FC-AFC-FCA and mixing modeler: a Microsoft® Excel© spreadsheet program for modeling geochemical differentiation of magma by crystal fractionation, crustal assimilation and mixing

by

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1. The goal of the study

Several petrological processes modifying the geochemical composition of the magma are graphically programmed using Microsoft® Excel© spreadsheet on the basis of differentiation equations.

The ***FC-AFC-FCA and mixing modeler*** is a spreadsheet program that models the consequent theoretical vectors of

- **Fractional crystallisation (FC)**
- **Combined fractional crystallisation and assimilation (AFC)**
- **Decoupled fractional crystallisation and assimilation (FCA)**
- **Mixing (Mix)**

2. Introduction

Magmatic rocks are differentiated by

* different degrees of enrichment processes in the source
* different degrees of melting of the source rocks
* crystal fractionation in magma chambers
* contamination of the magma via assimilation of the wall-rocks
* mixing of magmas of different compositions

may occur as combined (AFC) *or*

may occur as decoupled (FCA)

3. Modeling the Magmatic Processes

1. CRYSTALLISATION of MAGMAS

a. Equilibrium Crystallisation

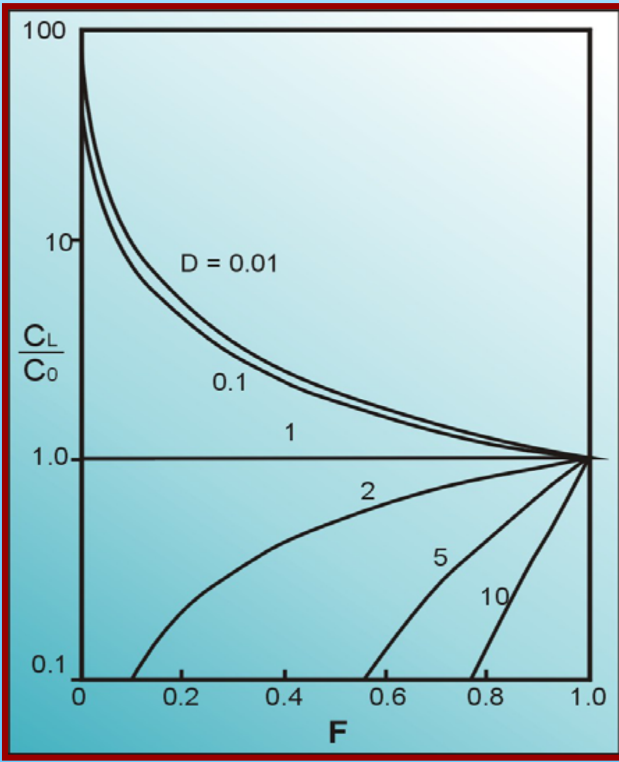
solid phases remain in the melt and stays in chemical equilibrium with the liquid phase

$$C_l^{EC} = C_0/[F + D(1 - F)]$$

b. Fractional Crystallisation

solid phases fractionate from melt
the new composition of the melt remaining:

$$C_l^{FC} = C_0 F^{(D-1)}$$



3. Modeling the Magmatic Processes

2. COMBINED FRACTIONAL CRYSTALLIZATION AND ASSIMLATION (DePaolo 1981)

During the AFC process there is a strict relationship between the amount of material assimilated and the amount of material crystallized during cooling of the magma.

for elements

$$C_l^{AFC} = C_0[F^{-z} + (\frac{r}{r-1})\frac{C_a}{zC_0}(1-F^{-z})]$$

for isotopes

$$IC_l^{AFC} = \frac{(\frac{r}{r-1})(\frac{C_a}{z})(1-F^{-z})Ic_a + C_0F^{-z}Ic_0}{(\frac{r}{r-1})(\frac{C_a}{z})(1-F^{-z}) + C_0F^{-z}}$$

$$r = \frac{m_a}{m_c}$$

$$z = \frac{r+D-1}{r-1}$$

C_l^{AFC} Ic_l^{AFC} concentration of an element and ratio of an isotope in the resulting magma

C_0 Ic_0 concentration of an element and ratio of an isotope in the original magma

C_a Ic_a concentration of an element and ratio of an isotope in the assimilant

m_a amount of assimilated material

m_c amount of crystallized material

D bulk partition coefficient

F fraction of melt remaining

3. Modeling the Magmatic Processes

3. DECOUPLED FRACTIONAL CRYSTALLIZATION AND ASSIMLATION (Cribb & Barton 1996)

Assimilation and fractional crystallization in a magma system are not strictly related; the mass assimilated may be decoupled from mass crystallized, and therefore varies independently.

$$C_l^{FCA} = \frac{C_0 R M_c + C_f (1 - M_c)}{F}$$

C_l^{FCA} concentration of an element in the resulting magma

C_0 concentration of an element in the original magma

C_f concentration of an element resulting from fractional crystallization

M_c amount of crystallized material

F fraction of melt remaining

3. Modeling the Magmatic Processes

4. Mixing Process (e.g., Powell 1984)

Trace element and isotope composition of a magma resulted from mixing of magmas *a* and *b*:

$$C_m = X(C_a - C_b) + C_b$$

$$Ic_m = Ic_a\left(\frac{C_a X}{C_m}\right) + Ic_b\left(\frac{C_b(1-X)}{C_m}\right)$$

4. Other parameters in the program

$$Eu/Eu^* = Eu_N / \sqrt{(Sm_N)\times(Gd_N)}$$

$$Mg\# = MgO/(MgO + FeO_t)$$

$$\varepsilon Sr = \frac{({}^{87}Sr/{}^{86}Sr)_{sample} - ({}^{87}Sr/{}^{86}Sr)_{chondrite}}{({}^{87}Sr/{}^{86}Sr)_{chondrite}} \times 10^4$$

$$\varepsilon Nd = \frac{({}^{143}Nd/{}^{144}Nd)_{sample} - ({}^{143}Nd/{}^{144}Nd)_{chondrite}}{({}^{143}Nd/{}^{144}Nd)_{chondrite}} \times 10^4$$

$$\tau_{DM}^{Nd} = \frac{1}{\lambda} \times \ln\left(\frac{({}^{143}Nd/{}^{144}Nd)_{sample} - ({}^{143}Nd/{}^{144}Nd)_{DM}}{({}^{147}Sm/{}^{144}Nd)_{sample} - ({}^{147}Sm/{}^{144}Nd)_{DM}} + 1\right.$$

5. Structure of the Program

A. Data input section
B. Data output section

The data input section contains two sheets:

(1) **parameters** *and*

(2) **samples**

The output section is consist of

(1) **modeling**

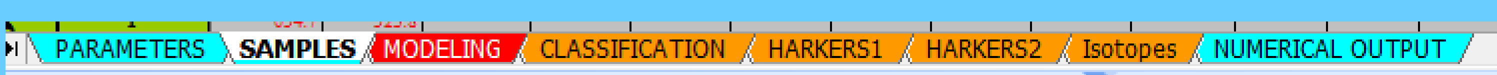
(2) **classification**

(3) **Harker1** (for major elements)

(4) **Harker2** (for trace elements)

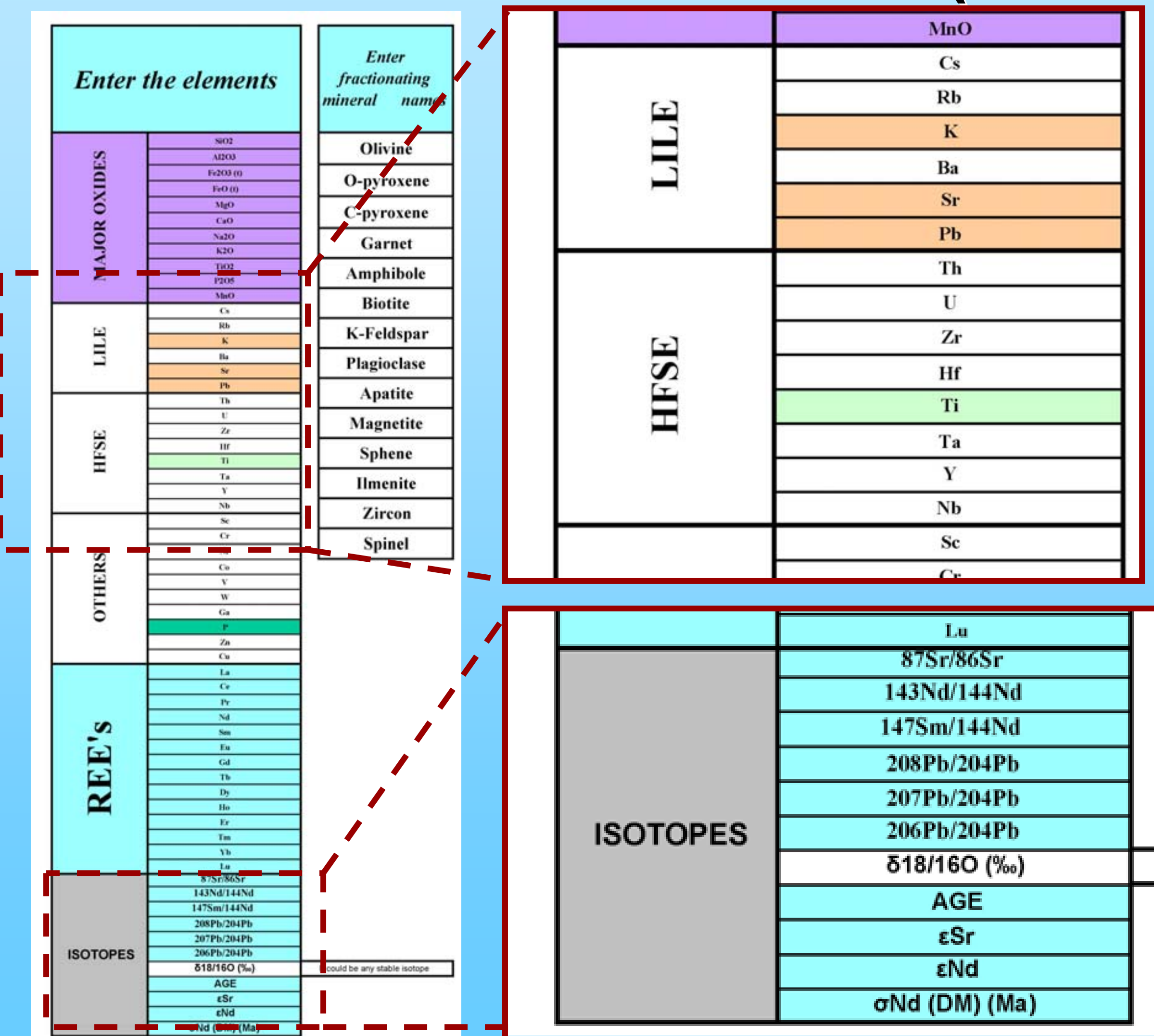
(5) **isotopes**, *and*

(6) **numerical output**



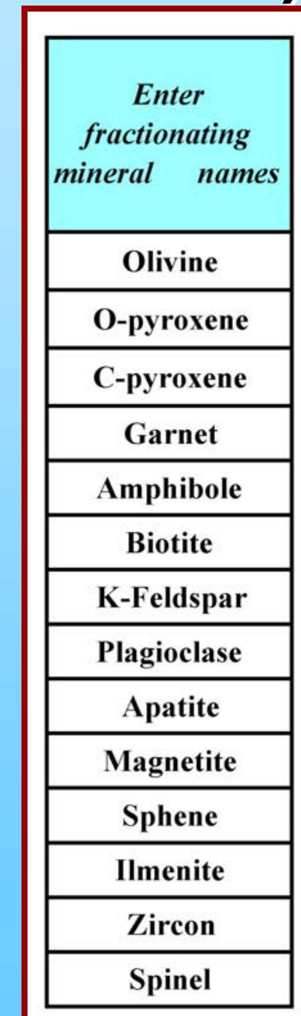
5. Structure of the Program

1. PARAMETERS SHEET (elements and minerals)



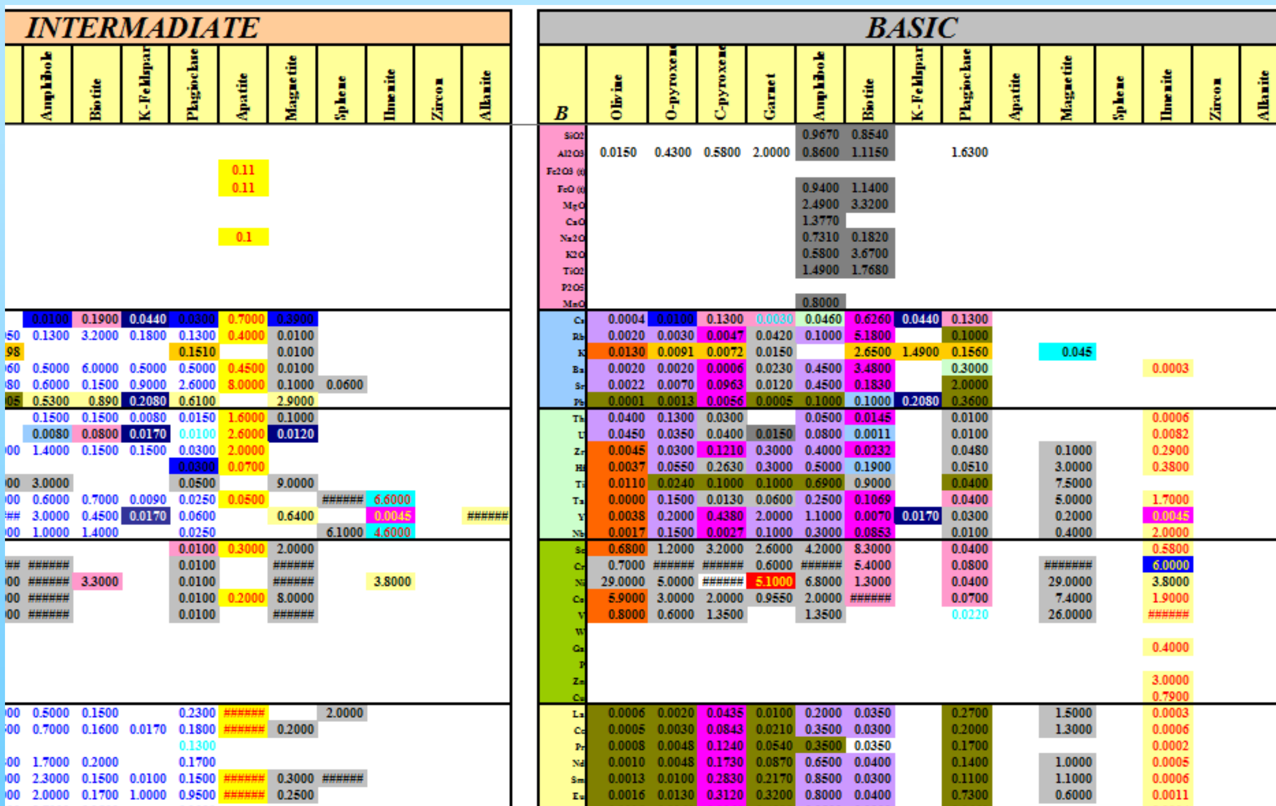
The user can change only uncolored cells

The cangings are simultaneously reflected to the other sheets



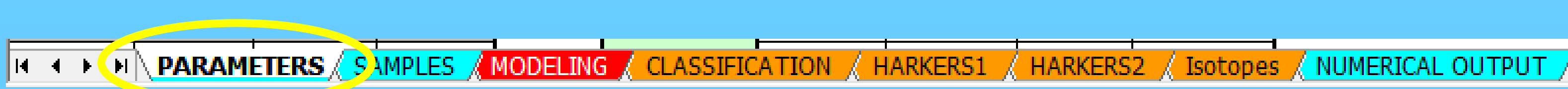
5. Structure of the Program

1. PARAMETERS SHEET (partition coefficients)



The partition coefficients for eny element and any mineral are entered to these tables.

The partition coefficient tables have been prepared for “acid”, intermediate” and “basic” melt compositions.



5. Structure of the Program

1. PARAMETERS SHEET (assimilants)

ASSIMILANTS (Ca)							
	Upper Continental Crust (Taylor & McLennan 1995)	Bulk Continental Crust (Taylor & McLennan 1995)	Lower Continental Crust (Taylor & McLennan 1995)	Rahmanlar	Menderes Massif Gneisses	UC (Cribb Barton)	Upper Continental Crust (Hart et al. 1999)
SiO2			58.94	71.4625	70.03	66.22	45.8
Al2O3			14.95	13.4375	15.23	14.99	15.53
Fe2O3 (t)			8.05	2.41	2.47	4.62	
FeO (t)							**9.02**
MgO			5.15	0.24	0.9	2.33	6.66
CaO			7.4	0.955	1.95	4.05	12.88
Na2O			2.48	2.9425	2.59	3.34	2.07
K2O			1.97	4.63	3.32	3.44	0.56
TiO2			0.17	0.3625	0.4	0.2	1.12
P2O5			0.76	0.2075	0.19	0.71	0.11
MnO			0.15	0.0375	0.02	0.1	0.17
LOI				3	2.1		
Mg#							
Cs	3.700	1.000	0.100	6.275	3.800		0.173
Rb	112.000	32.000	5.300	158.075	115.500	110.000	9.040
K			16353.561	38435.019	27560.316	28556.472	4648.728
Ba	550.000	250.000	150.000	1007.050	649.500	700.000	16.850
Sr	350.000	260.000	230.000	150.000	158.800	350.000	117.500
Pb	20.000	8.000	4.000	20.000	27.700	20.000	0.690
Th	10.700	3.500	1.060	14.550	13.900	10.500	0.072
U	2.800	0.910	0.280	5.450	2.100	2.800	0.321
Zr	190.000	100.000	70.000	277.700	184.700	240.000	67.000
Hf	5.800	3.000	2.100	8.875	4.900	5.800	
Ti			1013.030	2160.138	2383.600	1191.800	6674.080
Ta	2.200	1.000	0.600	1.375	0.600	2.200	
Y	22.000	20.000	19.000	59.500	36.900	22.000	32.000

PARAMETERS | SAMPLES | MODELING | CLASSIFICATION | HARKERS1 | HARKERS2 | Isotopes | NUMERICAL OUTPUT

Several assimilant factors can be entered by the user to this table. Upper, bulk and lower continental crust values of Taylor and McLennan (1995) have already been entered to the program. These parameters also changed by the users.

These factors, later can be selected in order to model the AFC, FCA and mixing processes.

5. Structure of the Program

1. PARAMETERS SHEET (normalizing factors)

NORMALIZING VALUES				
	E-MORB (Sun & McDonough 1989)	N-MORB (Sun & McDonough 1989)	PM (Sun & McDonough 1989)	C1-chondrite (Sun & McDonough 1989)
SiO2				
Al2O3				
Fe2O3 (t)				
FeO (t)				
MgO				
CaO				
Na2O				
K2O				
TiO2				
P2O5				
MnO				
LOI				
Mg#				
Cs	0.063	0.007	0.032	0.188
Rb	5.010	0.560	0.635	2.320
K	2100.000	600.000	250.000	545.000
Ba	57.000	6.300	6.989	2.410
Sr	156.000	90.000	21.100	7.260
Pb				
Th	0.600	0.120	0.085	0.029
U	0.180	0.047	0.021	0.008
Zr	73.000	74.000	11.200	3.870
Hf				
Ti	6000.000	7600.000	1300.000	445.000
Ta				
Y	22.000	28.000	4.550	1.570

Several normalizing factors can be entered by the user to this table. E-MORB, N-MORB, PM and C1-chondritic values of Sun and McDonough (1989) have already been entered to the program. These parameters also changed by the users.

These factors, later can be selected in order to plot normalized REE and multy-element diagrams.

PARAMETERS | SAMPLES | MODELING | CLASSIFICATION | HARKERS1 | HARKERS2 | Isotopes | NUMERICAL OUTPUT

5. Structure of the Program,

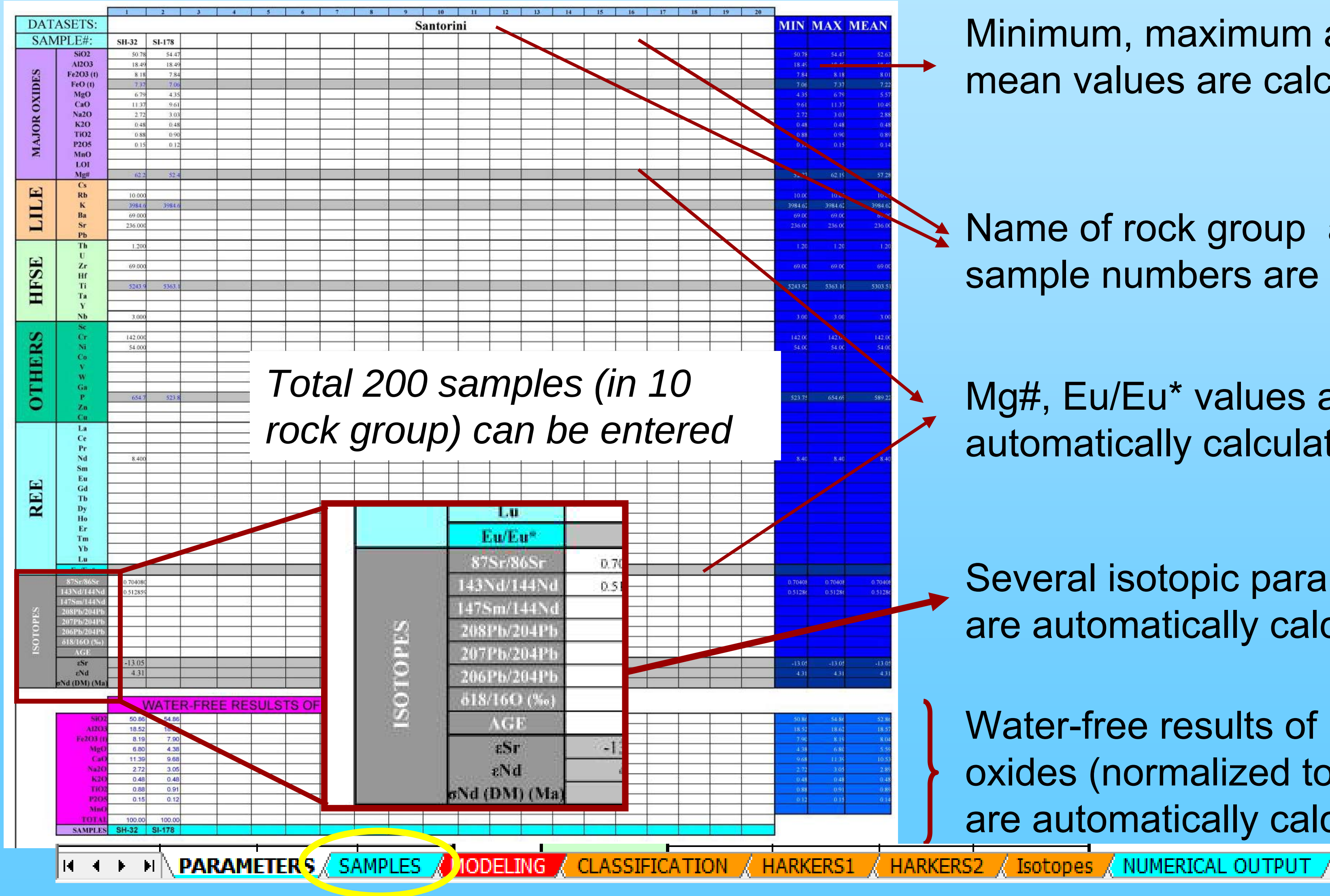
1. PARAMETERS SHEET (isotope values)

Isotope ratios	Value	Type
(87Sr/86Sr) standard (for εSr)	0.705000	chondrite
(143Nd/144Nd) standard (for εNd)	0.512638	chondrite
(143Nd/144Nd) standard (for PM model age)	0.513150	PM
(143Sm/144Sm) standard (for PM model age)	0.213700	PM

These values, which will be used to calculate several parameters on the “sample” sheet, can also be changed by the users

5. Structure of the Program

2. "SAMPLES" SHEET (1 of 10 sample tables)



Total 200 samples (in 10 rock group) can be entered

Minimum, maximum and mean values are calculated

Name of rock group and sample numbers are entered

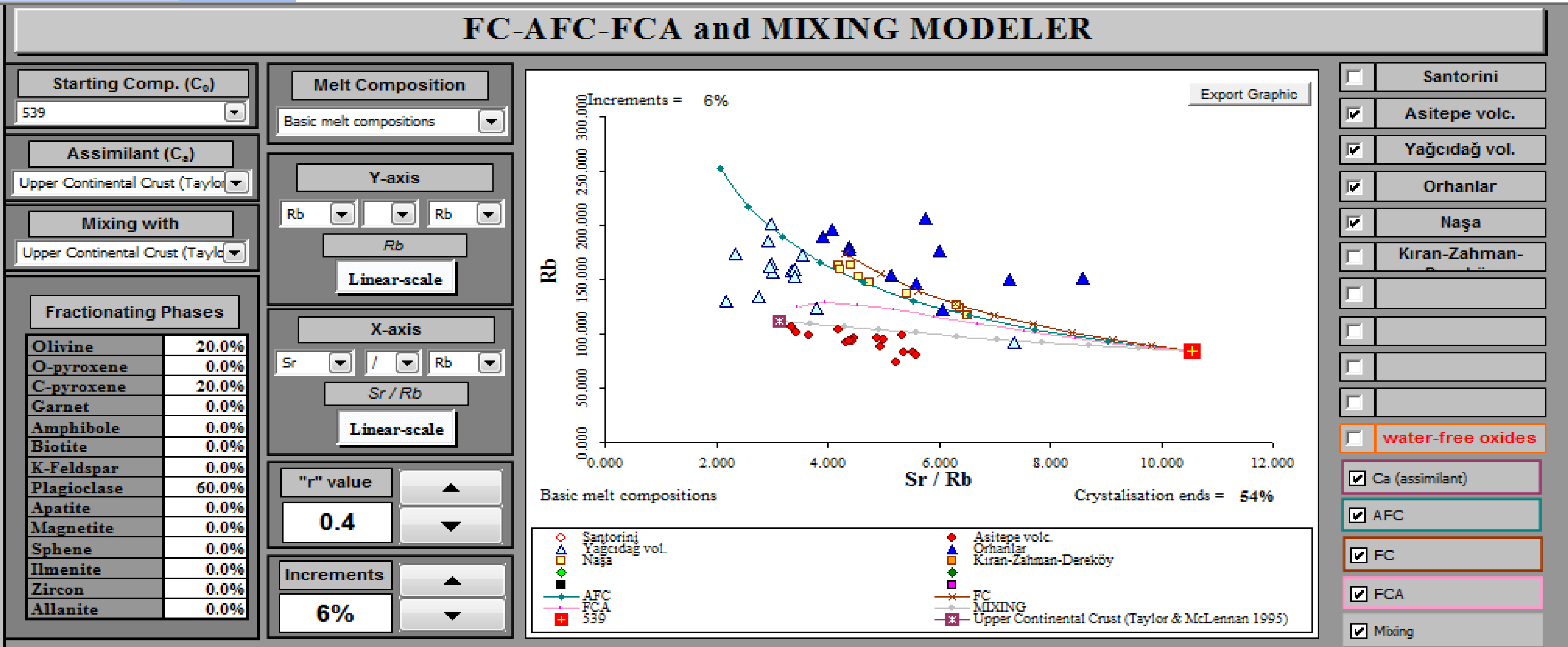
Mg#, Eu/Eu* values are automatically calculated

Several isotopic parameters are automatically calculated

Water-free results of major oxides (normalized to 100) are are automatically calculated

5. Structure of the Program

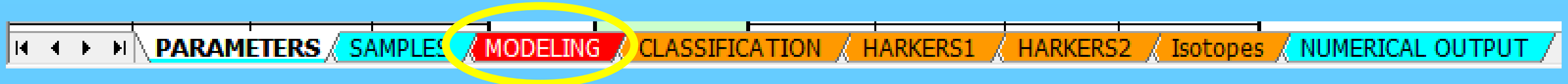
3. “MODELING” SHEET (upper section)



A bivarite diagram can be constructed.

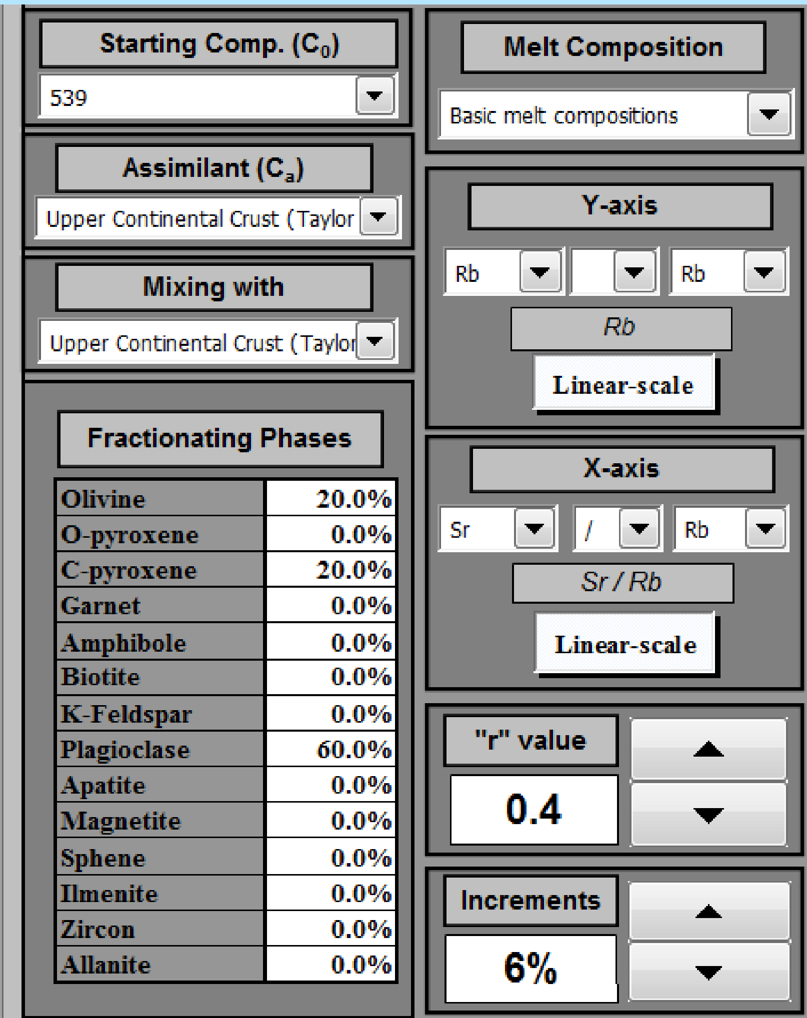
The parameters that can be changed are:

starting composition, assimilant material, the material mixing with the starting composition, fractionating phase, melt composition, “*r*” value for AFC and FCA models, increments for model curves and axes of the bivariate diagram



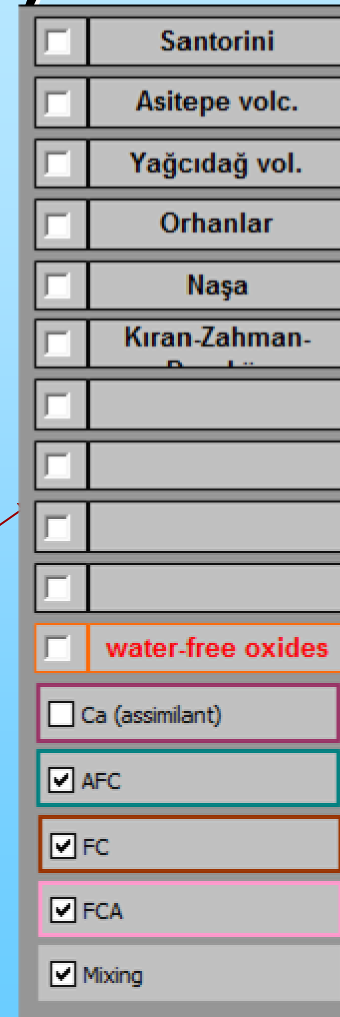
5. Structure of the Program

3. “MODELING” SHEET (upper section)



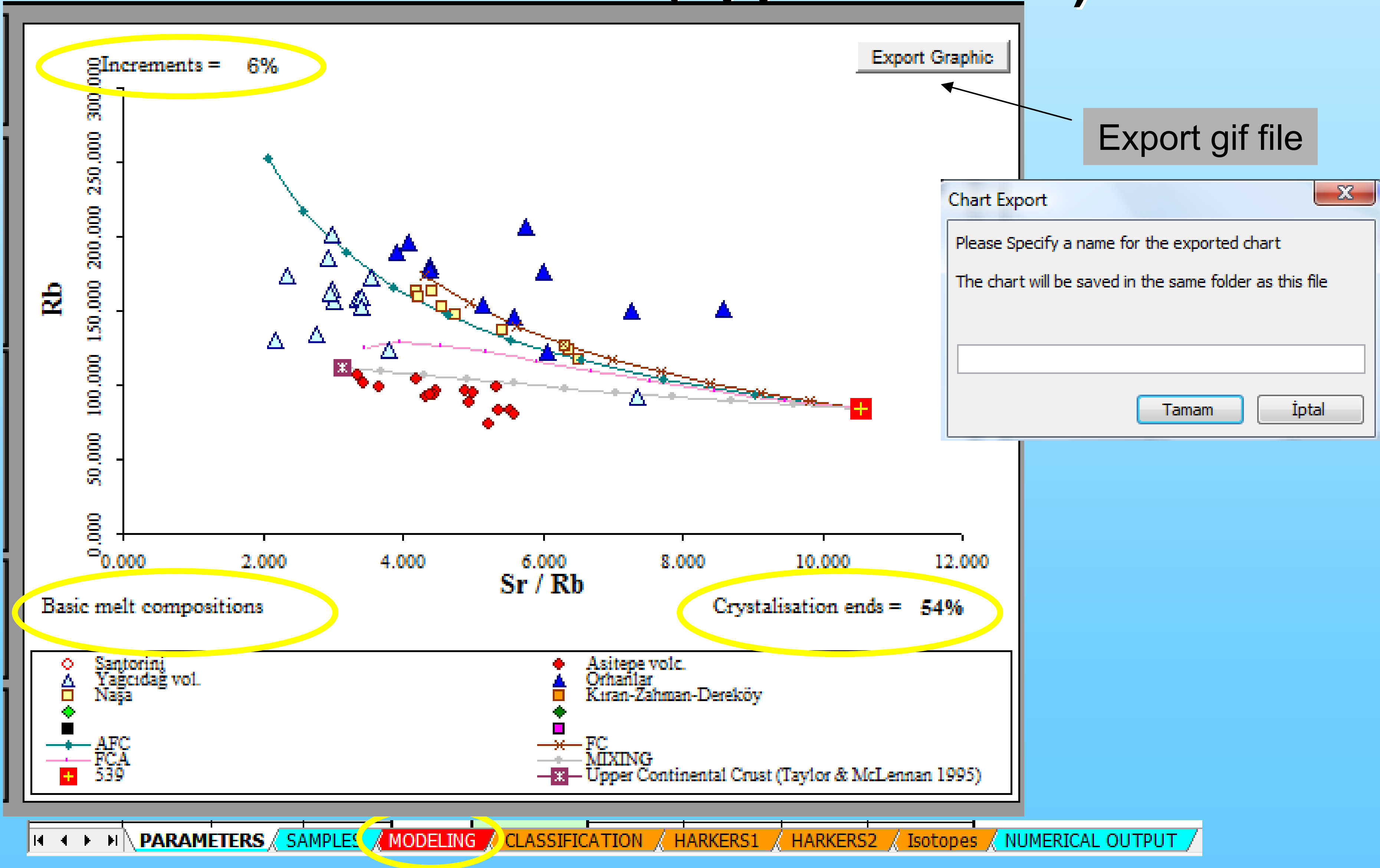
The parameters to models on the bivarite diagram

To show on the diagram these can be selected



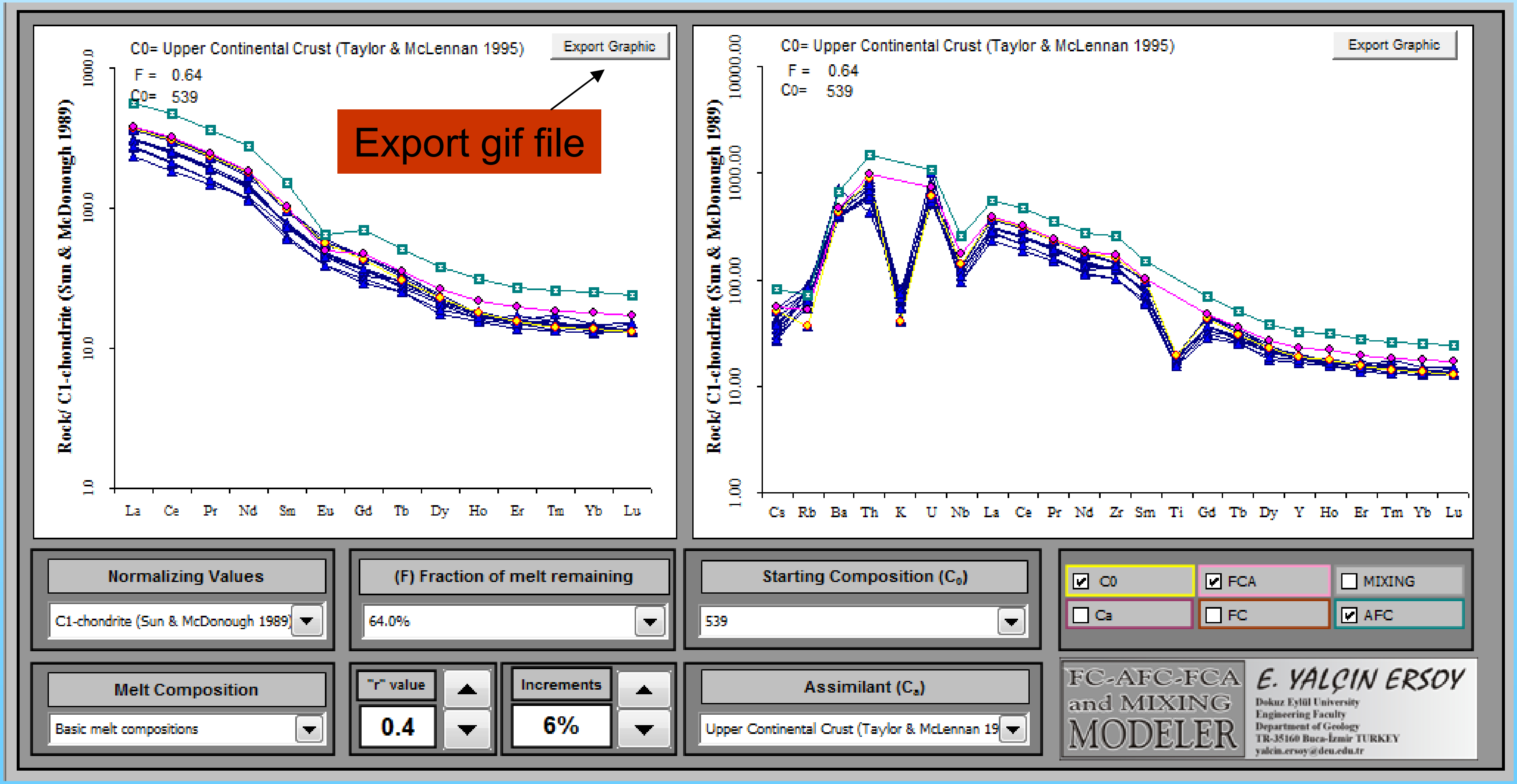
5. Structure of the Program

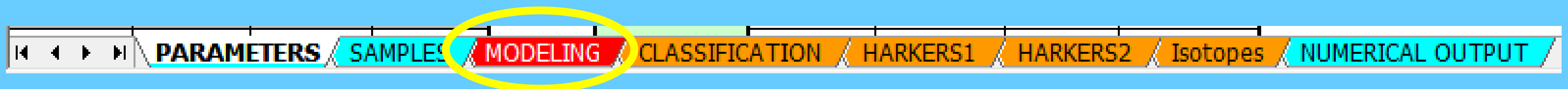
3. "MODELING" SHEET (upper section)



5. Structure of the Program

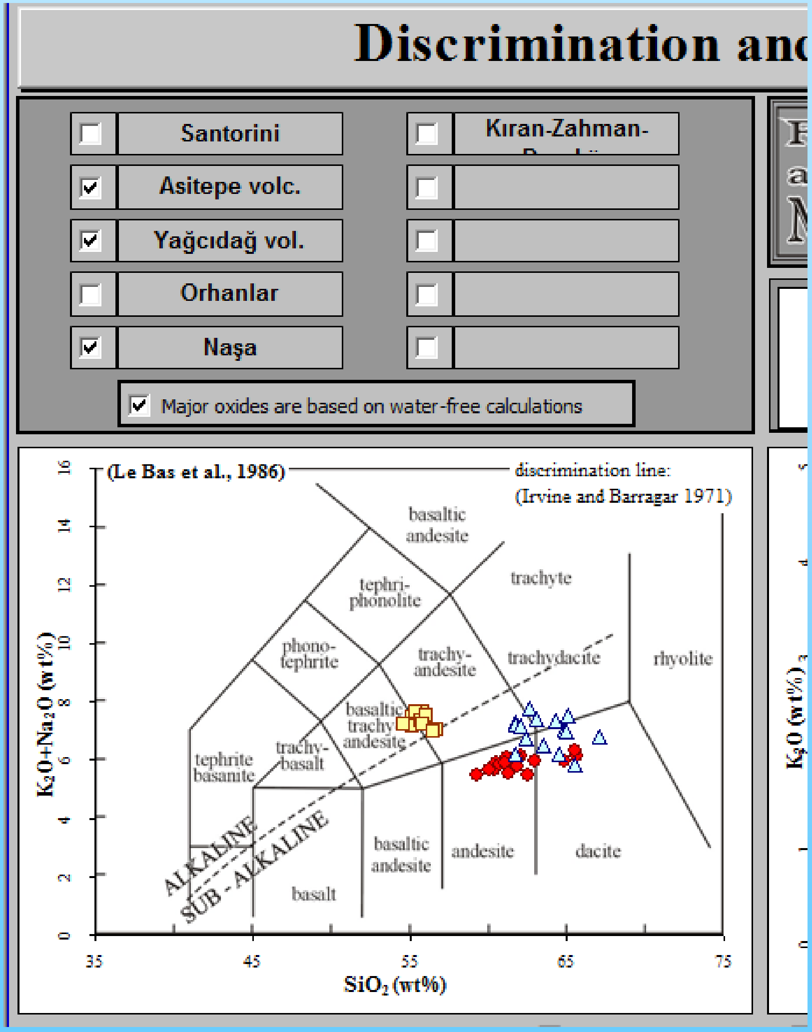
3. “MODELING” SHEET (lower section)





5. Structure of the Program

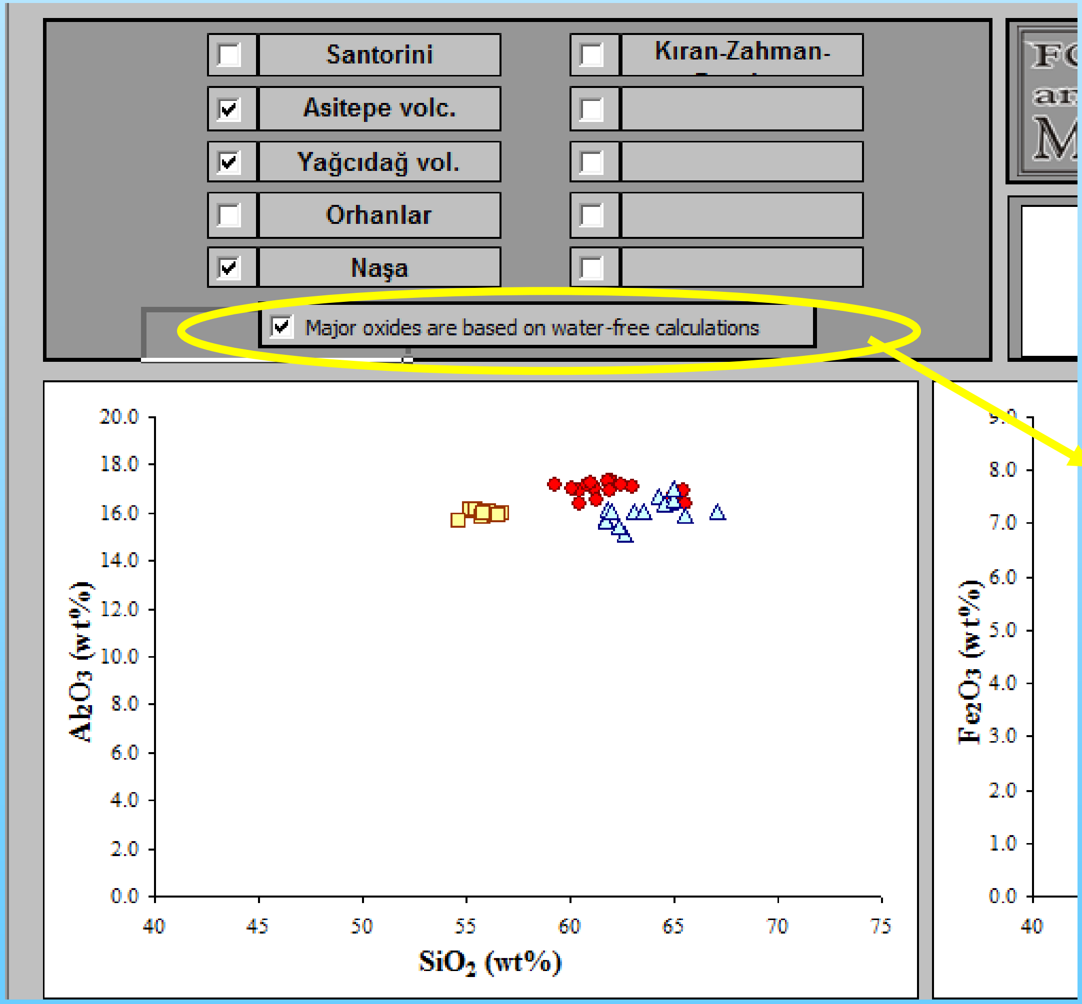
4. "CLASSIFICATION" SHEET (lower section)



* TAS diagram of LeBas et al (1986) with alkaline-subalkaline discrimination of Irvine and Baragar (1971)
* K2O-SiO2 diagram of LeMaitre (2002)
* TAS diagram of Cox et al (1978)
* K2O-Na2O diagram of Peccerillo and Taylor (1976)
* Th/Yb – Ta/Yb diagram of Pearce (1983)
* Sr/Y–Sr diagram of Castillo (2006)

5. Structure of the Program

5. “HARKERs” SHEET

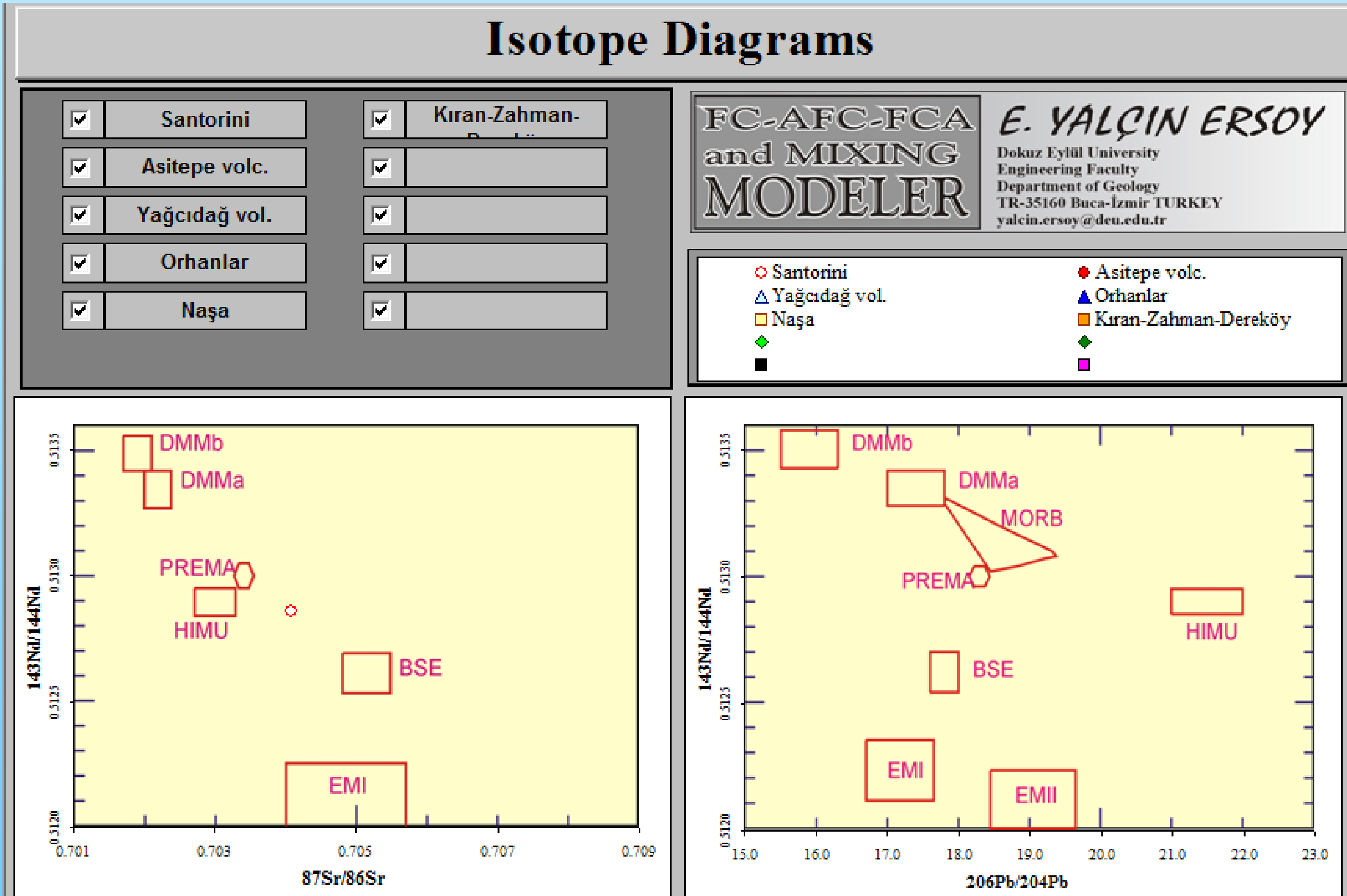


Major and trace elements canbe plotted on SiO2-dependet Harker variation diagrams.

Major elements can also be plotted on the basis of water-free contents

5. Structure of the Program

6. “ISOTOPES” SHEET



Four isotope diagrams can be plotted on this sheet.

5. Structure of the Program

7. “NUMERICAL OUTPUT” SHEET

	AFC RESULTS									
r=	0.40	F (fraction of melt remaining)								
	0.00%	6.0%	12.0%	18.0%	24.0%	30.0%	36.0%	42.0%	48.0%	54.0%
SiO2	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK
Al2O3	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK
Fe2O3 (t)	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK
FeO (t)	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK
MgO	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK
CaO	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK
Na2O	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK
K2O	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK
TiO2	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK
P2O5	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK
MnO	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK
Cs	9.60	10.26	11.00	11.84	12.80	13.91	15.21	16.76	18.62	20.93
Rb	84.00	93.55	104.33	116.60	130.70	147.09	166.38	189.44	217.52	252.51
K	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK
Ba	1023.60	1092.04	1168.32	1254.00	1351.03	1462.02	1590.46	1741.14	1920.88	2139.72
Sr	886.90	845.98	805.15	764.40	723.76	683.22	642.79	602.49	562.33	522.32
Pb	2.10	3.03	4.05	5.20	6.50	7.98	9.68	11.66	14.01	16.85
Th	25.40	27.42	29.71	32.33	35.36	38.89	43.08	48.12	54.30	62.06
U	4.90	5.32	5.79	6.34	6.97	7.70	8.57	9.61	10.89	12.49
Zr	610.10	653.51	702.55	758.43	822.70	897.46	985.56	1090.98	1219.53	1379.92
Hf	15.80	16.91	18.16	19.58	21.20	23.09	25.30	27.93	31.12	35.08
Ti	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK	#YOK
Ta	2.10	2.32	2.57	2.86	3.19	3.58	4.03	4.58	5.26	6.10
Y	29.10	31.55	34.30	37.42	40.99	45.10	49.92	55.63	62.54	71.07
Nb	34.70	37.95	41.65	45.88	50.77	56.50	63.29	71.48	81.55	94.23
Sc	26.00	25.92	25.83	25.74	25.65	25.55	25.45	25.34	25.22	25.09
Cr	554.24	287.87	143.74	68.93	31.91	14.57	6.96	3.86	2.71	2.33
Ni	218.80	96.21	40.41	16.32	6.55	2.84	1.55	1.15	1.03	1.00

PARAMETERS / SAMPLES / MODELING / CLASSIFICATION / HARKERS1 / HARKERS2 / Isotopes / NUMERICAL OUTPUT

Numerical results for AFC, FC, FCA and Mixing modelings can be taken İnto tables from this sheet.

6. RESULTS

*** The FC-AFC-FCA and mixing modeler program is a Microsoft® Excel© spreadsheet program designed on the basis of already proposed magmatic differentiation equations for crystal fractionation, assimilation and mixing processes in magmatic systems.**

*** The results of geochemical analyses of magmatic rocks can easily be transferred to the program.**

*** The program also has the advantage that the user can output the graphical and/or numerical results of FC, AFC, FCA and mixing processes in addition to several geochemical parameters.**

*** The program allows the users to change the several parameters and to see the different modeling results on the same diagram.**

*** The graphical results of any modeling can be exported and saved as a GIF file.**

*** The numerical results can also be taken into tables.**

The program will be available at:
Computers and Geosciences, Elsevier **(***accepted to be published***)**

Acknowledgements

Ercan Aldanmaz and Mehmet Keskin are thanked for their help and comments during preparing the program