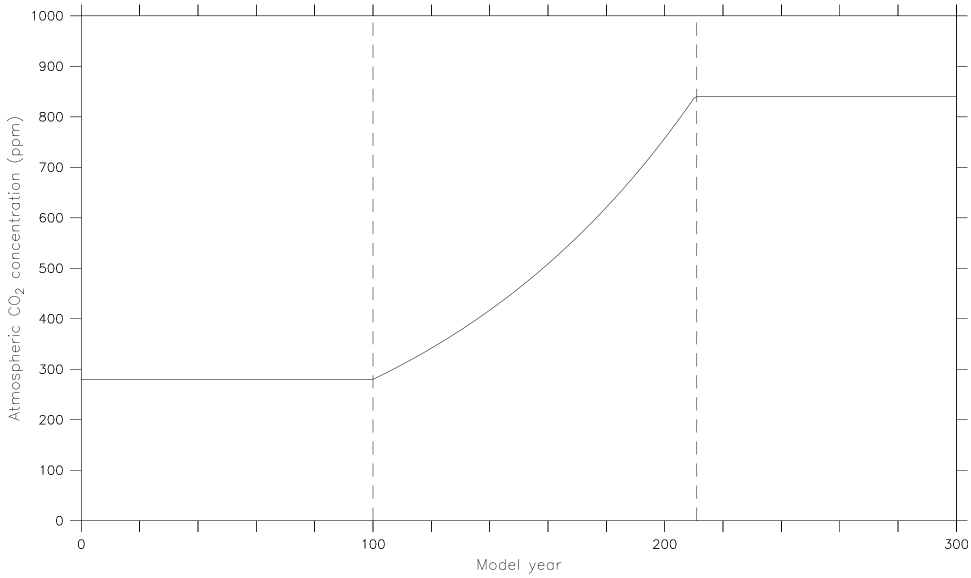

Figure A.1: The atmospheric carbon dioxide concentration for the $3\times CO_2$ stabilisation experiments. After being held constant at the pre-industrial concentration of 280 ppm for the first 100 years, the carbon dioxide concentration was increased at 1% per year, until it reached 840 ppm (three times the pre-industrial concentration) in year 211. It was held constant thereafter.

A.4.3 $3\times CO_2$ stabilisation experiments

Configuration

For the $3\times CO_2$ stabilisation experiments, the only change to the configuration of the coupled model, relative to the control runs, was an increase in the atmospheric carbon dioxide concentration. The experiments began in year 101, with the carbon dioxide concentration being increased at 1% per year. It reached 840 ppm, three times the pre-industrial level, in year 211, and was held constant thereafter. The resulting carbon dioxide concentrations are shown in Figure A.1.

Initial state

As for the mid-Holocene experiments, the coupled model was initialised from the end of year 100 of the appropriate control run.

Appendix B

Details of simulations

The simulations presented herein were conducted primarily at the Australian Partnership for Advanced Computing National Facility (*Australian Partnership for Advanced Computing*, 2005) in Canberra. Two different machines were used:

AlphaServer SC 126 Compaq AlphaServer SC nodes, each containing:
- 4 × 1GHz EV68 (Alpha 21264C) CPUs
- between 4 and 16GB of RAM
Tru64 UNIX operating system

Linux Cluster 152 Dell Precision 350 nodes, each containing:
- 1 × 2.66GHz Intel Pentium 4 CPU
- 1GB RAM
Linux operating system

Some of the simulations conducted on the AlphaServer SC were completed on an equivalent facility located at the Interactive Virtual Environments Centre in Perth, Western Australia.

Statistics are provided in Tables B.1, B.2 and B.3, for the atmosphere model, ocean model and coupled model simulations respectively.

Simulation	**Facility**	**Original name**	**Duration (years)**
A-DEF	APAC AlphaServer SC	c15	50
A-EFF	APAC AlphaServer SC	c17	50
A-SHF	APAC AlphaServer SC	c16	50

Table B.1: Atmosphere model simulations: the name used herein, the facility on which it was conducted, the name used on that facility, and the duration.

Simulation	Facility	Original name	Duration (years)
O-5d	APAC Linux Cluster	h73	4500
O-7.5d	APAC Linux Cluster	h74	3500
O-10d	APAC Linux Cluster	h69	3500
O-15d	APAC Linux Cluster	h70	4500
O-30d	APAC Linux Cluster	h71	5500
O-40d	APAC Linux Cluster	h72	5500
O-60d	APAC Linux Cluster	h75	5500
O-80d	APAC Linux Cluster	h76	6500
O-0.25psu	APAC Linux Cluster	h57	4500
O-0.5psu	APAC Linux Cluster	h56	4500
O-1psu	APAC Linux Cluster	h55	4500
O-DEF	APAC Linux Cluster	h53	4500
O-EFF	APAC Linux Cluster	h65	8600
O-SHF	APAC Linux Cluster	h61	500

Table B.2: Ocean model simulations: the name used herein, the facility on which it was conducted, the name used on that facility, and the duration.

Simulation	Facility	Original name	Model years
Control runs			
CON-DEF	APAC AlphaServer SC iVEC AlphaServer SC	d73	1–176 177–1400*
CON-EFF	APAC AlphaServer SC iVEC AlphaServer SC	d70	1–623 624–1100*
CON-SHF	APAC AlphaServer SC iVEC AlphaServer SC	d68	1–630 631–1100*
mid-Holocene experiments			
6ka-DEF	APAC Linux Cluster	d95	101–900*
6ka-EFF	APAC Linux Cluster	d94	101–900*
6ka-SHF	APAC Linux Cluster	d92	101–900*
$3\times CO_2$ stabilisation experiments			
3CO2-DEF	APAC AlphaServer SC iVEC AlphaServer SC	d86	101–185 186–1400*
3CO2-EFF	APAC AlphaServer SC iVEC AlphaServer SC	d85	101–638 639–1100*
3CO2-SHF	APAC AlphaServer SC iVEC AlphaServer SC	d83	101–637 638–1100*

Table B.3: Coupled model simulations: the name used herein, the facility on which it was conducted, the name used on that facility, and the model years which were conducted on that facility. The mid-Holocene and $3\times CO_2$ stabilisation experiments began at model year 101. *The simulation is still underway at the time of writing.