WEBASED VISUALIZATION OF SURFACE COMPLEXATION-ION EXCHANGE





(L-SCIE) DATABASE

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L-SCIE Database

L-SCIE Database Development:

In collaboration with RES3T, we are building a data digitization pipeline that merges the Dzombak & Morel approach (data mining, digitization, model fitting) with the RES3T workflow (reaction constant and metadata mining). This integrated framework supports surface complexation model (SCM) development and future machine learning (ML) applications.

Current content: 683 references and 75,601 digitized sorption data points with metadata

Focus: raw sorption data from RES3T and related literature

Structure: Microsoft Access relational database (linked tables for references, datasets, and parameters) Recent update (Clemson): added sorption data for radionuclides including Se-79, Eu-152, Ra-226,

Np-237, U-234/235/238, Pu-238/239/242, and Am-241 on iron (hydro)oxides

Applications: used in several studies to test and refine SCM model strategies

Why the website?

L-SCIE Data Visualization Tool:

The L-SCIE database is a valuable global resource but requires familiarity with SQL, Python, and PHREEQC, which can limit access for users without programming experience. To overcome this barrier, we developed an **interactive**, **web-based visualization platform** that enables users to easily explore and analyze L-SCIE data.

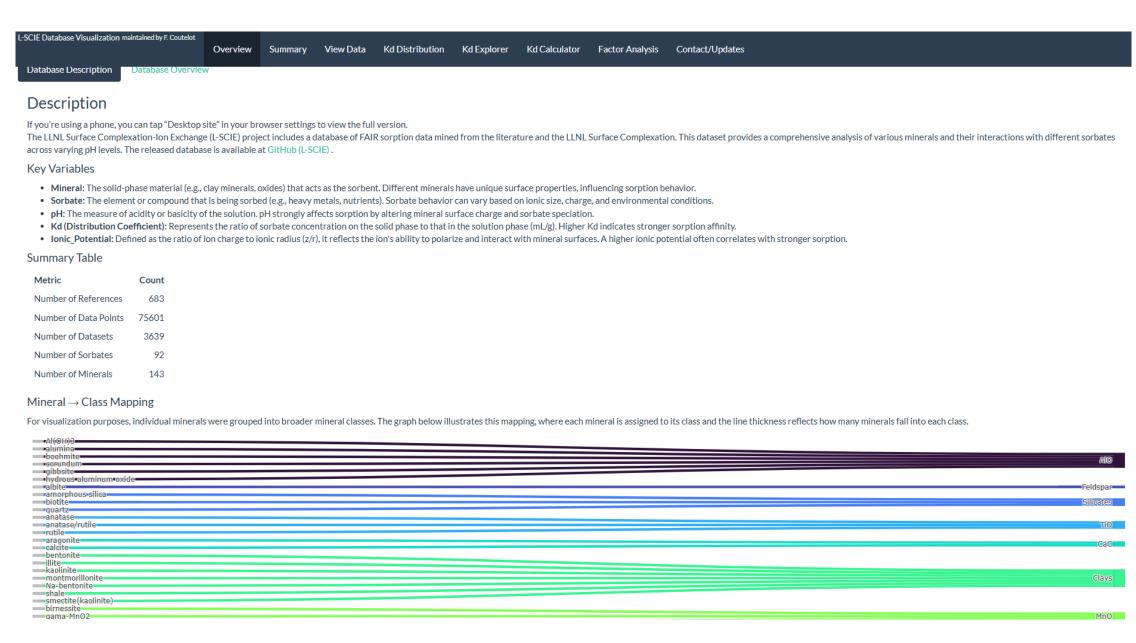
Explore: visualize pH, Kd, and sorbed value distributions by element or mineral.

Compare: contrast two minerals or sorbates across key variables.

Analyze: perform built-in statistical analyses (e.g., PCA, clustering) to identify trends.

This tool accelerates data exploration for both new and experienced users—eliminating the need for manual SQL queries—and will soon be freely accessible online.

OVERVIEW tab



The Overview tab provides an entry point into the L-SCIE database, allowing users to filter, sort, and preview sorption datasets directly in the browser. Users can quickly browse key metadata—such as mineral type, sorbate, pH range, and experimental conditions—and view the corresponding subset of data in an interactive, searchable table.

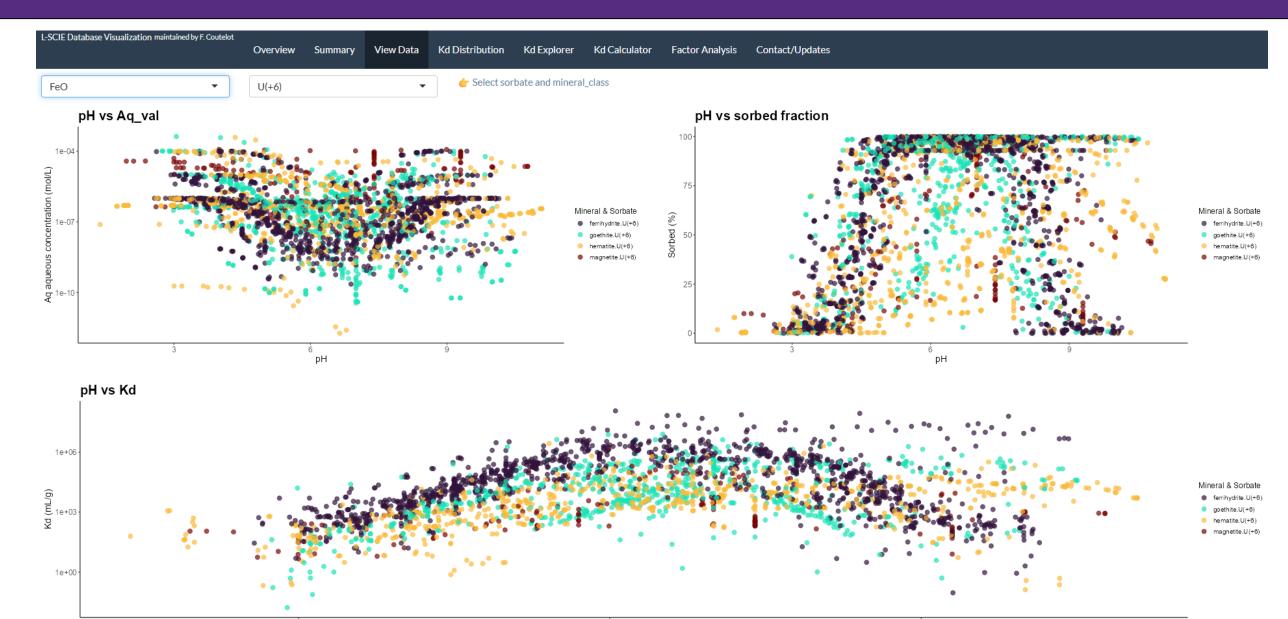
This interface is designed to help both new and experienced users understand the scope and structure of the database, identify relevant studies, and prepare datasets for further analysis in the *Compare* and *Analyze* tabs

L-SC	.IE Database Visualizat	ion maintained by F. Cout		Overview	Summary	View Data	Kd Distribution	Kd Explorer	Kd Calculator	Factor Analysis	Contact/Updates				
	Database Description	Database Ove	erview												
M	/lineral:						Sorbate:					Reference:			
	All		•				All		•			All	•		
how	25 ventries													Search:	
X	(Reference	Source Set	∳ S	SetID	ineral 🌲 Mi	ineral_formula ﴿	Mineral_source	Temp Ele	ectrolyte1 Ele	ctrolyte1_val 🛊 Ele	ectrolyte1_SD	yte1_units Electrolyte2	Electrolyte2_val	Electrolyte2_SD \(\phi\)	Electrolyte2_unit
L	0 rgrjh14	CLEMSON rgrjh1	.4_f1c 1	l sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
2	1 rgrjh14	CLEMSON rgrjh1	.4_f1c 2	2 sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
3	2 rgrjh14	CLEMSON rgrjh1	.4_f1c 3	3 sm	nectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
ļ	3 rgrjh14	CLEMSON rgrjh1	.4_f1c 4	sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
5	4 rgrjh14	CLEMSON rgrjh1	.4_f1c 5	sm sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
5	5 rgrjh14	CLEMSON rgrjh1	.4_f1c 6	sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
7	6 rgrjh14	CLEMSON rgrjh1	.4_f1c 7	7 sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
3	7 rgrjh14	CLEMSON rgrjh1	.4_f1c 8	3 sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
)	8 rgrjh14	CLEMSON rgrjh1	.4_f1c 9	sm sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
0	9 rgrjh14	CLEMSON rgrjh1	.4_f1c 1	lO sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
1	10 rgrjh14	CLEMSON rgrjh1	.4_f1c 1	l1 sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
2	11 rgrjh14	CLEMSON rgrjh1	.4_f1c 1	l2 sm	ectite			Κ(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
13	12 rgrjh14	CLEMSON rgrjh1	.4_f1c 1	l3 sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
4	13 rgrjh14	CLEMSON rgrjh1	.4_f1c 1	L4 sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
15	14 rgrjh14	CLEMSON rgrjh1	.4_f1c 1	L5 sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
6	15 rgrjh14	CLEMSON rgrjh1	.4_f1c 1	l6 sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
7	16 rgrjh14	CLEMSON rgrjh1	.4_f1c 1	L7 sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
18	17 rgrjh14	CLEMSON rgrjh1	.4_f1c 1	l8 sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
9	18 rgrjh14	CLEMSON rgrjh1	.4_f1c 1	l9 sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
20	19 rgrjh14	CLEMSON rgrjh1	.4_f1c 2	20 sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
21	20 rgrjh14	CLEMSON rgrjh1	.4_f1c 2	21 sm	ectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
		CLEMSON rgrjh1	.4_f1c 2	22 sm	nectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
23	22 rgrjh14	CLEMSON rgrjh1	.4_f1c 2	23 sm	nectite			K(+1)	0.01	0.0005 mol/L	CI(+7)	0.01	0.0005	5 mol/L
24	23 azbn00	LLNL azbn0	0_f1 1	l qu	artz SiG	02		Na	a(+1)	0.1	0.005 mol/L	CI(+7)	0.1	0.005	5 mol/L
25	24 azbn00	LLNL azbn0	0_f1 2	2 qu	artz SiG	02		Na	a(+1)	0.1	0.005 mol/L	CI(+7)	0.1	0.005	5 mol/L

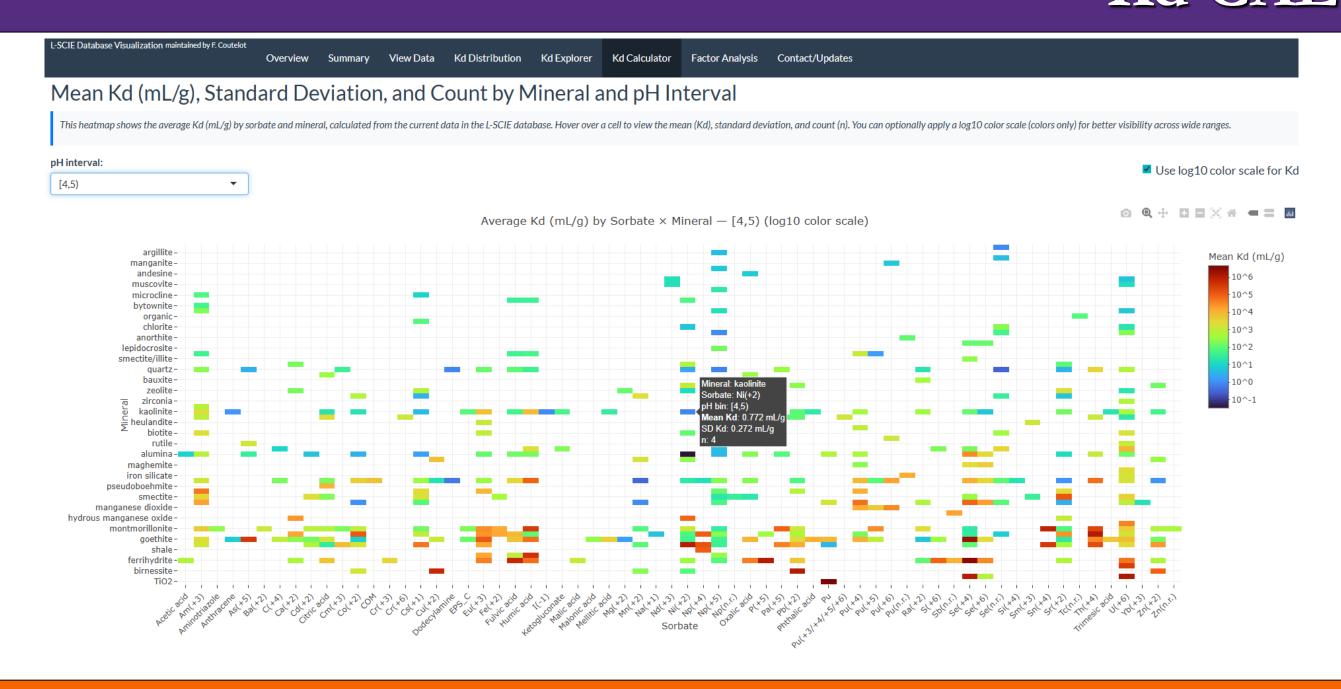
VIEW DATA tab

The View Data tab enables users to visualize relationships between experimental variables in the L-SCIE database through interactive scatter plots. Users can select any combination of parameters (e.g., pH, Kd, sorbate concentration, temperature, or mineral type) to explore data trends and correlations in real time.

Each plot is fully interactive—points can be hovered for metadata, zoomed, or filtered—making it easy to identify **outliers**, **clusters**, **and patterns** across studies. This feature provides a rapid and intuitive way to **examine raw data distributions** before moving to more advanced statistical analysis.



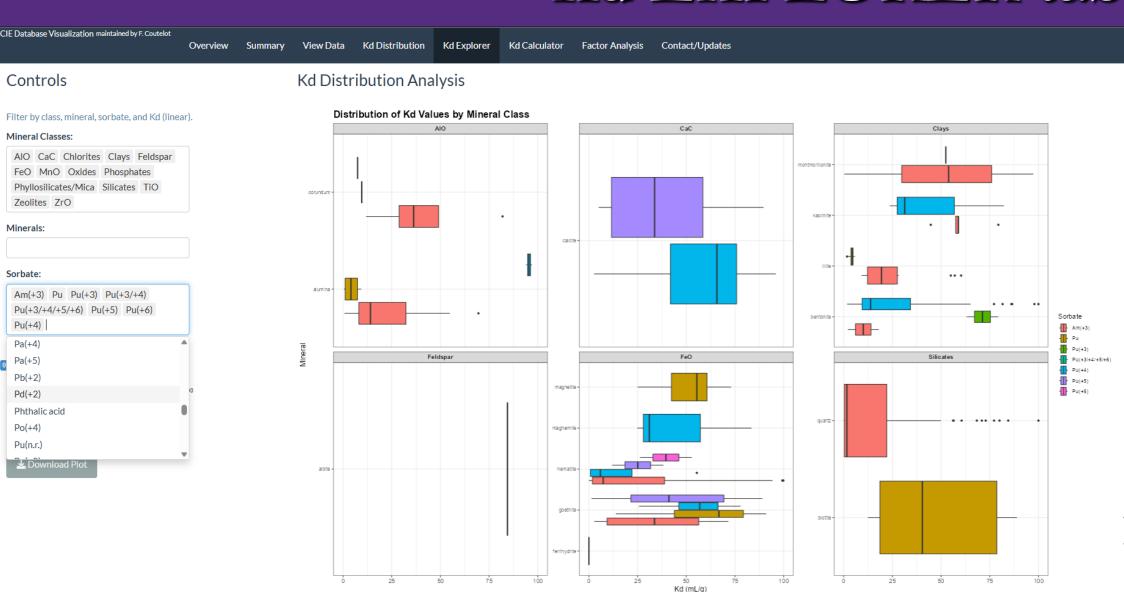
Kd CALCULATOR tab



The View Data tab enables users to visualize relationships between experimental variables in the L-SCIE database through interactive scatter plots. Users can select any combination of parameters (e.g., pH, Kd, sorbate concentration, temperature, or mineral type) to explore data trends and correlations in real time.

Each plot is fully interactive—points can be hovered for metadata, zoomed, or filtered—making it easy to identify **outliers**, **clusters**, **and patterns** across studies. This feature provides a rapid and intuitive way to **examine raw data distributions** before moving to more advanced statistical analysis.

Kd EXPLORER tab



Kd Explorer Tab:

Visualize Kd distributions across minerals, sorbates, and pH ranges using interactive boxplots.

Quickly identify patterns and variability in sorption behavior.

And much more, explore the website →

Aug. 2023, doi: 10.1016/j.apgeochem.2023.105731.

Link to the website

Link to the database



References

Acknowledgements

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[2]S.-C. Han, E. Chang, S. Zechel, F. Bok, and M. Zavarin, "Application of community data to surface complexation modeling framework development: Iron oxide protolysis," J. Colloid Interface Sci., Oct. 2023, doi: 10.1016/j.jcis.2023.06.054.

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