```
TITLE
UBGH2-1-1
END

RUNTIME
time_units              years
timestep_max            500.0
timestep_init           1.E-12
time_tolerance          0.1
hindmarsh               true
correction_max          2.0
debye-huckel            true
database_sweep          false
speciate_only           false
gimrt                   true
graphics                kaleidagraph
fix_saturation          1.0
database                carbon_cycle.dbs
screen_output           50
Steady_state            false
END

OUTPUT
time_units              years
Spatial_profile         400000
END

PRIMARY_SPECIES
HCO3-
H13CO3-
CH4(aq)
13CH4(aq)
NH4+
HPO4--
HS-
SO4--
Fe++
H+
```

H2(aq)
Cl-
Ca++
Na+
Mg++
END

SECONDARY_SPECIES
CO2(aq)
13CO2(aq)
CO3--
13CO3--
NH3(aq)
H3PO4(aq)
H2PO4-
PO4---
H2S(aq)
S--
END

GASES
CO2(g)
13CO2(g)
H2S(g)
CH4(g)
13CH4(g)
END

MINERALS
Calcite-Ca -rate -9.7
Calcite-Mg -rate -10.7
CH2O_SO4 -rate -9.6
CH2O_ME -associate CH2O_SO4 -rate -9.8
Pyrite_FeS -rate -14.8
Mackinawite
END

AQUEOUS_KINETICS

```
AOM
13AOM
CO2_reduction
13CO2_reduction
END

TRANSPORT
distance_units centimeters
time_units    seconds
fix_diffusion                 1.000e-5
D_25    Cl-                   2.055e-5
D_25    Na+                    1.349e-5
D_25    H+                     9.328e-5
D_25    Mg++                   7.040e-6
D_25    Ca++                   8.075e-6
D_25    Fe++                   7.060e-6
D_25    HCO3-                  1.194e-5
D_25    H13CO3-                1.191e-5
D_25    CH4(aq)               1.850e-5
D_25    13CH4(aq)             1.821e-5
D_25    NH3(aq)               2.280e-5
D_25    HPO4--                 7.685e-6
D_25    HS-                    1.726e-5
D_25    SO4--                 1.068e-5
D_25    H2(aq)                5.126e-5
D_25    CO2(aq)               1.916e-5
D_25    13CO2(aq)             1.910e-5
D_25    CO3--                  9.305e-6
D_25    13CO3--                9.287e-6
D_25    NH4+                   1.983e-5
D_25    H3PO4(aq)              9.595e-6
D_25    H2PO4-                 9.595e-6
D_25    PO4---                6.195e-6
D_25    H2S(aq)               2.100e-5
D_25    S--                   1.068e-5
diffusion_activation    4.539
cementation_exponent      1.9
END
```

```
BOUNDARY_CONDITIONS
x_begin      surface        Dirichlet
x_end        bottom         Dirichlet
END

INITIAL_CONDITIONS
surface 1-200
END

ION_EXCHANGE
exchange     X-
convention Gaines-Thomas
END

Condition surface
units                  mol/kg
pH                     7.8
set_porosity       0.8
HCO3-                  2.2e-3
H13CO3-                0.02472184E-3
CH4(aq)                1e-9
13CH4(aq)              0.010731526e-9
NH4+                   1e-4
HPO4--                 1e-5
HS-                    1e-9
SO4--                  28e-3
Fe++                   0.2e-2
H2(aq)                 1e-9
Cl-                    0.55
Ca++                   0.01
Na+                    charge
Mg++                   0.05
Calcite-Ca             2e-2 1
Calcite-Mg             2e-2 1
CH2O_SO4               0.04 1
CH2O_ME                0.04 1
Pyrite_FeS         0.01 1
```

```
Mackinawite          0.01 1
X- -cec 1.5e-4
SolidDensity CalculateFromMinerals
END

Condition bottom
units                mol/kg
set_porosity         0.486
pH                   7.6
HCO3-                70e-3
H13CO3-              0.79258219E-3
CH4(aq)              10e-3
13CH4(aq)            0.103719356e-3
NH4+                 5e-3
HPO4--               1e-5
HS-                  0
SO4--                0
Fe++                 0.7e-2
H2(aq)               1e-9
Cl-                  0.55
Ca++                 0.0045
Na+                  charge
Mg++                 0.05
Calcite-Ca           2e-2 1
Calcite-Mg           2e-2 1
CH2O_SO4             0.04 1
CH2O_ME              0.04 1
Pyrite_FeS           0.01 1
Mackinawite          0.01 1
X- -cec 1.5e-4
SolidDensity CalculateFromMinerals
END

POROSITY
read_PorosityFile    UBGH2-1-1_porosity.txt
END

TEMPERATURE
```

```
set_temperature             1.3
temperature_gradient    0.1
END

DISCRETIZATION
xzones 200 0.1
distance_units meters
END

EROSION/BURIAL
time_units          years
distance_units meters
read_burialfile alkalinity_burial.dat FullForm
END
```