Title: Predicting Radioactive Waste Glass Dissolution with Machine Learning

Supplementary Data

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Supplementary Tables

Table S1*: A brief summary of machine learning methods employed. See Krishnan et al.* [1] *for additional descriptions on several of the methods.*

Machine Learning Method	Description
Neural Network [2]	Neural networks formulate a non-linear relationship between output and input variables. They do this by adjusting the weight and bias values of basic units (known as neurons). Individual neuron outputs act as subsequent inputs to other neurons in the network, and it is the combined effect of the various individual neuron input-outputs that ultimately yields the overall network output prediction. This study uses feed-forward neural nets with a single hidden layer, whereby the number of hidden layer neurons is optimised by examining their effect on R^2 and mean square error (MSE) test set errors. As a simple example, were one neuron to have silicon concentration ([Si]) as an output variable, and both pH (pH) and temperature (T) as input variables, there would be some learnable mathematical relationship; [Si] = f (w1*pH + w2*T + b)). This is where w1 and w2 are the weights associated with the two input variables, b is the associated neuron bias vector, and f is the neuron activation function.
Multiple, Lasso, Ridge, and Elastic Net Regression [3]	Multiple linear regression formulates a linear correlation between an independent variable and several dependent variables. Additional regularisation parameters can be included that add either an L2 penalty (Lasso), L1 penalty (Ridge), or a combination (Elastic Net). These penalties help

	weight the relative contribution of predictive variance versus bias. Here, regularisation parameters are adjusted by studying their effect on R^2 and MSE test errors.
Support Vector Machine (SVM) Regression [4]	SVM regression is a non-parametric kernel based approach. The aim is to find a function of the predictor (input) for which predicted function outputs lie within an error range of the target response values. This study considers Gaussian, linear, and polynomial kernel functions to examine kernel performance variability.
Gaussian Process Regression (GPR) [5]	GPR is a kernel-based method that learns a probability distribution for the prediction learning function instead of computing exact function parameter values. This study considers MATLAB 'exponential', 'squaredexponential', and 'ardsquaredexponential' kernel functions to examine kernel performance variability.
Individual Regression Trees, Boosted Ensembles, and Bagged Random Forests [6]	These are methods of regression that formulate decision making through tree like binary splitting. The data is split and used to train different models for which the output results are then subsequently aggregated. The results of either single or collective regression trees are considered. Key parameters that are optimised with respect to R^2 and MSE test errors include leaf size in the case of individual regression trees and number of trees in the case of either boosting or bagging.

Table S2: *'Whole Experiment' mean R^2/MSE Dataset A-D test errors as a function of I/O combinations and machine learning algorithms. The complete Dataset A-D was used in the model training. I/O numbers are given in Table 1 of the full paper. Machine learning algorithm numbers correspond to the algorithms given at the beginning of Section 3 of the full paper.*

I/O	Error	Machine Learning Algorithm													
		1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	R^2	0.40	-0.04	-2.5E+02	-0.04	0.83	-4.8E+04	0.90	0.97	0.97	0.96	0.95	0.96	0.94	0.61
	MSE	21.54	43.44	9.1E+03	41.73	6.49	2.1E+06	4.35	1.11	1.24	1.61	2.15	1.93	4.19	14.91
2	R^2	0.72	-0.04	-2.7E+02	-0.04	0.85	-6.5E+05	0.90	0.97	0.97	0.96	0.96	0.93	0.94	0.63
	MSE	9.23	42.55	1.1E+04	44.35	5.62	2.1E+07	4.34	1.08	1.20	1.57	1.77	3.77	2.06	13.10
3	R^2	0.80	0.15	0.91	-1.1E+25	0.91	0.87	0.90	0.97	0.97	0.96	0.95	0.96	0.93	0.70
	MSE	6.98	34.32	3.35	4.6E+26	3.22	4.80	4.33	1.11	1.24	1.78	2.30	2.52	5.67	11.51
4	R^2	0.81	-0.01	-1.6E+02	-0.04	0.83	-1.9E+05	0.90	0.97	0.90	0.86	0.95	0.97	0.85	0.75
	MSE	7.40	42.14	5.8E+03	42.86	6.37	7.0E+06	4.16	1.22	3.80	4.94	2.22	0.99	7.52	9.56
5	R^2	0.64	-0.03	-3.3E+02	-0.04	0.84	-8.5E+02	0.90	0.97	0.97	0.96	0.95	0.92	0.93	0.57
	MSE	14.01	42.80	1.2E+04	40.74	5.98	2.1E+04	4.34	1.14	1.25	1.61	1.96	4.21	4.46	15.73
6	R^2	0.44	-0.03	-1.9E+02	-0.06	0.85	-3.0E+03	0.90	0.97	0.97	0.95	0.95	0.97	0.97	0.77
	MSE	19.06	40.09	6.5E+03	42.87	5.97	1.4E+05	4.24	1.10	1.19	1.86	2.44	1.09	1.28	9.68
7	R^2	-4.1E+02	-0.01	-3.4E+11	-0.04	0.32	0.32	0.53	-1.51	-0.29	-3.12	0.32	0.45	0.48	-0.21
	MSE	1.0E+04	38.38	1.2E+13	40.29	23.51	24.66	17.33	74.92	45.99	117.73	24.28	33.51	17.76	46.39
8	R^2	0.62	-0.03	-2.7E+02	-0.05	0.85	-4.3E+04	0.89	0.97	0.97	0.96	0.95	0.97	0.94	0.59
	MSE	15.16	43.44	1.2E+04	42.23	5.73	1.3E+06	4.81	1.03	1.19	1.57	2.01	1.23	2.83	14.24
9	R^2	0.61	-0.04	-9.5E+02	-0.05	0.83	0.78	0.89	0.90	0.90	0.86	0.86	0.97	0.85	0.45
	MSE	15.46	41.11	2.9E+04	41.69	6.59	8.33	4.29	3.82	3.80	4.94	5.33	0.99	7.52	19.52
10	R^2	0.50	-0.03	-1.3E+02	-0.06	0.80	-1.8E+06	0.90	0.96	0.96	0.95	0.93	0.89	0.78	0.70
	MSE	21.13	42.13	4.5E+03	41.65	7.35	5.3E+07	4.36	1.34	1.42	2.08	2.80	5.73	12.88	11.27
11	R^2	0.68	-0.04	-1.4E+02	-0.05	0.85	-1.1E+04	0.90	0.97	0.97	0.96	0.95	0.97	0.96	0.61
	MSE	10.49	43.38	6.0E+03	39.93	5.81	3.3E+05	4.35	1.10	1.23	1.61	2.08	1.78	0.94	14.30
12	R^2	0.73	0.00	-2.3E+02	-0.06	0.88	0.79	0.94	0.97	0.97	0.96	0.95	0.98	0.94	0.65
	MSE	12.06	42.73	8.2E+03	42.38	4.51	8.08	2.55	1.12	1.24	1.62	1.95	1.32	3.20	12.68
13	R^2	-0.79	-0.03	-2.5E+08	-0.04	0.81	-2.3E+06	0.89	0.96	0.95	0.93	0.94	0.90	0.93	0.47
	MSE	59.66	40.97	1.4E+10	44.61	7.64	6.5E+07	4.97	1.69	2.00	2.41	2.74	4.94	3.42	18.90
14	R^2	0.96	-0.05	-1.1E+02	-0.04	0.83	-2.1E+05	0.83	0.96	0.96	0.96	0.95	0.96	0.89	0.89
	MSE	1.49	44.29	4.4E+03	41.65	5.71	1.2E+07	7.39	1.43	1.44	1.51	2.00	2.29	2.17	4.07
15	R^2	-11.70	0.00	-3.6E+03	-0.05	0.37	0.34	0.55	-0.25	0.23	-0.60	0.26	0.60	0.39	-0.18
	MSE	4.3E+02	38.51	1.3E+05	41.28	25.08	24.63	17.40	44.19	30.35	52.20	27.20	19.13	29.57	42.15
16	R^2	-20.67	-0.01	-4.0E+03	-0.05	0.36	0.34	0.54	-0.23	-0.04	-0.77	0.35	0.31	0.46	-0.15
	MSE	7.0E+02	41.98	1.4E+05	40.94	23.84	26.79	17.52	42.80	37.76	57.63	25.00	34.85	19.58	42.44
17	R^2	-59.82	-0.01	-3.2E+03	-0.04	0.35	0.33	0.55	-0.23	-0.05	-0.97	0.36	0.49	0.50	0.11
	MSE	2.4E+03	38.92	1.3E+05	41.15	25.80	24.71	16.92	43.46	38.27	63.27	24.80	18.39	13.72	35.10

Table S3: *'Whole Experiment' mean R^2/MSE Dataset B-D test errors as a function of I/O combinations and machine learning algorithms. The complete Dataset A was used for model training. I/O numbers are given in Table 1 of the full paper. Machine learning algorithm numbers correspond to the algorithms given at the beginning of Section 3 of the full paper.*

I/O	Error	Machine Learning Algorithm													
		1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	R^2	-2.1E+08	-1.91	-1.7E+03	-2.81	-3.48	-1.9E+02	-5.18	-2.3E+03	-2.1E+03	-2.4E+03	0.29	0.77	0.35	-5.3E+01
	MSE	2.3E+09	31.77	1.9E+04	41.55	48.83	2.1E+03	67.40	2.5E+04	2.3E+04	2.6E+04	7.80	2.47	7.13	5.9E+02
2	R^2	-2.3E+07	-1.85	-1.8E+03	-2.80	-3.31	-2.5E+03	-4.67	-2.4E+03	-2.3E+03	-2.5E+03	0.32	0.79	0.84	-7.0E+01
	MSE	2.5E+08	31.37	2.0E+04	41.88	47.45	2.8E+04	62.47	2.6E+04	2.5E+04	2.7E+04	7.49	2.36	1.81	7.8E+02
3	R^2	-2.0E+06	-4.45	-3.5E+02	-1.9E+06	-16.12	-2.6E+04	-4.52	-7.7E+01	-1.6E+02	-2.0E+02	0.26	0.78	0.35	-4.9E+01
	MSE	2.2E+07	59.41	3.8E+03	2.0E+07	1.9E+02	2.8E+05	60.17	8.5E+02	1.8E+03	2.2E+03	8.03	2.35	7.04	5.4E+02
4	R^2	-7.6E+05	-1.87	-2.1E+03	-2.81	-3.36	-5.1E+02	-4.48	-2.7E+03	-1.5E+03	-1.6E+03	0.27	0.38	0.33	-5.8E+01
	MSE	8.3E+06	31.34	2.3E+04	41.57	47.56	5.6E+03	59.76	3.0E+04	1.6E+04	1.7E+04	7.97	6.78	7.33	6.4E+02
5	R^2	-3.2E+05	-1.85	-1.5E+03	-2.82	-3.22	-1.7E+03	-4.74	-1.8E+03	-2.2E+03	-2.4E+03	0.29	0.81	0.77	-4.6E+01
	MSE	3.5E+06	31.11	1.7E+04	41.62	46.07	1.9E+04	62.64	2.0E+04	2.4E+04	2.6E+04	7.70	2.02	2.54	5.1E+02
6	R^2	-5.1E+06	-1.89	-9.6E+02	-2.79	-3.60	-6.4E+04	-4.43	-1.5E+03	-1.7E+03	-1.8E+03	0.30	0.80	0.34	-5.1E+01
	MSE	5.5E+07	31.50	1.0E+04	41.35	50.23	7.0E+05	59.27	1.6E+04	1.8E+04	2.0E+04	7.65	2.18	7.18	5.7E+02
7	R^2	-5.6E+06	-2.42	-9.8E+04	-3.91	-2.20	-3.89	-2.48	-1.1E+06	-6.2E+05	-1.0E+06	-9.82	-10.80	-13.14	-1.3E+02
	MSE	5.0E+07	30.92	8.8E+05	44.36	28.92	44.17	31.47	9.9E+06	5.6E+06	9.1E+06	97.76	1.1E+02	127.71	1.2E+03
8	R^2	-1.6E+08	-1.85	-1.4E+03	-2.87	-3.59	-1.6E+02	-4.36	-2.6E+03	-2.4E+03	-2.5E+03	0.25	0.79	0.23	-5.5E+01
	MSE	1.8E+09	31.04	1.5E+04	42.18	50.08	1.8E+03	58.46	2.9E+04	2.6E+04	2.7E+04	8.14	2.31	8.36	6.2E+02
9	R^2	-3.0E+07	-1.87	-7.8E+02	-2.86	-3.07	-1.2E+02	-8.09	-1.5E+03	-1.5E+03	-1.6E+03	0.25	0.38	0.33	-5.4E+01
	MSE	3.2E+08	31.34	8.6E+03	42.15	44.36	1.3E+03	99.14	1.7E+04	1.6E+04	1.7E+04	8.14	6.78	7.33	6.0E+02
10	R^2	-6.7E+08	-1.92	-3.9E+03	-2.76	-2.71	-2.7E+07	-5.40	-2.0E+03	-2.3E+03	-3.0E+03	0.84	0.57	0.76	-4.9E+01
	MSE	7.3E+09	31.91	4.2E+04	41.06	40.43	2.9E+08	69.79	2.2E+04	2.5E+04	3.3E+04	1.76	4.66	2.61	5.4E+02
11	R^2	-6.4E+07	-1.85	-1.5E+03	-2.72	-3.33	-3.0E+03	-4.85	-2.4E+03	-2.2E+03	-2.4E+03	0.35	0.81	0.47	-7.5E+01
	MSE	7.0E+08	31.12	1.7E+04	40.63	47.21	3.3E+04	63.86	2.6E+04	2.3E+04	2.6E+04	7.11	2.03	5.82	8.3E+02
12	R^2	-8.2E+08	-2.37	-1.5E+03	-2.87	-5.29	-1.5E+01	-6.10	-2.4E+03	-2.3E+03	-2.4E+03	0.22	0.77	0.19	-5.5E+01
	MSE	8.9E+09	36.71	1.6E+04	42.23	68.58	1.7E+02	77.44	2.6E+04	2.5E+04	2.6E+04	8.54	2.49	8.83	6.1E+02
13	R^2	-1.9E+04	-1.95	-7.2E+03	-2.98	-1.60	-1.7E+09	-9.92	-2.7E+03	-2.2E+03	-2.4E+03	0.84	-1.33	0.41	-7.8E+01
	MSE	2.0E+05	31.29	7.6E+04	42.28	27.59	1.8E+10	115.99	2.8E+04	2.3E+04	2.6E+04	1.65	24.71	6.30	8.4E+02
14	R^2	-5.3E+03	-1.91	-1.6E+03	-2.86	-3.41	-4.8E+02	-16.29	-5.3E+03	-5.9E+03	-5.9E+03	0.29	0.79	0.53	-2.2E+02
	MSE	5.8E+04	31.70	1.7E+04	42.15	48.14	5.2E+03	188.61	5.8E+04	6.4E+04	6.5E+04	7.80	2.33	5.16	2.4E+03
15	R^2	-5.7E+06	-2.76	-7.7E+04	-4.24	-2.12	-4.29	-1.23	-9.7E+05	-7.0E+05	-9.3E+05	-8.93	-13.95	-2.82	-2.7E+01
	MSE	5.1E+07	33.59	6.8E+05	46.86	27.92	47.32	19.94	8.7E+06	6.2E+06	8.3E+06	88.73	1.3E+02	34.10	2.5E+02
16	R^2	-5.2E+06	-2.70	-6.9E+04	-4.36	-2.12	-4.09	-1.10	-5.6E+05	-3.0E+05	-5.4E+05	-9.63	-7.92	-13.69	-2.0E+01
	MSE	4.6E+07	33.07	6.2E+05	47.88	27.88	45.48	18.76	5.0E+06	2.7E+06	4.8E+06	94.92	79.64	1.3E+02	1.9E+02
17	R^2	-4.1E+06	-2.72	-7.5E+04	-4.32	-2.27	-4.28	-1.22	-5.6E+05	-3.0E+05	-5.4E+05	-9.03	-8.73	-12.25	-3.1E+01
	MSE	3.7E+07	33.24	6.7E+05	47.51	29.24	47.17	19.82	5.0E+06	2.7E+06	4.8E+06	89.60	86.90	1.2E+02	2.8E+02

Table S4: *'Missing Data' mean R^2/MSE Dataset A-D test errors as a function of I/O combinations and machine learning algorithms. The complete Dataset A-D was used for model training. I/O numbers are given in Table 1 of the full paper. Machine learning algorithm numbers correspond to the algorithms given at the beginning of Section 3 of the full paper.*

I/O	Error	Machine Learning Algorithm													
		1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	R^2	0.99	-0.01	-1.7E+02	-0.01	0.91	-1.9E+04	0.94	0.99	0.98	0.99	0.97	0.99	0.97	0.99
	MSE	0.59	41.28	6.9E+03	41.67	3.67	5.8E+05	2.80	0.58	0.61	0.60	1.46	0.43	1.03	0.46
2	R^2	0.98	0.01	-5.3E+02	-0.01	0.91	-60.31	0.95	0.99	0.99	0.99	0.97	0.96	0.98	0.98
	MSE	0.60	41.01	2.0E+04	40.59	3.52	2.3E+03	2.22	0.60	0.57	0.59	1.47	1.65	1.02	0.62
3	R^2	0.99	0.17	0.91	-1.4E+26	0.93	0.91	0.97	0.99	0.98	0.99	0.97	0.98	0.98	0.99
	MSE	0.59	34.38	3.68	5.9E+27	2.88	3.99	1.45	0.60	0.61	0.60	1.28	0.93	0.86	0.40
4	R^2	0.99	0.01	-1.2E+02	-0.01	0.90	-4.3E+04	0.96	0.99	0.98	0.99	0.97	0.98	0.97	0.98
	MSE	0.59	39.94	4.9E+03	41.64	3.92	1.4E+06	1.85	0.58	0.61	0.60	1.48	0.69	1.03	0.73
5	R^2	0.99	0.00	-1.8E+02	-0.01	0.91	0.76	0.96	0.99	0.98	0.99	0.96	0.97	0.97	0.99
	MSE	0.59	41.12	7.4E+03	42.17	3.72	8.88	1.71	0.59	0.61	0.60	1.49	1.13	0.97	0.46
6	R^2	0.99	-0.01	-1.7E+02	0.00	0.91	-5.9E+02	0.96	0.99	0.98	0.99	0.97	0.98	0.97	0.99
	MSE	0.57	41.85	6.6E+03	42.16	3.80	1.8E+04	1.76	0.59	0.61	0.60	1.51	0.67	0.98	0.59
7	R^2	0.39	0.05	-4.3E+04	-0.01	0.51	0.48	0.86	0.41	0.40	0.40	0.81	0.83	0.71	0.71
	MSE	23.71	36.57	1.6E+06	39.02	18.73	19.95	5.33	22.76	23.17	22.12	7.44	8.45	12.45	10.77
8	R^2	0.98	-0.01	-1.6E+03	-0.01	0.91	-1.2E+04	0.95	0.99	0.99	0.99	0.97	0.98	0.96	0.98
	MSE	0.60	41.08	6.5E+04	41.51	3.77	4.0E+05	2.28	0.59	0.58	0.61	1.35	0.65	1.43	0.86
9	R^2	0.95	0.00	-4.7E+02	0.00	0.90	0.88	0.98	0.95	0.95	0.95	0.96	0.96	0.95	0.94
	MSE	2.00	41.95	1.9E+04	40.47	4.14	4.98	0.79	2.04	2.04	2.00	1.66	2.23	1.97	2.53
10	R^2	0.98	-0.01	-6.9E+02	-0.01	0.88	-1.3E+03	0.96	0.98	0.98	0.98	0.95	0.98	0.97	0.99
	MSE	0.75	42.04	2.6E+04	41.84	4.91	5.3E+04	1.94	0.77	0.77	0.77	2.17	0.77	1.19	0.54
11	R^2	0.99	-0.01	-1.9E+02	-0.01	0.91	0.80	0.96	0.99	0.99	0.99	0.96	0.97	0.97	0.99
	MSE	0.59	41.01	7.7E+03	42.24	3.70	8.66	1.62	0.59	0.60	0.59	1.55	1.39	1.53	0.58
12	R^2	0.99	0.24	-1.1E+02	-0.01	0.99	0.98	0.99	0.99	0.98	0.98	0.97	0.97	0.98	0.99
	MSE	0.60	31.60	4.6E+03	41.04	0.44	0.88	0.48	0.60	0.63	0.62	1.49	1.15	0.90	0.46
13	R^2	0.92	0.00	-2.4E+08	-0.01	0.87	-9.9E+02	0.97	0.98	0.97	0.98	0.95	0.97	0.95	0.97
	MSE	3.20	41.22	1.2E+10	41.89	5.47	4.1E+04	1.44	1.02	1.03	0.97	2.40	1.36	2.14	1.12
14	R^2	0.97	0.00	-2.2E+02	-0.01	0.91	-1.3E+06	0.94	0.97	0.97	0.97	0.97	0.98	0.97	0.96
	MSE	1.08	40.95	9.5E+03	41.41	3.62	5.3E+07	2.64	1.06	1.12	1.07	1.37	0.60	1.00	1.67
15	R^2	0.49	0.03	-4.3E+03	-0.01	0.50	0.50	0.87	0.50	0.49	0.49	0.81	0.82	0.64	0.57
	MSE	20.72	38.36	1.7E+05	40.69	19.39	19.75	5.22	19.33	20.25	20.03	7.54	7.16	11.81	16.92
16	R^2	0.48	0.04	-4.6E+03	0.00	0.50	0.48	0.88	0.48	0.48	0.49	0.78	0.87	0.68	0.66
	MSE	20.72	37.83	1.8E+05	40.55	20.16	20.91	4.73	20.72	20.40	20.23	8.76	4.99	13.53	13.44
17	R^2	0.17	0.03	-4.4E+03	0.00	0.50	0.49	0.89	0.49	0.48	0.49	0.78	0.88	0.67	0.63
	MSE	37.91	39.37	1.7E+05	39.48	19.97	21.14	4.47	20.27	20.31	20.17	8.70	3.76	13.74	14.79

Table S5: *'Missing Data' mean R^2/MSE Dataset B-D test errors as a function of I/O combinations and machine learning algorithms. The complete Dataset A was used for model training. I/O numbers are given in Table 1 of the full paper. Machine learning algorithm numbers correspond to the algorithms given at the beginning of Section 3 of the full paper.*

I/O	Error	Machine Learning Algorithm													
		1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	R^2	-1.5E+03	-1.85	-1.0E+03	-2.87	-3.76	-3.5E+03	-5.59	-1.3E+03	-8.3E+02	-1.7E+03	0.29	0.80	0.58	-5.9E+01
	MSE	1.7E+04	31.10	1.1E+04	42.19	51.94	3.8E+04	71.88	1.4E+04	9.1E+03	1.8E+04	7.78	2.14	4.61	6.5E+02
2	R^2	-1.5E+03	-1.80	-1.0E+03	-2.77	-3.46	-3.5E+02	-5.25	-1.2E+03	-1.5E+03	-1.8E+03	0.32	0.77	0.75	-5.5E+01
	MSE	1.7E+04	30.81	1.1E+04	41.49	49.14	3.9E+03	68.78	1.4E+04	1.7E+04	1.9E+04	7.49	2.55	2.73	6.2E+02
3	R^2	-1.1E+03	-4.36	-5.0E+01	-6.8E+08	-15.74	-4.9E+03	-6.73	-8.0E+02	-3.6E+02	-1.4E+02	0.29	0.77	0.58	-4.3E+01
	MSE	1.2E+04	58.49	5.6E+02	7.4E+09	1.8E+02	5.3E+04	84.33	8.7E+03	3.9E+03	1.5E+03	7.71	2.46	4.61	4.8E+02
4	R^2	-1.6E+03	-1.87	-9.7E+02	-2.84	-3.44	-5.4E+02	-5.62	-1.0E+03	-1.1E+03	-2.0E+03	0.30	0.83	0.58	-6.1E+01
	MSE	1.8E+04	31.27	1.1E+04	41.85	48.43	5.9E+03	72.25	1.1E+04	1.2E+04	2.2E+04	7.60	1.85	4.61	6.7E+02
5	R^2	-2.1E+03	-1.84	-9.8E+02	-2.83	-3.66	-6.7E+03	-5.93	-1.1E+03	-1.3E+03	-2.0E+03	0.27	0.78	0.58	-7.1E+01
	MSE	2.3E+04	30.98	1.1E+04	41.77	50.78	7.3E+04	75.60	1.2E+04	1.4E+04	2.2E+04	7.95	2.38	4.61	7.9E+02
6	R^2	-1.4E+03	-1.82	-3.7E+02	-2.81	-3.74	-7.9E+02	-5.81	-6.7E+02	-7.7E+02	-1.3E+03	0.30	0.77	0.58	-6.5E+01
	MSE	1.5E+04	30.80	4.0E+03	41.58	51.68	8.6E+03	74.27	7.3E+03	8.4E+03	1.4E+04	7.60	2.51	4.61	7.2E+02
7	R^2	-1.1E+06	-2.45	-7.1E+04	-3.89	-1.76	-4.42	-0.78	-8.4E+05	-6.4E+05	-5.9E+05	-12.52	-9.58	-9.33	-3.3E+02
	MSE	9.9E+06	31.12	6.4E+05	44.16	24.92	48.97	16.08	7.6E+06	5.8E+06	5.3E+06	1.2E+02	9.6E+01	9.3E+01	3.0E+03
8	R^2	-1.8E+03	-1.83	-8.3E+02	-2.82	-3.90	-1.7E+03	-5.12	-1.7E+03	-1.7E+03	-1.9E+03	0.30	0.73	0.54	-5.6E+01
	MSE	1.9E+04	30.90	9.0E+03	41.61	53.44	1.9E+04	66.75	1.8E+04	1.8E+04	2.0E+04	7.66	2.90	5.01	6.2E+02
9	R^2	-3.9E+03	-1.89	-4.3E+02	-2.82	-3.33	-8.3E+03	-6.36	-1.0E+03	-6.2E+02	-7.6E+02	0.30	0.35	0.14	-5.8E+01
	MSE	4.3E+04	31.48	4.6E+03	41.66	47.21	9.0E+04	80.34	1.1E+04	6.7E+03	8.2E+03	7.63	7.06	9.38	6.4E+02
10	R^2	-2.1E+03	-1.85	-3.8E+03	-2.83	-2.90	-4.2E+07	-5.42	-6.6E+02	-7.9E+02	-1.2E+03	0.82	0.67	0.82	-5.1E+01
	MSE	2.2E+04	31.08	4.1E+04	41.79	42.59	4.6E+08	70.05	7.2E+03	8.6E+03	1.3E+04	1.94	3.61	1.95	5.7E+02
11	R^2	-1.5E+03	-1.84	-9.3E+02	-2.84	-3.81	-1.9E+04	-6.00	-1.0E+03	-8.3E+02	-1.7E+03	0.32	0.76	0.14	-6.4E+01
	MSE	1.7E+04	31.01	1.0E+04	41.91	52.49	2.1E+05	76.33	1.1E+04	9.1E+03	1.8E+04	7.45	2.61	9.41	7.1E+02
12	R^2	-1.6E+03	-2.35	-9.9E+02	-2.87	-5.34	-12.45	-8.54	-8.7E+02	-7.6E+02	-1.7E+03	0.19	0.77	0.58	-6.8E+01
	MSE	1.7E+04	36.50	1.1E+04	42.21	69.19	1.5E+02	1.0E+02	9.5E+03	8.3E+03	1.8E+04	8.80	2.50	4.61	7.5E+02
13	R^2	-1.0E+03	-1.96	-6.6E+03	-3.01	-2.12	-2.1E+09	-9.22	-2.3E+03	-1.7E+03	-1.4E+03	0.86	-1.27	0.82	-5.7E+01
	MSE	1.1E+04	31.43	7.0E+04	42.60	33.10	2.2E+10	1.1E+02	2.5E+04	1.8E+04	1.5E+04	1.48	24.09	1.89	6.2E+02
14	R^2	-4.4E+03	-1.86	-8.6E+02	-2.84	-3.76	-21.50	-17.75	-4.4E+03	-4.8E+03	-5.3E+03	0.32	0.76	0.67	-8.9E+03
	MSE	4.8E+04	31.22	9.4E+03	41.89	51.92	2.5E+02	2.0E+02	4.8E+04	5.2E+04	5.7E+04	7.40	2.63	3.59	9.8E+04
15	R^2	-1.5E+06	-2.68	-4.4E+04	-4.26	-1.91	-4.01	-1.35	-9.1E+05	-4.6E+05	-5.6E+05	-17.41	-8.52	-51.11	-1.3E+02
	MSE	1.4E+07	32.88	3.9E+05	47.00	26.02	44.78	21.02	8.2E+06	4.1E+06	5.0E+06	1.6E+02	8.5E+01	4.7E+02	1.2E+03
16	R^2	-8.7E+05	-2.64	-4.0E+04	-4.24	-1.84	-4.17	-1.44	-3.4E+05	-2.6E+05	-2.7E+05	-14.24	-9.36	-9.43	-8.4E+01
	MSE	7.8E+06	32.54	3.6E+05	46.77	25.34	46.19	21.83	3.0E+06	2.3E+06	2.4E+06	1.4E+02	9.2E+01	9.3E+01	7.6E+02
17	R^2	-7.9E+05	-2.68	-3.2E+04	-4.29	-1.92	-3.99	-1.53	-3.2E+05	-2.6E+05	-2.7E+05	-17.01	-11.35	-9.43	-9.8E+01
	MSE	7.1E+06	32.82	2.9E+05	47.25	26.11	44.60	22.58	2.9E+06	2.3E+06	2.4E+06	1.6E+02	1.1E+02	9.3E+01	8.9E+02

Table S6: *'Forecasting' mean R^2/MSE Dataset A test errors as a function of I/O combinations and machine learning algorithms. The complete Dataset A was used for model training. I/O numbers are given in Table 1 of the full paper. Machine learning algorithm numbers correspond to the algorithms given at the beginning of Section 3 of the full paper.*

I/O	Error	Machine Learning Algorithm													
		1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	R^2	0.97	-0.44	0.95	-0.26	0.9	0.88	0.96	0.97	0.97	0.97	0.93	0.98	0.95	0.93
	MSE	1.27	84.7	2.99	70.2	4.75	5.62	3.29	1.23	1.21	1.19	3.77	0.34	0.85	3.43
2	R^2	0.97	-0.38	0.95	-0.23	0.9	0.89	0.97	0.98	0.97	0.97	0.94	0.99	0.97	0.89
	MSE	1.29	75.9	2.76	66.84	4.7	5.42	2.43	1.2	1.19	1.17	3.59	0.33	0.47	3.79
3	R^2	0.98	0.06	0.95	-0.22	0.97	0.95	0.97	0.98	0.98	0.97	0.93	0.98	0.96	0.93
	MSE	1.21	54.29	3.09	71.31	1.54	3.21	2.73	1.22	1.24	1.19	4.07	0.54	0.91	3.12
4	R^2	0.97	-0.42	0.95	-0.26	0.91	0.91	0.98	0.97	0.97	0.97	0.93	0.99	0.96	0.93
	MSE	1.32	75.91	2.67	72.18	4.4	4.41	1.59	1.19	1.2	1.19	4.04	0.43	0.79	3.05
5	R^2	0.97	-0.43	0.95	-0.26	0.9	0.9	0.97	0.97	0.97	0.97	0.94	0.99	0.97	0.94
	MSE	1.32	78.6	2.72	70.34	4.72	5	2.34	1.17	1.17	1.2	3.57	0.46	0.67	3.56
6	R^2	0.97	-0.42	0.94	-0.25	0.9	0.91	0.96	0.97	0.97	0.97	0.93	0.99	0.93	0.94
	MSE	1.3	81.68	3.43	75.36	5.31	5.23	3.64	1.2	1.21	1.18	3.99	0.46	1.2	3.14
7	R^2	0.38	-0.39	0.01	-0.24	-0.09	-0.16	0.25	0.39	0.39	0.42	-0.03	0.67	0.52	0.26
	MSE	34.74	76.86	50.97	65.2	52.23	54.98	33.63	29.29	29.51	29.66	44.99	9.34	13.22	40.72
8	R^2	0.97	-0.41	0.95	-0.23	0.91	0.9	0.96	0.97	0.97	0.97	0.93	0.97	0.96	0.95
	MSE	1.3	76.13	3.14	69.42	4.83	5.89	3.1	1.23	1.21	1.18	4.16	0.41	0.88	2.76
9	R^2	0.96	-0.4	0.95	-0.24	0.89	0.91	0.97	0.96	0.96	0.96	0.94	0.96	0.97	0.92
	MSE	1.94	84.42	3.17	69.3	5.25	4.25	1.58	1.78	1.78	1.7	3.73	0.58	0.77	4.41
10	R^2	0.95	-0.38	0.93	-0.27	0.82	0.7	0.96	0.96	0.96	0.96	0.89	0.98	0.94	0.91
	MSE	2.14	76.04	3.4	75.45	8.69	14.02	3.16	1.89	1.84	1.87	5.94	0.68	0.83	4.22
11	R^2	0.97	-0.45	0.95	-0.29	0.92	0.92	0.95	0.98	0.98	0.97	0.94	0.98	0.98	0.91
	MSE	1.26	80	3.26	79.15	4.79	4.92	4.17	1.17	1.19	1.18	3.35	0.26	0.87	3.53
12	R^2	0.97	-0.27	0.95	-0.22	0.93	0.97	0.95	0.97	0.97	0.98	0.94	0.98	0.98	0.92
	MSE	1.33	75.12	3.02	71.77	3.77	1.6	3.24	1.16	1.17	1.16	3.69	0.46	1.15	4.56
13	R^2	0.95	-0.43	0.92	-0.26	0.8	0.93	0.92	0.96	0.95	0.96	0.9	0.96	0.96	0.93
	MSE	2.56	83.78	4.06	73.65	9.45	3.25	5.7	2.25	2.2	2.19	5.55	1.23	2.28	3.67
14	R^2	0.96	-0.41	0.95	-0.23	0.91	0.9	0.89	0.97	0.96	0.96	0.93	0.98	0.98	0.96
	MSE	2.01	75.65	2.77	70.24	4.61	4.89	6.93	1.67	1.59	1.59	3.63	0.39	0.96	2.01
15	R^2	0.37	-0.39	0.02	-0.25	-0.15	-0.23	0.27	0.43	0.43	0.43	0.02	0.37	0.35	0.14
	MSE	33.07	76.16	56.03	73.43	59.71	63.08	36.29	28.78	28.85	29.63	47.13	11.01	10.21	40.09
16	R^2	0.38	-0.43	0.06	-0.23	-0.14	-0.23	0.36	0.45	0.45	0.47	0.08	0.57	0.42	0.19
	MSE	31.67	83.49	48.85	64.86	54.27	58.04	29.03	27.31	27.08	27.62	48.46	10.43	14.45	36.41
17	R^2	0.4	-0.4	0.04	-0.24	-0.17	-0.27	0.36	0.46	0.46	0.47	0.09	0.68	0.77	0.28
	MSE	34.55	79.99	51.72	68.49	56.96	60.77	29.85	27.36	27.19	27.62	45.61	7.18	9.5	37.73

Table S7: *'Forecasting' mean R^2/MSE Dataset A-D test errors as a function of I/O combinations and machine learning algorithms. The complete Dataset A-D was used in the model training. I/O numbers are given in Table 1 of the full paper. Machine learning algorithm numbers correspond to the algorithms given at the beginning of Section 3 of the full paper.*

I/O	Error	Machine Learning Algorithm													
		1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	R^2	0.04	4.33	7.3E+03	10.18	0	0.91	0	0.04	0.05	0.05	0.57	0.32	0.03	4.19
	MSE	3.4	88.01	2.0E+03	79.27	39.36	9.5E+02	27.08	3.23	3.17	3.57	25.19	42.97	13.62	7.75
2	R^2	0.04	4.23	1.7E+08	10.65	0	1.38	0	0.04	0.05	0.05	0.51	0.63	0.03	3.9
	MSE	3.21	82.16	1.6E+08	83.08	39.6	4.7E+02	28.37	3.4	3.12	3.5	22.24	31.65	27.8	8.68
3	R^2	0.04	3.75	1.1E-01	6.3E+19	0	0.01	0	0.04	0.04	0.05	0.54	1.19	0.06	3.33
	MSE	3.69	82.43	3.8E+00	2.2E+24	45.95	4.9E+03	26.64	3.79	3.01	3.57	22.25	28.69	11.62	7.26
4	R^2	0.04	4.59	7.4E+03	10.38	0.06	1.66	0	0.04	0.04	0.05	0.52	0.94	0.04	3.49
	MSE	3.47	88.59	1.7E+03	80.97	40.3	1.1E+03	28.83	3.32	3.3	3.57	22.3	24.25	21.6	7.43
5	R^2	0.04	4.1	7.2E+03	9.63	0	1.32	0	0.05	0.04	0.05	0.44	0.12	0.03	3.52
	MSE	3.34	82.47	1.6E+03	77.33	37.82	5.2E+02	25.63	3.88	3.77	3.58	21.24	19.04	21.44	6.76
6	R^2	0.04	4.04	1.4E+04	10.15	0	2.05	0	0.05	0.04	0.05	0.42	0.32	0.11	3.74
	MSE	3.2	87.43	4.2E+03	80.58	38.89	6.7E+02	26.98	3.64	3.02	3.59	23.17	13.96	17.13	6.96
7	R^2	4.05	3.98	9.1E+11	9.48	0.58	2.56	1.68	4.58	4.76	4.65	4.42	1.26	1.09	38.52
	MSE	75.39	74.79	8.3E+11	72.98	61.53	69.17	62.17	92.49	94.18	82.82	48.95	26.2	45.67	129.19
8	R^2	0.04	4.4	5.7E+03	9.99	0	1.3	0	0.05	0.05	0.05	0.48	0.25	0.01	3.86
	MSE	2.94	88.09	2.5E+03	80.24	38.4	4.6E+02	27.28	3.64	3.32	3.42	22.02	33.03	29.49	6.73
9	R^2	0.21	4.35	4.5E+09	10.42	0	1.74	0	0.24	0.24	0.2	0.58	1.14	0.06	7.27
	MSE	23.86	85.93	2.8E+09	78.37	42.89	2.6E+02	30.35	23.97	23.93	21.94	24.06	30.78	41.46	25.14
10	R^2	0.07	4.12	1.7E+04	9.92	0	1.84	0	0.11	0.1	0.1	0.51	0.57	0.09	4.33
	MSE	3.86	80.43	3.3E+03	78.25	45.42	85.8	31.3	3.23	4.12	4.2	25.74	24.02	13.18	8.49
11	R^2	0.04	4.11	1.2E+04	9.86	0	1.49	0	0.04	0.04	0.05	0.55	0.14	0.16	6.63
	MSE	3.78	85.28	3.7E+03	75.76	37.22	7.9E+02	26.55	3.21	3.04	3.67	22.25	19.18	12.72	8.72
12	R^2	0.04	4.14	1.4E+04	10.34	0	1.74	0	0.05	0.05	0.06	0.47	1.25	0.43	3.62
	MSE	2.07	84.06	2.4E+03	79.42	20.5	18.1	27.67	1.69	1.63	1.55	23.27	23.33	36.97	6.11
13	R^2	0.14	4.1	8.4E+10	10.67	0.01	1.53	0	0.14	0.16	0.15	0.45	1.18	0.07	11.36
	MSE	3.93	81.97	7.4E+10	84.22	62.69	65.55	33.55	3.78	2.94	3.74	22.52	21.45	16.1	14.53
14	R^2	0.09	4.46	9.6E+03	9.92	0.28	2.88	0	0.09	0.09	0.1	0.5	0.96	0.02	1.1
	MSE	3.99	87.55	2.3E+03	79.4	40.11	4.3E+02	35.61	4.43	3.82	4.52	24.04	25.08	19.31	12.94
15	R^2	2.68	4.11	1.1E+05	9.32	0.72	2.42	0.53	2.9	2.97	2.97	4.32	1.78	1.84	40.63
	MSE	59.33	76.09	1.0E+05	74.77	60.04	73.57	55.75	69.49	70.01	57.44	52.89	64.86	76.17	116.27
16	R^2	1.9	4.38	2.8E+11	9.32	0.69	2.68	0.22	2.07	2.13	2.08	3.28	1.2	0.68	35.61
	MSE	80.03	79.3	2.7E+11	74.45	58.56	69.82	54.43	92.4	87.84	93.56	52.43	39.06	63.26	120.07
17	R^2	1.97	3.91	8.4E+04	9.54	0.63	3.27	0.24	2.03	2.02	2.06	3.98	0.52	0.86	61.71
	MSE	88.55	74.1	7.8E+04	75.6	60.16	72.62	56.31	112.57	110.94	95.36	54.18	37.99	65.47	194.67

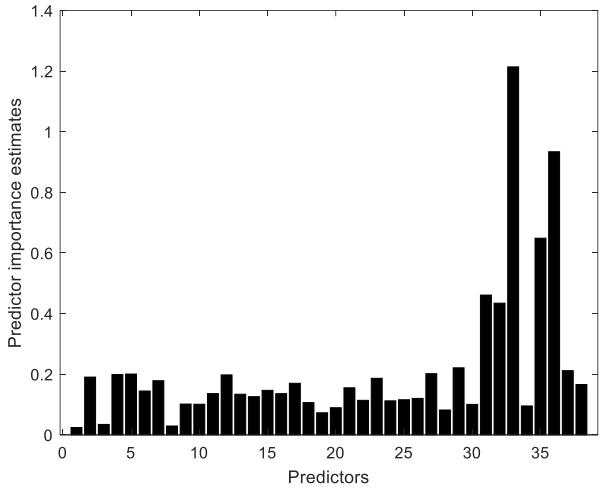
Table S8: *Mean R^2/MSE Dataset E-J test errors as a function of I/O combinations and machine learning algorithms. The complete Dataset E-J was used for model training. I/O numbers are given in Table 2 of the full paper. Machine learning algorithm numbers correspond to the algorithms given at the beginning of Section 3 of the full paper.*

I/O	Error	Machine Learning Algorithm													
		1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	R^2	0.81	0.35	0.83	-5.5	0.91	0.90	0.93	0.85	0.85	0.85	0.82	0.83	0.91	0.92
	MSE	0.19	0.68	0.17	6.8	0.10	0.10	0.07	0.15	0.16	0.16	0.19	0.17	0.09	0.08
2	R^2	-0.11	-0.01	0.15	-3.8E+02	0.36	0.33	0.56	0.00	-0.05	-0.08	0.37	0.37	0.03	0.56
	MSE	6.15	5.87	4.50	3.4E+03	3.46	3.74	1.97	4.31	4.71	4.41	2.89	3.02	3.96	1.95
3	R^2	0.77	0.79	0.75	-7.9E+07	0.85	0.84	0.85	0.78	0.78	0.78	0.83	0.82	0.83	0.86
	MSE	0.24	0.21	0.26	7.9E+07	0.15	0.17	0.16	0.22	0.22	0.22	0.18	0.18	0.17	0.14
4	R^2	0.06	0.24	0.07	-2.9E+04	0.44	0.30	0.37	0.08	0.08	0.08	0.40	0.35	0.22	0.43
	MSE	5.20	4.55	4.59	1.4E+05	2.53	2.94	3.03	4.17	4.17	3.72	2.43	3.00	3.17	2.49

Table S9: *Mean R^2/MSE Dataset F-J test errors as a function of I/O combinations and machine learning algorithms. The complete Dataset E was used for model training. I/O numbers are given in Table 2 of the full paper. Machine learning algorithm numbers correspond to the algorithms given at the beginning of Section 3 of the full paper.*

I/O	Error	Machine Learning Algorithm													
		1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	R^2	-1.77	-0.62	-0.80	-13	0.30	-0.32	0.03	-0.14	-0.43	-0.58	0.11	0.12	0.28	-1.26
	MSE	2.21	1.29	1.43	11	0.56	1.05	0.77	0.91	1.14	1.25	0.70	0.70	0.57	1.80
2	R^2	-1.20	-0.26	-0.29	-9.3E+02	-0.06	-0.14	-0.06	-0.18	-0.27	-0.33	-0.08	-0.10	-0.04	-1.58
	MSE	52.66	30.00	30.77	2.2E+04	25.43	27.30	25.42	28.16	30.25	31.79	25.74	26.26	24.84	61.58
3	R^2	-0.52	-0.18	-0.57	-2.1E+07	-0.03	-0.44	-0.24	-0.48	-0.50	-0.49	-0.05	-0.26	-0.12	-0.36
	MSE	1.21	0.94	1.25	1.7E+07	0.82	1.14	0.99	1.18	1.19	1.19	0.83	1.00	0.89	1.08
4	R^2	-0.31	-0.22	-0.28	-2.3E+04	-0.18	-0.18	-0.13	-0.30	-0.30	-0.30	-0.07	-0.23	-0.18	-0.31
	MSE	31.19	29.05	30.61	5.4E+05	28.14	28.30	27.00	30.96	31.01	30.98	25.59	29.30	28.23	31.41

Figure S1: *Predictor importance estimates as a function of predictors for the bagged random forest trained using Dataset A. Predictors 1-30 correspond to variables relevant to experimental initial conditions, whereas predictors 32-37 correspond to different species elemental releases.*



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