Potential Consequences of the Compositional Distribution of Trace Element Partitioning Experiments

Sui Tung[1], Gokce K. Ustunisik[1,2] and Roger L. Nielsen[1,3*] (roger.nielsen@sdsmt.edu)

[1]*Department of Geology and Geological Engineering, South Dakota School of Mines and Technology, Rapid City, SD, 57701*

[2]*Department of Earth and Planetary Sciences, American Museum of Natural History, New York, NY, 10024*

[3]*College of Earth, Ocean, and Atmospheric Sciences, Oregon State University, Corvallis, OR, 97331*

[*] *presenting author*

AGU 2018 V23I-3472 382100

Abstract

Our trace element partitioning study aims at evaluating the characteristics of the existing database used for the calibration of predictive models of trace element behavior in natural systems. How this goal is pursued and what each investigator defines as a relevant database varies dramatically from study to study. Over the past several years, we have developed traceDs as part of the IEDA initiative. Our goal in developing traceDs is to provide a transparent and accessible resource of experimental partitioning data for the community. traceDs now includes the experimental trace element partitioning data (>5400 experiments), including the experimental conditions, and the major and trace element composition of the phases. The existing databases has focused on data characteristics:

- Data quality – reflect reproducibility, precision, equilibration of phases, and quality of analysis
- Data relevance – indicate how the data are relevant to a modelled system
- Methodologies –for generating models

There is another important characteristic of the existing data that has yet to be fully examined – the data distribution in compositional space. Most models include regression parameters for composition as well as experimental conditions. This is because the mineral and melt component activities, the substitution of trace elements into specific sites and the role of paired substitutions are influenced by composition. The existing data illustrates that the number of experimental determinations is different from element to element – even for a series of elements such as the REE. For instance, there are more determinations for the partitioning of the LREE between plagioclase and melt than there are for the HREE. In addition, there are more determinations for the REE in plagioclase than there are for the HFSE, and equally important, the composition of the population of determinations also vary with different elements. For instance, the population of liquids for the experiments where Zr partitioning was determined for pyroxene are different from those where Sr partitioning was determined. This means that any regression analysis must "see through" these differences in order to be applicable for a wide range of composition and to provide a set of modelled partition coefficients characterized by a systematic "smooth" pattern.

Distribution of Experimental determinations by mineral and element

	Plagioclase	Clinopyroxene	Olivine	Garnet	Amphibole
Total:	269	898	941	279	179
Sr	146	181	25	99	28
La	88	247	30	106	83
Ce	77	111	17	99	38
Pr	38	43	11	68	9
Nd	87	124	14	111	36
Sm	79	208	30	140	60
Eu	92	91	28	93	36
Gd	47	139	39	94	45
Tb	10	38	106	73	9
Dy	26	89	16	95	36
Ho	5	106	50	64	23
Er	30	77	129	99	36
Tm	3	27	29	44	34
Yb	32	163	179	177	38
Lu	31	170	52	118	36
Ti	140	745	383	272	179
Zr	43	257	197	150	34
Hf	10	135	95	125	41
Nb	18	139	19	88	38
Ta	12	101	19	65	48

The table above documents the number of available experiments for these five major rock forming minerals where a specific element's partition coefficient is reported. Note that for some minerals, there is a wide range of values even within a group of elements, while for others there is more consistency.

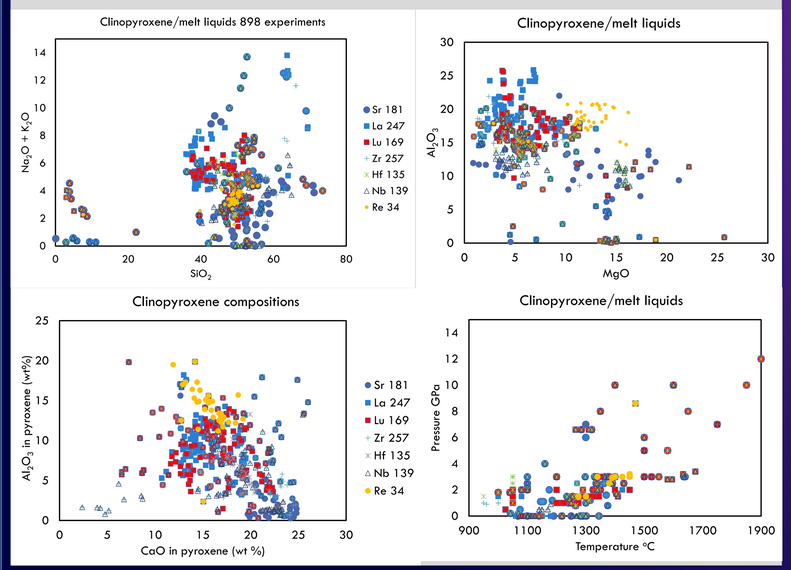
Distribution of the subject area of the experimental partitioning literature

	Olivine	Opx	Cpx	Plag	Amph	Spinel	Garnet
extraterrestrial	10	8	5	7	0	6	5
general/synthetic	15	5	13	7	1	5	4
mantle	23	20	30	3	1	6	14
arc/crustal	4	7	18	6	8	7	16
carbonatite	6	4	8	0	1	2	8
alkaline	2	1	6	0	4	1	0
total papers	60	45	80	23	15	27	47

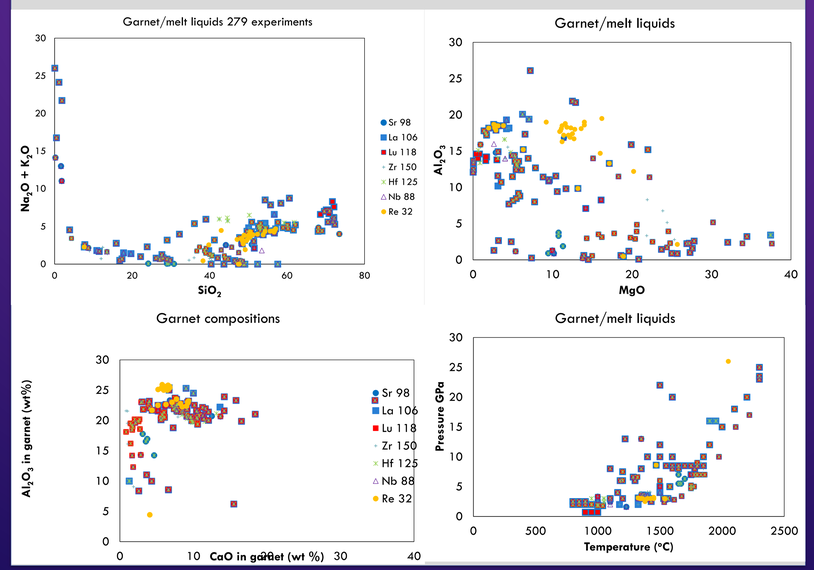
Documentation of where we have focused our efforts in the determination of partitioning behavior

The area of focus for each mineral is determined to some significant degree on the phase equilibria of the mineral and its significance in a specific environment. General/synthetic represents investigations focused on the general aspects of partitioning and/or studies that used starting materials that were simplified in some way (e.g. Fe free).

Distribution of experimental determinations by element of interest in the traceDs database



Distribution of experimental determinations by element of interest in the traceDs database



	Clinopyroxene/melt data. Total # experiments 898								Garnet/melt data. Total # experiments 279						
	Sr	Zr	Hf	Nb	La	Lu	Re		Sr	Zr	Hf	Nb	La	Lu	Re
Sr	181	137	85	75	120	73	2	Sr	98	97	82	74	88	81	10
Zr		258	110	132	127	82	3	Zr		150	111	87	98	101	11
Hf			135	133	91	80	3	Hf			125	72	86	106	11
Nb				139	71	48	3	Nb				88	73	75	10
La					247	103	3	La					106	92	10
Lu						170	3	Lu						118	10
Re							34	Re							32

Cross correlation of partitioning experiments for clinopyroxene and garnet. The self correlation (e.g. Sr vs Sr) represents the number of experimental determinations present in the literature for Sr partitioning in clinopyroxene (181 experiments) or garnet (98 experiments). The numbers in the cells represent the # experiments that have both elements determined. For example, for clinopyroxene, there are 258 experimental determinations for Zr partitioning (~29% of all experiments). Of those 258 experiments, 137 also have Sr determinations (e.g. ~ half). Note that the number of experiments varies within groups of elements (e.g. REE or HFSE), but to a lesser degree than between groups of elements (REE vs HFSE). Also note that the degree of cross correlation varies between minerals. In this case, the "coverage" is higher for garnet than it is for clinopyroxene. This means that experimental studies for garnet tend to report information on more elements than studies for clinopyroxene.

Trace element partitioning experiments for clinopyroxene

The distribution of liquids from published investigations for trace element partition between clinopyroxene and liquid. The number of experiments for each element are in the key (e.g. 181 experiments with Sr determinations. Note that the range of temperature, pressure and composition is determined by the phase equilibria of clinopyroxene, as well as the problem being addressed.

Trace element partitioning experiments for garnet

The distribution of liquids from published investigations for trace element partition between garnet and liquid. The number of experiments for each element are in the key (e.g. 98 experiments with Sr determinations). Note that the range of temperature, pressure and composition is determined by the phase equilibria of garnet, as well as the problem being addressed.

Conclusions and implications

The number and character of the distribution of partitioning data varies between elements and between minerals

This "heterogeneity" of the data produces several challenges to the methodologies applied to modeling trace element behavior

The two most important implications are:

- Nearest neighbor searches will pull very different numbers from the database. This is caused by the fact that not all elements are determined for each experiment – which is different from such searches within the LEPR database of major element phase equilibria
- The approach most likely to produce consistent results is the calibration of numerical expressions designed to predict partitioning behavior
- However, such models for trace element behavior, even within groups of trace elements, are calibrated using different databases, potentially producing internal systematic bias.