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

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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<sup>®</sup> Excel<sup>©</sup> 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 wallrocks
- \* mixing of magmas of different compositions
  - may occur as combined (AFC) or
  - may occur as decoupled (FCA)

### **1. CRYSTALLISATION of MAGMAS**

#### a. Equilibrium Crystallisation

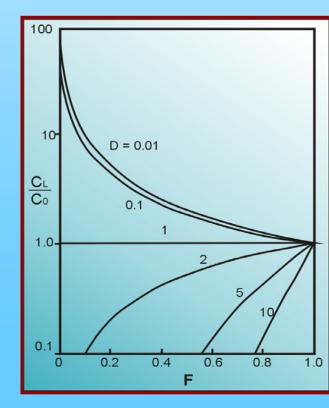
solid phases remain in the melt and stays in chemical equilibrium with the liquid phase

$$C_{l}^{EC} = C_{0}/[F + D(1-F)]$$

#### b. Fractional Crystallisation

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

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



# 2. COMBINED FRACTIONAL CRYSTALLIZATIONAND 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  $IC_{l}^{AFC} = \frac{(\frac{r}{r-1})(\frac{C_{a}}{z})(1-F^{-z})Ic_{a} + C_{0}F^{-z}Ic_{0}}{(\frac{r}{r-1})(\frac{C_{a}}{z})(1-F^{-z}) + C_{0}F^{-z}}$ 

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

- $Ic_0$  concentration of an element and ratio of an isotope in the original magma
  - concentration of an element and ratio of an isotope in the assimilant
- $m_{\rm a}$  amount of assimilated material
- $m_{\rm c}$  amount of crystallized material
- *D* bulk partition coefficient

Ic.

 $C_0 \\ C_a$ 

*F* fraction of melt remaining

# 3. DECOUPLED FRACTIONAL CRYSTALLIZATIONAND 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.

$$C_{l}^{FCA} = \frac{C_{0}RM_{c} + C_{f}(1 - M_{c})}{F}$$

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

 $C_0$  concentration of an element in the original magma

- $C_{\rm f}$  concentration of an element resulting from fractional crystallization
- $M_{
  m c}$  amount of crystallized material
- *F* fraction of melt remaining

(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

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

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

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

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

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

#### A.Data input section B.Data output section

The data input section contains two sheets:

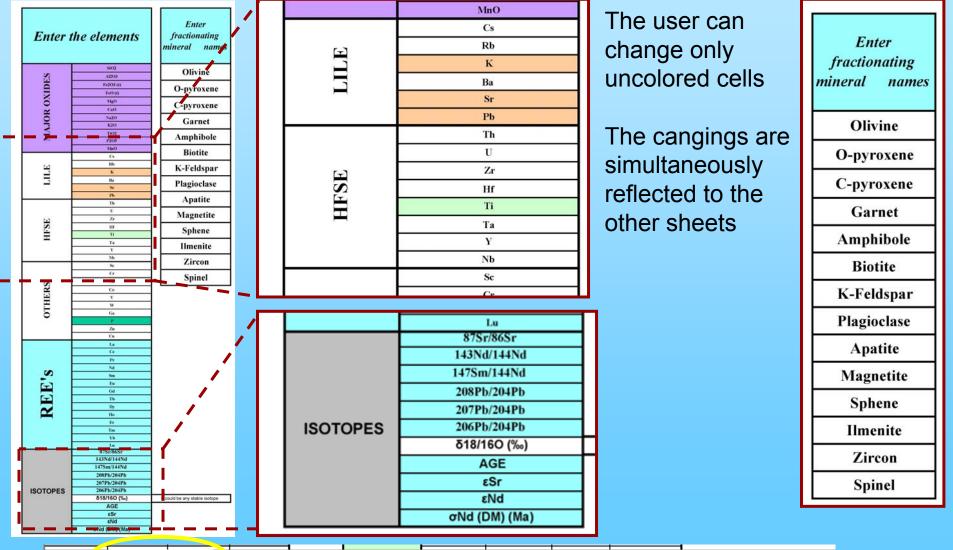
- (1) parameters and
- (2) samples

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

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

#### 1. PARAMETERS SHEET (elements and minerals)



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### 1. PARAMETERS SHEET (partition coefficients)

INTERMADIATE	BASIC			
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Amphilode Biotite Biotite Plagioclauc Apatite Spleae Spleae Zircon Albaite	R Olibriae O-pyroxea C-pyroxea Garaet Biotite Biotite Biotite Magnetite Magnetite Ilmenite Splene	Allanite		
	sic2 0.9670 0.8540			
0.11	A1203 0.0150 0.4300 0.5800 2.0000 0.8600 1.1150 1.6300			
0.11	F=0 m 0.9400 1.1400 Mg0 2.4900 3.3200			
	C10 1.3770			
0.1	Na10 0.7310 0.1820 820 0.5800 3.6700			
	TV02 1.4900 1.7680			
	P205 Ma0 0.8000			
0.0100 0.1900 0.0440 0.0300 0.7000 0.3900 50 0.1300 3.2000 0.1800 0.1300 0.4000 0.0100	c, 0.0004 0.0100 0.1300 0.0020 0.0460 0.6260 0.0440 0.1300 25 0.0020 0.0030 0.0047 0.0420 0.1000 5.1800 0.1000			
98 0.1510 0.0100	x 0.0130 0.0091 0.0072 0.0150 2.6500 1.4900 0.1560 0.045			
60 0.5000 6.0000 0.5000 0.5000 0.4500 0.0100 80 0.6000 0.1500 0.9000 2.6000 8.0000 0.1000 0.0600	B2         0.0020         0.0006         0.0230         0.4500         3.4800         0.3000         0.0003           sr         0.0022         0.0070         0.0963         0.120         0.4500         0.1830         2.0000         0.0003			
05 0.5300 0.890 0.2080 0.6100 2.9000 0.1500 0.1500 0.0080 0.0150 1.6000 0.1000	рь 0.0001 0.0013 0.0056 0.0005 0.1000 0.1000 0.2080 0.3600 ть 0.0400 0.1300 0.0300 0.0500 0.0145 0.0100 0.0006			
0.0080 0.0800 0.0170 0.0100 2.6000 0.0120	t 0.0450 0.0350 0.0400 0.0150 0.0800 0.0011 0.0100 0.0082			
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0.0100 0.3000 2.0000 ## ###### 0.0100 ######	s= 0.6800 1.2000 3.2000 2.6000 4.2000 8.3000 0.0400 0.5800 cr 0.7000 ###### ###### 0.6000 ###### 5.4000 0.0800 ######## 6.0000			
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	z. 3.0000 c. 0.7900			
00 0.5000 0.1500 0.2300 ###### 2.0000	Ls 0.0006 0.0020 0.0435 0.0100 0.2000 0.0350 0.2700 1.5000 0.0003			
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00 2,7000 0,1500 0,1300	CI 0.0015 0.0160 0.3360 0.4980 0.9500 0.0300 0.0660 0.0034			

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.

M 🔹 🕨 PARAMETERS / SAMPLES / MODELING / CLASSIFICATION / HARKERS1 / HARKERS2 / Isotopes / NUMERICAL OUTPUT /

#### 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 Continenta l Crust (Hart et al. 1999)		
SiO2			58.94	71.4625	70.03	66.22	45.8		
AI2O3			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		
K20			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		
РЬ	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		
н	5.800	3.000	2.100	8.875	4.900	5,800			
п			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		

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.

MODELING 🔏 CLASSIFICATION 🦼 HARKERS1 🔏 HARKER

Isotopes / NUMERICAL OUTPUT

### 1. PARAMETERS SHEET (normalizing factors)

NORMALIZING VALUES								
	E-MORB N-MORB (sun & Cun & PM (sun & McDonough 1989) 1989) 1989		C1-chondrite (Sun & McDonough 1989)					
SiO2								
Al2O3								
Fe2O3 (t)								
FeO (t)								
MgO				2				
CaO								
Na2O								
K2O				23				
TiO2								
P2O5								
MnO								
LOI								
Mg#				(z				
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 Sr	57.000 156.000	6.300 90.000	6.989 21.100	2.410 7.260				
Sr Pb	150.000	90.000	21.100	7.200				
Th	0.600	0.120	0.085	0.029				
U	0.180	0.047	0.003	0.029				
Zr	1007.001	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 multyelement diagrams.

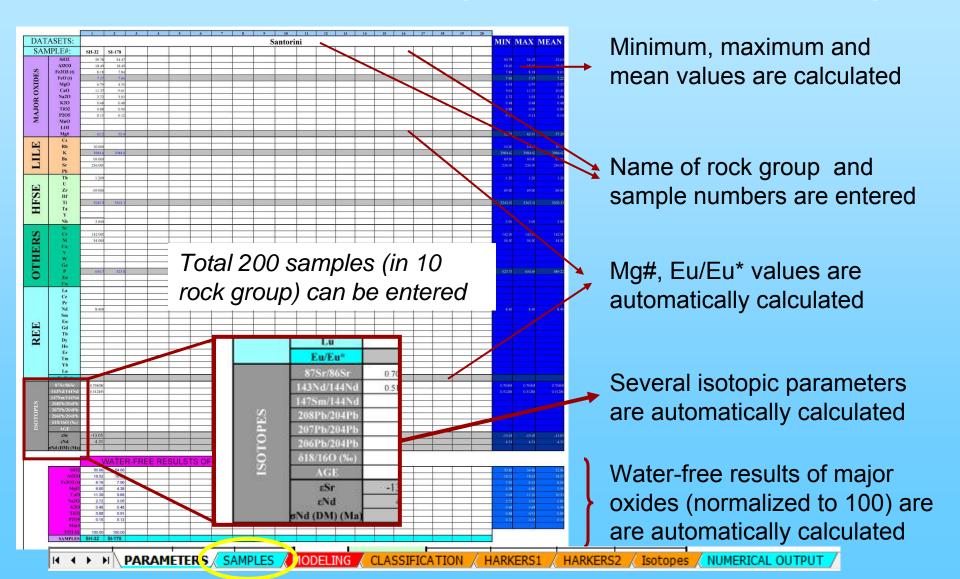
H A F N PARAMETERS SAMPLES MODELING CLASSIFICATION HARKERS1 HARKERS2 Isotopes NUMERICAL OUTPUT

#### 1. PARAMETERS SHEET (isotope values)

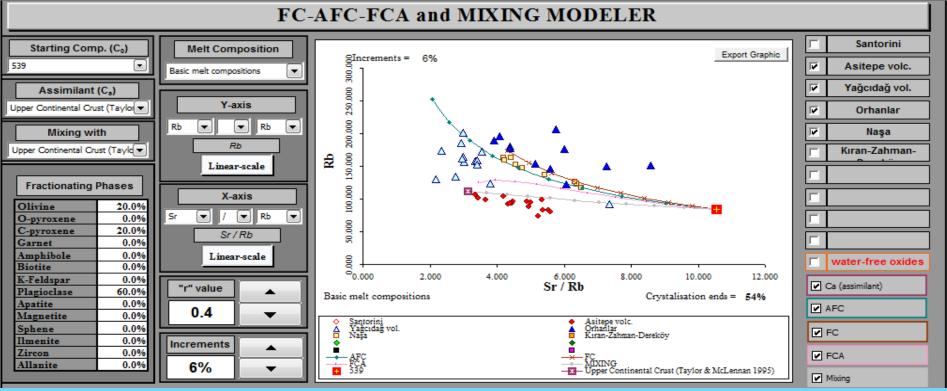
Isotope ratios	Value	Туре
(87Sr/86Sr) standard (for εSr)	0.705000	chondrite
(143Nd/144Nd) standard (for εNd)	0.512638	chondrite
(143Nd/144Nd) standard (for PM model age)	0.513150	РМ
(143Sm/144Sm) standard (for PM model age)	0.213700	РМ

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

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



### 3. "MODELING" SHEET (upper section)



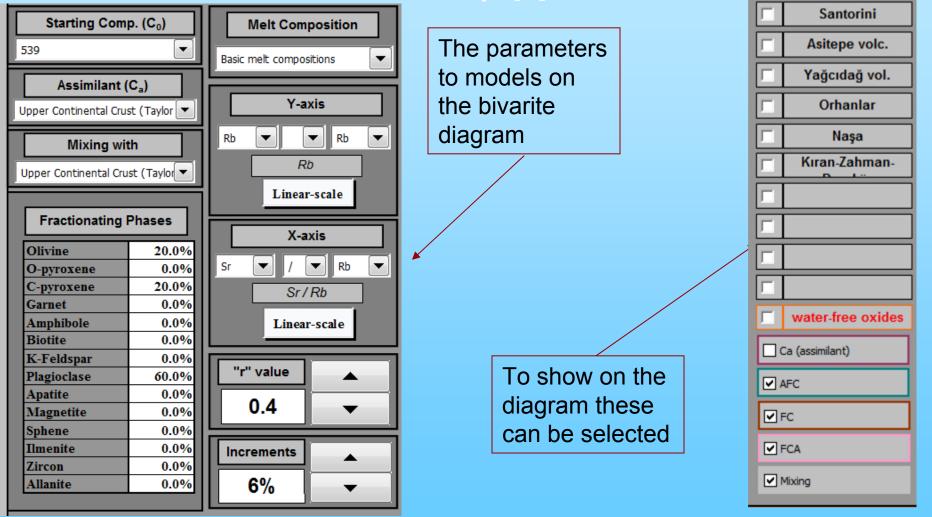
A bivarite diagram can be constructed.

#### 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

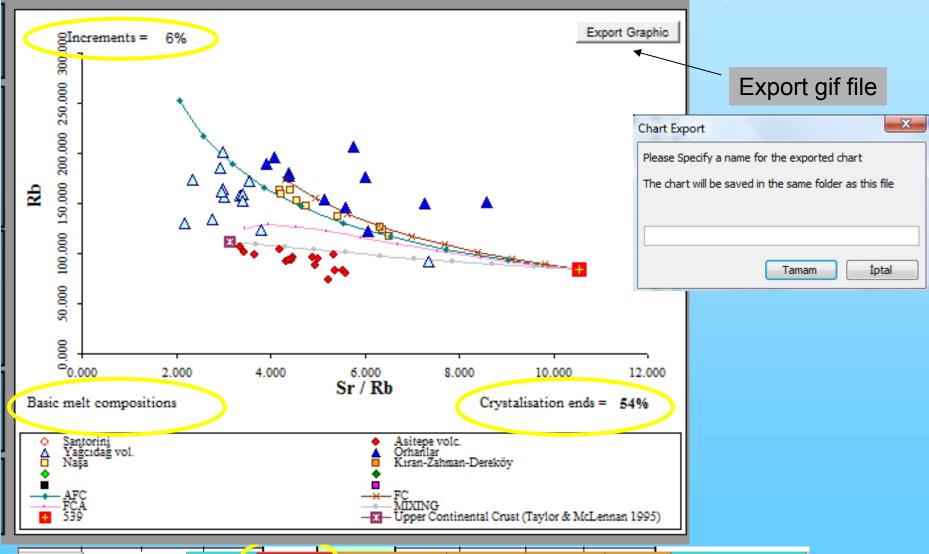
H + + H PARAMETERS SAMPLES MODELING CLASSIFICATION / HARKERS1 / HARKERS2 / Isotopes NUMERICAL OUTPUT

#### 3. "MODELING" SHEET (upper section)



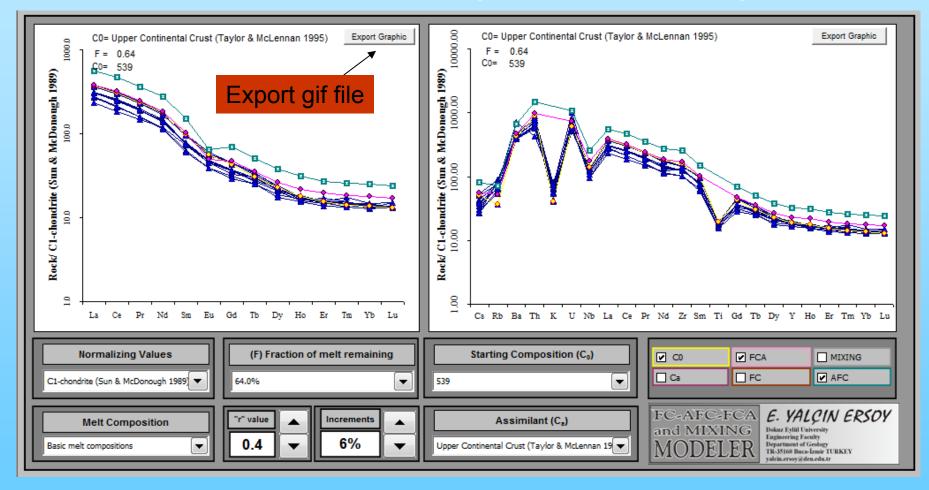
H + + H PARAMETERS SAMPLES MODELING CLASSIFICATION (HARKERS1 / HARKERS2 / Isotopes NUMERICAL OUTPUT )

#### 3. "MODELING" SHEET (upper section)



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#### 3. "MODELING" SHEET (lower section)



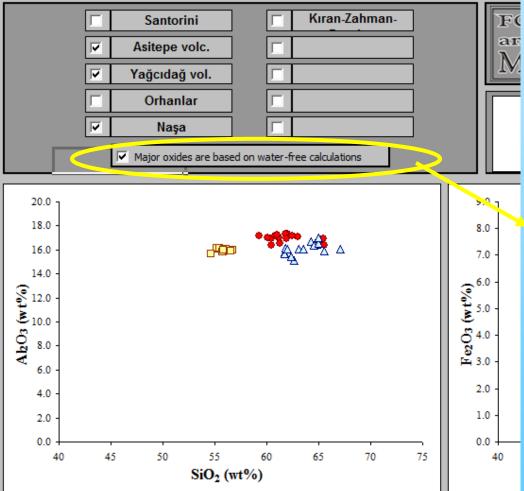
N A MARKERS SAMPLES MODELING CLASSIFICATION A HARKERS1 A HARKERS2 A Isotopes NUMERICAL OUTPUT

#### 4. "CLASSIFICATION" SHEET (lower section)

<b>Discrimination and</b>							
	Γ	Santorini F Kıran-Zahman-	F				
	•	Asitepe volc.	a				
	•	Yağcıdağ vol.					
	Γ	Orhanlar 🗾					
	•	Naşa					
		Major oxides are based on water-free calculations					
2	Τ¢	Le Bas et al., 1986) discrimination line: (Irvine and Barragar 1971)					
ž	ł	basaltic andesite					
2	ł	tephri- phonolite trachyte	7				
( <b>w</b> t%) 10	ł	phono- tephrite trachy- andesite trachydacite rhyolite	¢) ،				
$K_20+Na_20$ (w $t\%$ )	t	trachy- andesite -	Kş0 (w1%) <sub>3</sub>				
K <sub>2</sub> 0+	Ť	tephrite dospit	1 3				
*	ł	basanite ousait basanite basaltic andesite dacite basalt basalt basaltic andesite dacite					
5	t	N LIB - A basalt basalt					
•	35	45 55 65 75 SiO <sub>2</sub> (wt%)	6				
	_	5107(1179)					

- \* 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. "HARKERs" SHEET

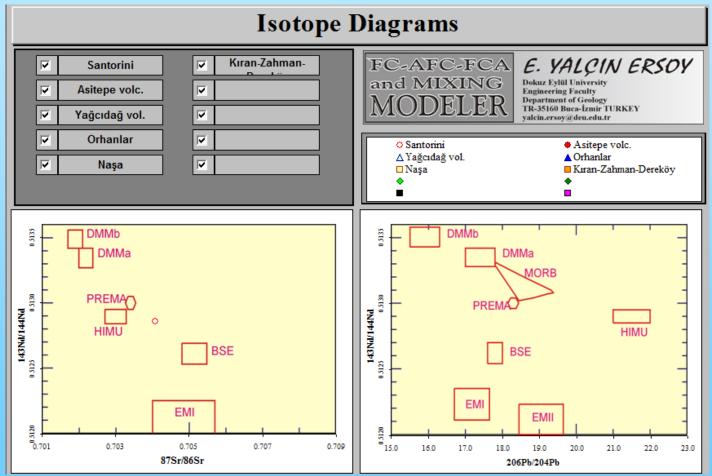


Major and trace elements canbe plotted on SiO2-dependet Harker variation diagrams.

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

H A > > > PARAMETERS SAMPLES MODELING CLASSIFICATION HARKERS1 HARKERS2 Is topes NUMERICAL OUTPUT

#### 6. "ISOTOPES" SHEET



Four isotope diagrams can be plotted on this sheet.

H A A H PARAMETERS SAMPLES MODELING CLASSIFICATION HARKERS1 HARKERS2 Stopes NUMERICAL OUTPUT

#### 7. "NUMERICAL OUTPUT" SHEET

	AFC RESULTS									
	0.40 F (fraction of melt remaining)									
-1										
	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
. C.	,50.00		40.05	40.04	20.00	24.42	20.00	0100 A	22.20	10.02

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

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

# 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