

Supplement of Solid Earth, 10, 1409–1428, 2019
<https://doi.org/10.5194/se-10-1409-2019-supplement>
© Author(s) 2019. This work is distributed under
the Creative Commons Attribution 4.0 License.



Supplement of

Chemical heterogeneities in the mantle: progress towards a general quantitative description

Massimiliano Tirone

Correspondence to: Massimiliano Tirone (max.tirone@gmail.com)

The copyright of individual parts of the supplement might differ from the CC BY 4.0 License.

S1 Supplementary Data

This section describes the additional material available through an external data repository.

The public link to access all the files is:

<https://figshare.com/collections/G-KINB/4079111>

List of the available files:

- TWOPD-G-KIN.DATA.ZIP
- TWOPD-G-KIN.MOVIE1.AVI
- TWOPD-G-KIN.MOVIE5.AVI
- 2D-G-KIN.DATA.ZIP
- 2D-G-KIN.MOVIE5A.AVI
- 2D-G-KIN.MOVIE5B.AVI

S1.1 1-D Simulations

The zip file TWOPD-G-KIN.DATA.ZIP includes the data of three 1-D simulations assuming that the initial proportion of the two assemblages is 1:1, 5:1 and 50:1 ($f = 1, 5, 50$). The details of the models are discussed in the main text. For every simulation there are two data files: TWOPD-G-KIN1.1.DAT and TWOPD-G-KIN2.1.DAT for the case with 1:1 proportion, TWOPD-G-KIN1.5.DAT, TWOPD-G-KIN2.5.DAT and TWOPD-G-KIN1.50.DAT, TWOPD-G-KIN2.50.DAT for the models with initial proportion 5:1 and 50:1, respectively. The data files are divided in blocks, each block of data refers to a particular time step.

The first data file for each simulation (TWOPD-G-KIN1.1.DAT, TWOPD-G-KIN1.5.DAT and TWOPD-G-KIN1.50.DAT) includes in every block, distance, G^* (joules) and the grid step size for the two sub-systems. The number of grid points for sub-system *A* and *B* are 101 and 101 in the first simulation, 501 and 101 in the second simulation, 1001 and 101 in the third simulation. Time step is 4, 40 and 800 for the three simulations. Data are stored every 20, 20, 50 numerical time steps respectively. As discussed in the main text, time, distance and step size have arbitrary units.

The second data file of each simulation (TWOPD-G-KIN2.1.DAT, TWOPD-G-KIN2.5.DAT and TWOPD-G-KIN2.50.DAT) includes in every block, distance and abundance of nine oxides (grams or wt%) which describes the bulk composition at every grid point. The listed oxides are: SiO_2 , TiO_2 , Al_2O_3 , Fe_2O_3 , Cr_2O_3 , FeO , MgO , CaO and Na_2O .

Two 1-D animations TWOPD-G-KIN.MOVIE1.AVI and TWOPD-G-KIN.MOVIE5.AVI are based on the simulations with $f = 1$ and $f = 5$. The relative data are included in the zip file TWOPD-G-KIN.DATA.ZIP.

S1.2 2-D Simulations

The results of two 2-D simulations are included in the zip file 2D-G-KIN.DATA.ZIP. For both simulations the initial proportion of the two assemblages is set to 5:1. The interface between the two sub-systems is a vertical line. The first simulation assumes that assemblage *A* becomes mobile downwards at time=1000000 (arbitrary units), while in the second simulation the dynamic assemblage is *B*. The velocity of the moving assemblages is set to 0.00625 (arbitrary units). New material entering from the top side has the same bulk composition of the initial assemblage. The composition is reported in the main text and in the data files here below. Output data are stored every 400 time steps and the simulation time step is 16 (arbitrary units). Each block of data defined by the label "ZONE" provides information related to a particular time step.

The first data file of each simulation (2D-G-KIN1.5A.DAT and 2D-G-KIN1.5B.DAT) includes the distance x-direction,

y-direction and G^* . The number of grid points in the x-direction is 251 and 51 in sub-system *A* and *B*, respectively (total initial distance is 500 and 100 in arbitrary units). The number of grid points in the y-direction is 51 (total distance is 50 in arbitrary units). A block of data is divided in sub-blocks. Each sub-block consists of $(251 + 51) \times 51$ data points. The first sub-block contains the x-coordinate defining the numerical grid, the second sub-block the y-coordinate and the third sub-block the G^* values at the corresponding grid points.

The second data file of each simulation (2D-G-KIN2 . 5A . DAT and 2D-G-KIN2 . 5B . DAT) follows the same data structure, except that instead of G^* , nine bulk oxides are listed in nine sub-blocks. The sequence of oxides is the same reported for the 1-D models.

The data in the zip file 2D-G-KIN . DATA . AVI have been used to create two animations, 2D-G-KIN . MOVIE5A . AVI and 2D-G-KIN . MOVIE5B . AVI, both are available following the link to the external data repository.

S2 Supplementary Table

The following table reports the initial bulk composition and the proportion factor f of the two sub-systems for all the 43 cases considered in this study (see sections 2.1 and 2.2 in the main text).

Table S1. Initial bulk composition of the two assemblages and proportion factor f .

bulk comp.	(A ₀)	(B ₀)	(A ₀)	(B ₀)	(A ₀)	(B ₀)	(A ₀)	(B ₀)	(A ₀)	(B ₀)
oxides (g or wt%)	#1(f=1)		#2(f=1.2)		#3(f=1.3)		#4(f=1.6)		#5(f=2)	
SiO ₂	45.200	48.860	45.200	48.860	45.200	48.860	45.200	48.860	45.200	48.860
TiO ₂	0.200	0.370	0.200	0.370	0.200	0.370	0.200	0.370	0.200	0.370
Al ₂ O ₃	3.940	17.720	3.940	17.720	3.940	17.720	3.940	17.720	3.940	17.720
Fe ₂ O ₃	0.200	0.840	0.200	0.840	0.200	0.840	0.200	0.840	0.200	0.840
Cr ₂ O ₃	0.400	0.030	0.400	0.030	0.400	0.030	0.400	0.030	0.400	0.030
FeO	8.100	7.610	8.100	7.610	8.100	7.610	8.100	7.610	8.100	7.610
MgO	38.400	9.100	38.400	9.100	38.400	9.100	38.400	9.100	38.400	9.100
CaO	3.150	12.500	3.150	12.500	3.150	12.500	3.150	12.500	3.150	12.500
Na ₂ O	0.410	2.970	0.410	2.970	0.410	2.970	0.410	2.970	0.410	2.970
sum	100	100	100	100	100	100	100	100	100	100
	#6(f=5)		#7(f=20)		#8(f=100)		#9(f=500)		#10(f=1000)	
SiO ₂	45.200	48.860	45.200	48.860	45.200	48.860	45.200	48.860	45.200	48.860
TiO ₂	0.200	0.370	0.200	0.370	0.200	0.370	0.200	0.370	0.200	0.370
Al ₂ O ₃	3.940	17.720	3.940	17.720	3.940	17.720	3.940	17.720	3.940	17.720
Fe ₂ O ₃	0.200	0.840	0.200	0.840	0.200	0.840	0.200	0.840	0.200	0.840
Cr ₂ O ₃	0.400	0.030	0.400	0.030	0.400	0.030	0.400	0.030	0.400	0.030
FeO	8.100	7.610	8.100	7.610	8.100	7.610	8.100	7.610	8.100	7.610
MgO	38.400	9.100	38.400	9.100	38.400	9.100	38.400	9.100	38.400	9.100
CaO	3.150	12.500	3.150	12.500	3.150	12.500	3.150	12.500	3.150	12.500
Na ₂ O	0.410	2.970	0.410	2.970	0.410	2.970	0.410	2.970	0.410	2.970
sum	100	100	100	100	100	100	100	100	100	100
	#11(f=1)		#12(f=1.5)		#13(f=2)		#14(f=5)		#15(f=20)	
SiO ₂	47.434	48.860	47.434	48.860	47.434	48.860	47.434	48.860	47.434	48.860
TiO ₂	0.317	0.370	0.317	0.370	0.317	0.370	0.317	0.370	0.317	0.370
Al ₂ O ₃	7.978	17.720	7.978	17.720	7.978	17.720	7.978	17.720	7.978	17.720
Fe ₂ O ₃	0.582	0.840	0.582	0.840	0.582	0.840	0.582	0.840	0.582	0.840
Cr ₂ O ₃	0.288	0.030	0.288	0.030	0.288	0.030	0.288	0.030	0.288	0.030
FeO	7.595	7.610	7.595	7.610	7.595	7.610	7.595	7.610	7.595	7.610
MgO	26.035	9.100	26.035	9.100	26.035	9.100	26.035	9.100	26.035	9.100
CaO	7.902	12.500	7.902	12.500	7.902	12.500	7.902	12.500	7.902	12.500
Na ₂ O	1.869	2.970	1.869	2.970	1.869	2.970	1.869	2.970	1.869	2.970
sum	100	100	100	100	100	100	100	100	100	100
	#16(f=100)		#17(f=500)		#18(f=1.32)		#19(f=2)		#20(f=5)	
SiO ₂	47.434	48.860	47.434	48.860	48.940	48.860	48.940	48.860	48.940	48.860
TiO ₂	0.317	0.370	0.317	0.370	0.393	0.370	0.393	0.370	0.393	0.370
Al ₂ O ₃	7.978	17.720	7.978	17.720	10.394	17.720	10.394	17.720	10.394	17.720
Fe ₂ O ₃	0.582	0.840	0.582	0.840	0.820	0.840	0.820	0.840	0.820	0.840
Cr ₂ O ₃	0.288	0.030	0.288	0.030	0.237	0.030	0.237	0.030	0.237	0.030
FeO	7.595	7.610	7.595	7.610	7.074	7.610	7.074	7.610	7.074	7.610
MgO	26.035	9.100	26.035	9.100	18.887	9.100	18.887	9.100	18.887	9.100
CaO	7.902	12.500	7.902	12.500	10.505	12.500	10.505	12.500	10.505	12.500
Na ₂ O	1.869	2.970	1.869	2.970	2.751	2.970	2.751	2.970	2.751	2.970
sum	100	100	100	100	100	100	100	100	100	100

Table S1. (continue) Initial bulk composition of the two assemblages and proportion factor f .

bulk comp.	(A ₀)	(B ₀)	(A ₀)	(B ₀)	(A ₀)	(B ₀)	(A ₀)	(B ₀)	(A ₀)	(B ₀)
oxides (g or wt%)	#21(f=20)		#22(f=100)		#23(f=500)		#24(f=1)		#25(f=10)	
SiO ₂	48.940	48.860	48.940	48.860	48.940	48.860	49.619	48.860	49.619	48.860
TiO ₂	0.393	0.370	0.393	0.370	0.393	0.370	0.426	0.370	0.426	0.370
Al ₂ O ₃	10.394	17.720	10.394	17.720	10.394	17.720	11.372	17.720	11.372	17.720
Fe ₂ O ₃	0.820	0.840	0.820	0.840	0.820	0.840	0.918	0.840	0.918	0.840
Cr ₂ O ₃	0.237	0.030	0.237	0.030	0.237	0.030	0.219	0.030	0.219	0.030
FeO	7.074	7.610	7.074	7.610	7.074	7.610	6.745	7.610	6.745	7.610
MgO	18.887	9.100	18.887	9.100	18.887	9.100	16.074	9.100	16.074	9.100
CaO	10.505	12.500	10.505	12.500	10.505	12.500	11.518	12.500	11.518	12.500
Na ₂ O	2.751	2.970	2.751	2.970	2.751	2.970	3.109	2.970	3.109	2.970
sum	100	100	100	100	100	100	100	100	100	100
	#26(f=20)		#27(f=100)		#28(f=500)		#29(f=1)		#30(f=5)	
SiO ₂	49.619	48.860	49.619	48.860	49.619	48.860	45.200	45.931	45.200	45.931
TiO ₂	0.426	0.370	0.426	0.370	0.426	0.370	0.200	0.199	0.200	0.199
Al ₂ O ₃	11.372	17.720	11.372	17.720	11.372	17.720	3.940	18.599	3.940	18.599
Fe ₂ O ₃	0.918	0.840	0.918	0.840	0.918	0.840	0.200	0.351	0.200	0.351
Cr ₂ O ₃	0.219	0.030	0.219	0.030	0.219	0.030	0.400	0.015	0.400	0.015
FeO	6.745	7.610	6.745	7.610	6.745	7.610	8.100	8.576	8.100	8.576
MgO	16.074	9.100	16.074	9.100	16.074	9.100	38.400	17.507	38.400	17.507
CaO	11.518	12.500	11.518	12.500	11.518	12.500	3.150	7.623	3.150	7.623
Na ₂ O	3.109	2.970	3.109	2.970	3.109	2.970	0.410	1.199	0.410	1.199
sum	100	100	100	100	100	100	100	100	100	100
	#31(f=20)		#32(f=100)		#33(f=500)		#34(f=1)		#35(f=5)	
SiO ₂	45.200	45.931	45.200	45.931	45.200	45.931	45.200	45.914	45.200	45.914
TiO ₂	0.200	0.199	0.200	0.199	0.200	0.199	0.200	0.216	0.200	0.216
Al ₂ O ₃	3.940	18.599	3.940	18.599	3.940	18.599	3.940	18.582	3.940	18.582
Fe ₂ O ₃	0.200	0.351	0.200	0.351	0.200	0.351	0.200	0.296	0.200	0.296
Cr ₂ O ₃	0.400	0.015	0.400	0.015	0.400	0.015	0.400	0.005	0.400	0.005
FeO	8.100	8.576	8.100	8.576	8.100	8.576	8.100	8.015	8.100	8.015
MgO	38.400	17.507	38.400	17.507	38.400	17.507	38.400	18.551	38.400	18.551
CaO	3.150	7.623	3.150	7.623	3.150	7.623	3.150	7.459	3.150	7.459
Na ₂ O	0.410	1.199	0.410	1.199	0.410	1.199	0.410	0.962	0.410	0.962
sum	100	100	100	100	100	100	100	100	100	100
	#36(f=20)		#37(f=100)		#38(f=500)		#39(f=1)		#40(f=5)	
SiO ₂	45.200	45.914	45.200	45.914	45.200	45.914	45.200	45.804	45.200	45.804
TiO ₂	0.200	0.216	0.200	0.216	0.200	0.216	0.200	0.281	0.200	0.281
Al ₂ O ₃	3.940	18.582	3.940	18.582	3.940	18.582	3.940	18.319	3.940	18.319
Fe ₂ O ₃	0.200	0.296	0.200	0.296	0.200	0.296	0.200	0.246	0.200	0.246
Cr ₂ O ₃	0.400	0.005	0.400	0.005	0.400	0.005	0.400	0.015	0.400	0.015
FeO	8.100	8.015	8.100	8.015	8.100	8.015	8.100	7.482	8.100	7.482
MgO	38.400	18.551	38.400	18.551	38.400	18.551	38.400	18.834	38.400	18.834
CaO	3.150	7.459	3.150	7.459	3.150	7.459	3.150	8.295	3.150	8.295
Na ₂ O	0.410	0.962	0.410	0.962	0.410	0.962	0.410	0.723	0.410	0.723
sum	100	100	100	100	100	100	100	100	100	100

Table S1. (continue) Initial bulk composition of the two assemblages and proportion factor f .

bulk comp.	(A_0)	(B_0)	(A_0)	(B_0)	(A_0)	(B_0)
oxides (g or wt%)	41($f=20$)		42($f=100$)		43($f=500$)	
SiO ₂	45.200	45.804	45.200	45.804	45.200	45.804
TiO ₂	0.200	0.281	0.200	0.281	0.200	0.281
Al ₂ O ₃	3.940	18.319	3.940	18.319	3.940	18.319
Fe ₂ O ₃	0.200	0.246	0.200	0.246	0.200	0.246
Cr ₂ O ₃	0.400	0.015	0.400	0.015	0.400	0.015
FeO	8.100	7.482	8.100	7.482	8.100	7.482
MgO	38.400	18.834	38.400	18.834	38.400	18.834
CaO	3.150	8.295	3.150	8.295	3.150	8.295
Na ₂ O	0.410	0.723	0.410	0.723	0.410	0.723
sum	100	100	100	100	100	100