Influence of Dissolution on Fate of Nanoparticles in Freshwater

Yubing Pu, Bertrand Laratte, and Rodica Elena Ionescu

***Abstract*—The fate of engineering nanoparticles (ENPs) determines how long they stay in a certain compartment such as freshwater. Many factors such as diameter of suspended particles in freshwater, depth of freshwater, may affect the fate of ENPs in freshwater with different extent. Dissolution rate (k_{diss}) of ENPs has been demonstrated as one of the most significant parameters. However, the influences of k_{diss} on relative importance of the other parameters are still not clear. In this study, the relative importance of four parameters has been calculated with the k_{diss} being fixed to eight different values respectively. The relative importance decreases along with the increasing k_{diss} values. The results are well fitted ($R^2 > 0.999$) by an exponential associate function, which simplifies the calculation of the relative importance of the studied parameters.**

***Index Terms*—Dissolution rate, fate model, nanoparticle, sensitivity analysis, exponential associate function.**

I. Introduction

The production and application of engineering nanoparticles (ENPs) are increasing rapidly due to their relatively specific characteristics compared to their bulk counterparts. Ref. [1]-[3] the wastewater treatment plant (WWTP) effluent is the main source of the ENPs in aquatic ecosystems. Ref. [4] fate describes the possible transport and destination of a substance. After the ENPs release into freshwater, many behaviors may occur (such as dissolution, aggregation, and transformation [5]) which are usually addressed as the fate of ENPs. Essentially, dissolution of ENPs is a transformation process from their solid form to the dissolved ionic form or other intermediates. Ref. [6] there are two important elements related to dissolution: solubility and dissolution rate. Solubility is the maximum amount of a solute (in this study is the ENPs) that a solvent can hold in solution at certain conditions. Dissolution rate presents how long it takes to get the saturation concentration of a solute. Solubility is an endpoint, while dissolution rate is a kinetic process. Although the solubility and dissolution rate are different concepts, they are related. Based on the famous Noyes-Whitney equation, when dissolution is limited by diffusion, dissolution rate has positive correlation with solubility [7].

The dissolution of various ENPs could differ from each other vastly due to their different physical-chemical properties. However, even the same ENPs may have very different solubility and dissolution rate because of the different environmental conditions. For example, titanium dioxide nanoparticles (nano-TiO_2) were assumed to be practically insoluble in freshwater in many studies, [8], [9] while they were confirmed being able to dissolve in acid aqueous NaCl solutions (pH < 3) at temperatures of 25 and 37 °C. [10] Dissolution of zinc oxide nanoparticles (nano-ZnO) was observed with 7.18-7.40 mg/L dissolved Zn in pure water, but with much higher dissolved Zn concentration (> 34 mg/L) in a cell culture medium [11].

In order to appropriately assess the potential environmental impact of ENPs, many fate models have been developed to predict the fate of ENPs in various environmental media, particularly the aquatic media. Ref. [8], [12] a recently published research has demonstrated that there are many factors affecting the output of fate model, such as dissolution rate of ENPs, diameter of suspended particles in freshwater, depth of freshwater. Among them, dissolution rate is one of the most significant factor for many subcontinental regions [12].

However, directly modeling the dissolution of ENPs to understand its influence on fate of ENPs is difficult. Many factors may affect dissolution of ENPs in freshwater, such as temperature, pH, ion strength, natural organic matters. Ref. [5], [13] Even though some studies have described the dissolution kinetics of ENPs under extreme oxidative, acidic, or alkaline conditions, [14] the modeling of dissolution rate of ENPs in freshwater is complex and still in its infancy. Ref. [11], [12] therefore, in practice, as an acceptable simplification, the dissolution rate constant of ENPs in freshwater is assumed to be 0-10^{-5} s^{-1} for different ENPs. [14]

In this study, four important input parameters of a fate model were selected. The influences of k_{diss} on fate model were indirectly investigated by studying the influences of k_{diss} on the relative importance of the four selected parameters.

II. Methods

A. Fate Model for Enps in Freshwater

Recently, a fate model based on colloid science has been

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proposed by our group to calculate the persistence time of ENPs in freshwater ecosystem. Ref. [12] its functionality was proved and it could be used to calculate ENPs' characterization factor (CF), an important input parameter in life cycle impact assessment (LCIA).

In the fate model, three behaviors have been considered as removal processes for freshwater after the ENPs released into freshwater: dissolution, sedimentation, and advection to other water compartments. In addition, the fate model considered 17 different subcontinental regions shown in Table I and gave the recommended values for each input parameter. Essentially, the fate model is a mathematical function with many input values. Thus, in this study, the fate model is defined as: $FF(\delta_1, \delta_2, \delta_3, \cdots)$. The δ_i (i = 1, 2, 3, ⋯) represents input parameters (such as radius of ENPs, depth of freshwater). More detailed information about the fate model could be found in the study of Pu, *et al.* [12].

TABLE I: THE 17 DIFFERENT SUBCONTINENTAL REGIONS CONSIDERED IN THE STUDY OF PU ET AL. [12]

Region ID	Region*
DEFAULT	Unknown region
W1	Central and west Asia
W2	Indochina
W3	Northern Australia
W4	Southern Australia & New Zealand
W5	Southern Africa
W6	North, West, East & Central Africa
W7	Argentina+
W8	Brazil+
W9	Central America+ & Caribbean
W10	USA & Southern Canada
W12	Northern Europe & Northern Canada
W13	Europe
W14	East Indies & Pacific
CHI	Eastern China
JAP	Japan & Korean peninsula
IND	India+

*The further details about the countries within each region can be found in the study of Shaked. [15]

B. Sensitivity Analysis of Fate Model

Since the input values of fate model may vary in different literature sources, a sensitivity analysis for studying the influences of main input parameters on output results was carried out in previous study.[12] By doing this, it was possible to determine which input parameter should receive more attention in the future. One of the methods used in the study was labeled as "Single Parameter SA".[12] It was performed by varying each selected parameter within its range while holding the others constant. There were 13 parameters involved in total. The recommended values and ranges of main input parameters are listed in Table II. The first five parameters with high relative importance follow the order shown in (1), while the relative importance of the other studied parameters was at least 3 orders of magnitude lower compared to the first fives.[12]

$$k_{diss} > r_{LSP} > \rho_{SNP} > \alpha_2 \approx Depth_{water} \quad (1)$$

where k_{diss} is the dissolution rate of ENPs in freshwater; r_{LSP} is the radius of larger suspended particles (LSP, > 450 nm) in freshwater; ρ_{SNP} is the density of the suspended particles in freshwater; α_2 is the attachment efficiency between ENPs and LSP; $Depth_{water}$ is the depth of freshwater.

TABLE II: RECOMMENDED VALUES AND RANGES OF FIVE INPUT PARAMETERS FOR THE SENSITIVITY ANALYSIS EXTRACTED FROM THE STUDY OF PU ET AL. [12]

Parameter	Unit	Value	Range	Reference
k_{diss}	s^{-1}	$5\cdot10^{-6}$	$0\text{-}1\cdot10^{-5}$	[12], [14]
r_{LSP}	m	$1.05\cdot10^{-5}$	$5\cdot10^{-7}\text{-}1\cdot10^{-4}$	[12], [16], [17]
ρ_{SNP}	kg m^{-3}	1230	1100-2500	[12], [16]
α_2	--	0.9	0.001-1	[8], [12]
$Depth_{water}$	m	--	0.5-2 $Depth_{water}$	[12], [18]

C. Sensitivity Analysis with Different Dissolution Rate

In the sensitivity analysis of fate model in the study of Pu *et al*. [12], the k_{diss} of ENPs was set as $5\cdot10^{-6}$ s^{-1} as shown in Table II by the method "Single Parameter SA" when assessing the other parameters' relative importance. However, because the k_{diss} of ENPs is the most important parameter for many studied regions [12] and could be any value between 0 and $1\cdot10^{-5}$ s^{-1}, [14] the different k_{diss} values may have big influences on the sensitivity analysis results. Thus, in this study, eight values of k_{diss} have been selected to explore their potential influence on sensitivity analysis results. The eight selected values of k_{diss} are 0, $1\cdot10^{-7}$ s^{-1}, $5\cdot10^{-7}$ s^{-1}, $1\cdot10^{-6}$ s^{-1}, $3\cdot10^{-6}$ s^{-1}, $5\cdot10^{-6}$ s^{-1}, $7\cdot10^{-6}$ s^{-1}, and $1\cdot10^{-5}$ s^{-1}, respectively.

In practice, the fate model is simplified as a model with five variables (Ⓐ, Ⓑ, Ⓒ, Ⓓ, Ⓔ) as shown in Fig. 1. From the aspect of computational mathematics, the fate model can be expressed as:

$$FF(k_{diss}, r_{LSP}, \rho_{SNP}, \alpha_2, Depth_{water}) \quad (2)$$

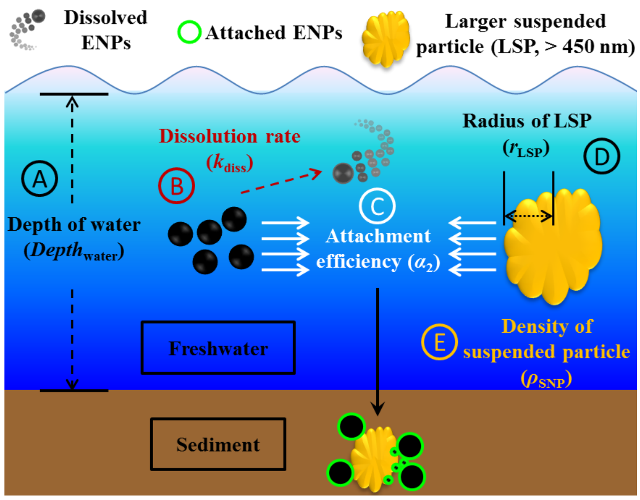

Fig. 1. The five fate model input parameters considered in this study: k_{diss}, $Depth_{water}$, α_2, r_{LSP}, and ρ_{SNP}.

The values and ranges of the four parameters (r_{LSP}, ρ_{SNP}, α_2, and $Depth_{water}$) are listed in Table II. All the other parameters are considered as constants and can be found in the study of Pu et al. [12] The method for doing sensitivity analysis is the same as "Single Parameter SA" by software MATLAB. [12], [19] When one parameter (δ) changes its value in its range, the other parameters stay as constants. In this way, a maximum ($FF(\delta)_{max}$) and minimum ($FF(\delta)_{min}$) value can be obtained. The difference between $FF(\delta)$max and $FF(\delta)$min is defined as $DFF(\delta)$:

$$DFF(\delta) = FF(\delta)_{\max} - FF(\delta)_{\min} \quad (3)$$

The value of $DFF(\delta)$ represents the relative importance of the parameter δ for one given region.

III. Results and Discussions

A. *Relative Importance of Four Studied Parameters in 17 Subcontinental Regions*

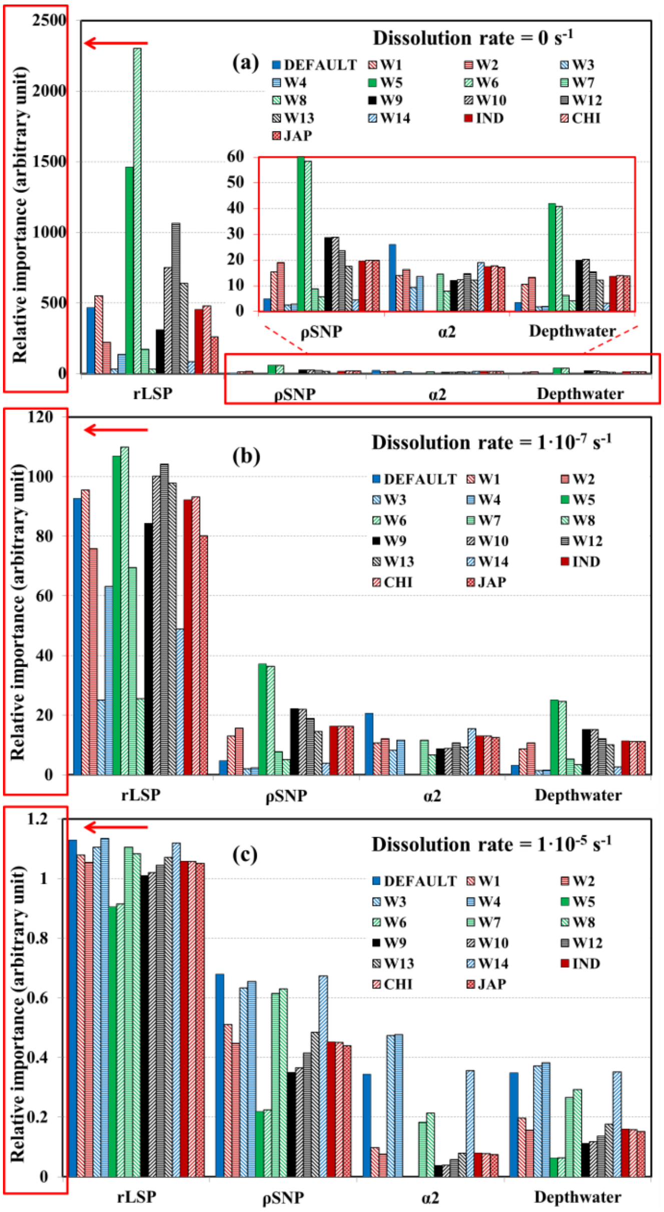

Fig. 2. Relative importance of the four studied parameters (r_{LSP}, ρ_{SNP}, α_2, and $Depth_{water}$) in 17 subcontinental regions for ENPs' fate model, when (a) k_{diss} = 0; (b) $k_{diss} = 1 \cdot 10^{-7}$ s^{-1}; (c) $k_{diss} = 1 \cdot 10^{-5}$ s^{-1}.

The tables in Appendix list the relative importance of the four studied parameters (r_{LSP}, ρ_{SNP}, α_2, and $Depth_{water}$) in 17 subcontinental regions for ENPs' fate model, when the k_{diss} respectively equals 0 (Table III), $1 \cdot 10^{-7}$ s^{-1} (Table IV), $5 \cdot 10^{-7}$ s^{-1} (Table V), $1 \cdot 10^{-6}$ s^{-1} (Table VI), $3 \cdot 10^{-6}$ s^{-1} (Table VII), $7 \cdot 10^{-6}$ s^{-1} (Table VIII), and $1 \cdot 10^{-5}$ (Table IX). The results related to $k_{diss} = 5 \cdot 10^{-6}$ s^{-1} were described in the study of Pu et al. [12] Here, three scenarios were shown by Fig. 2. Fig. 2(a) represents the case of insoluble ENPs with k_{diss} = 0, while Fig. 2(c) is the situation of the ENPs with very quick dissolution rate equaling $1 \cdot 10^{-5}$ s^{-1}. Fig. 2(b) shows a general case ($k_{diss} = 1 \cdot 10^{-7}$ s^{-1}) between the two extreme situations.

It is obvious that the relative importance of a certain parameter for the same region under different dissolution rates of ENPs has big differences. The scales of vertical axis for the three scenarios are 10^3 (k_{diss} = 0, Fig. 2(a)), 10^2 ($k_{diss} = 1 \cdot 10^{-7}$ s^{-1}, Fig. 2(b)) and 10^1 ($k_{diss} = 1 \cdot 10^{-5}$ s^{-1}, Fig. 2(c)), respectively. In addition, the relative importance of different parameters differs from each other even under the same dissolution rate of ENPs. For example, the relative importance of r_{LSP} for W6 region (2300.812) is more than 700 times higher than for W3 region (32.302).

B. *Influence of Dissolution Rate on Relative Importance of Four Studied Parameters*

When dissolution rate was fixed to one value, the relative importance of one studied parameter (such as r_{LSP} and ρ_{SNP}) for all the regions were calculated by summing the relative importance values of the same parameter for all the 17 subcontinental regions. The results are shown in Fig. 3. The relative importance of the four studied parameters follows the order below:

$$r_{LSP} > \rho_{SNP} > \alpha_2 \approx Depth_{water} \quad (4)$$

This order is the same as the one reported in the study of Pu *et al.*, which demonstrates that the change of dissolution rate will not change the priority of other parameters. However, it should be noted that the relative importance values of the four studied parameters decrease along with the increasing dissolution rates. The relative importance values have dropped dramatically with the dissolution rate lower than $1 \cdot 10^{-6}$ s^{-1}, while they decrease gradually with the dissolution rate between $1 \cdot 10^{-6}$ and $1 \cdot 10^{-5}$ s^{-1}.

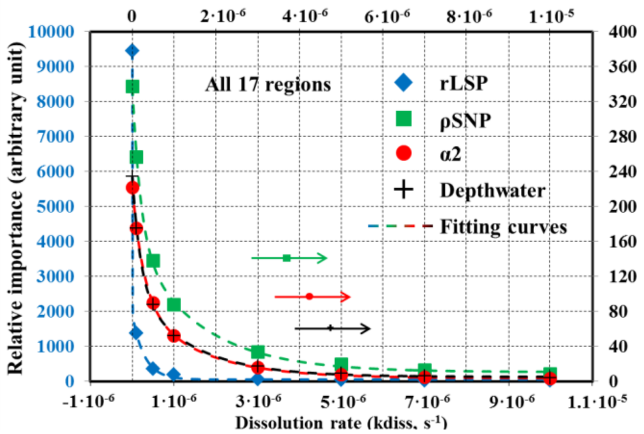

Fig. 3. Influence of dissolution rate on relative importance of the four studied parameters (r_{LSP}, ρ_{SNP}, α_2, and $Depth_{water}$) for 17 subcontinental regions.

The four curves in Fig. 3 were fitted by an exponential associate function using Origin 9.0, respectively. All the four coefficients of determination (R^2) are higher than 0.999, which indicates that the fitting is quite successful.

The fitting equation is shown in (5) and the values of fitting parameters are listed in Table X.

$$y = A + B \cdot (1 - e^{(-x/C)}) + D \cdot (1 - e^{(-x/E)}) \quad (5)$$

where y represents the relative importance of one given parameter (i.e. r_{LSP}, ρ_{SNP}, α_2, and $Depth_{water}$) for 17 subcontinental regions and x is the dissolution rate of ENPs. e is the mathematical constant which is approximately equal to 2.71828.

TABLE X: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	$9.44 \cdot 10^{3}$	$3.37 \cdot 10^{2}$	$2.21 \cdot 10^{2}$	$2.33 \cdot 10^{2}$
B	$-1.85 \cdot 10^{3}$	$-1.78 \cdot 10^{2}$	$-1.28 \cdot 10^{2}$	$-1.29 \cdot 10^{2}$
C	$2.90 \cdot 10^{-7}$	$2.05 \cdot 10^{-7}$	$2.75 \cdot 10^{-7}$	$2.04 \cdot 10^{-7}$
D	$-7.54 \cdot 10^{3}$	$-1.48 \cdot 10^{2}$	$-8.95 \cdot 10^{1}$	$-9.94 \cdot 10^{1}$
E	$6.40 \cdot 10^{-11}$	$1.59 \cdot 10^{-6}$	$1.49 \cdot 10^{-6}$	$1.38 \cdot 10^{-6}$
R^2	0.99974	0.99911	0.99971	0.99928

Interestingly, the relative importance of one studied parameter (such as r_{LSP}, ρ_{SNP}) for one subcontinental region (W1, W2, JAP, etc.) can also be well fitted by (5). One example of JAP region is shown in Fig. 4. The fitting parameters and coefficients of determination are listed in Table XI. The results for other regions are listed in tables from Table XII to Table XXVII, respectively.

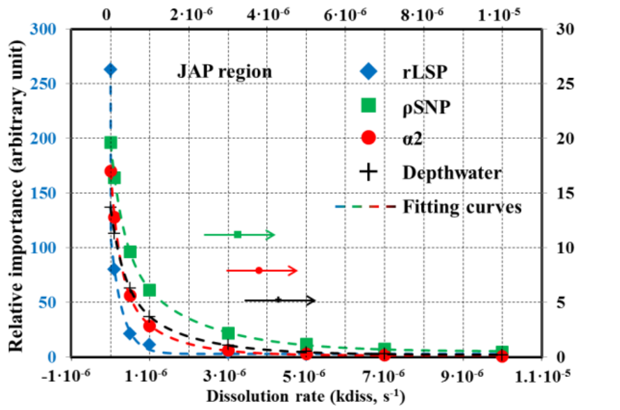

Fig. 4. Influence of dissolution rate on relative importance of the four studied parameters (r_{LSP}, ρ_{SNP}, α_2, and $Depth_{water}$) for JAP region.

Equation (5) and the parameters listed in Table X, Table XI-XXVII can be very practical for predicting the relative importance of the four studied parameters (r_{LSP}, ρ_{SNP}, α_2, and $Depth_{water}$) in 17 subcontinental regions (in total or in separate) by just introducing the k_{diss} value as input data. It is noteworthy that although all the fitting parameters were calculated essentially based on the previous fate model and the recommended values in literature, [12] the results reported in this study can be expediently updated with new available data.

IV. CONCLUSION

Modeling the fate of ENPs in freshwater is a way to estimate the persistence time of ENPs. Various input parameters (e.g. radius and density of ENPs, depth of freshwater) have different influences on the output of ENP's fate model. Dissolution rate (k_{diss}) of ENPs plays an important role in estimation of ENPs' fate in freshwater. It also has significant influence on the relative importance of the other input parameters. The relative importance of the four studied parameters (r_{LSP}, ρ_{SNP}, α_2, and $Depth_{water}$) decreases along with the increasing k_{diss} values. The results are well fitted (R^2 > 0.999) by an exponential associate function which could be used for predicting the relative importance of the four studied parameters in 17 subcontinental regions (in total or in separate).

APPENDIX

TABLE III: THE RELATIVE IMPORTANCE (RI, ARBITRARY UNITS) OF FOUR DIFFERENT INPUT PARAMETERS IN FATE MODEL FOR 17 SUBCONTIENTAL REGIONS; DISSOLUTION RATE OF ENPS IS EQUAL TO 0

Regions	RI(r_{LSP})	RI(ρ_{SNP})	RI(α_2)	RI($Depth_{water}$)
DEFAULT	467.005	4.886	26.134	3.415
W1	552.736	15.285	13.732	10.276
W2	221.949	18.773	16.169	13.084
W3	32.302	2.266	9.176	1.580
W4	139.565	2.603	13.351	1.817
W5	1462.919	60.067	0.000	41.941
W6	2300.812	58.223	0.000	40.676
W7	174.505	8.594	14.230	5.997
W8	32.991	5.547	7.640	3.845
W9	313.397	28.749	12.115	20.032
W10	752.095	28.645	12.242	20.004
W12	1064.061	23.522	14.496	15.120
W13	640.396	17.268	11.926	12.061
W14	85.272	4.248	18.793	2.964
IND	455.734	19.566	17.385	13.661
CHI	482.000	19.669	17.503	13.735
JAP	263.107	19.620	17.027	13.670

TABLE IV: THE RELATIVE IMPORTANCE (RI, ARBITRARY UNITS) OF FOUR DIFFERENT INPUT PARAMETERS IN FATE MODEL FOR 17 SUBCONTIENTAL REGIONS; DISSOLUTION RATE OF ENPS IS EQUAL TO 1.0 ·10-7 S-1

Regions	RI(r_{LSP})	RI(ρ_{SNP})	RI(α_2)	RI($Depth_{water}$)
DEFAULT	92.729	4.661	20.577	3.254
W1	95.623	13.260	10.944	8.915
W2	75.978	15.779	12.278	10.897
W3	25.249	2.216	8.348	1.544
W4	63.260	2.537	11.734	1.770
W5	106.936	37.137	0.000	25.072
W6	109.893	36.477	0.000	24.713
W7	69.548	7.915	11.860	5.507
W8	25.659	5.250	6.830	3.627
W9	84.373	22.239	8.789	15.251
W10	100.155	22.223	8.950	15.325
W12	104.265	19.031	10.836	12.240
W13	97.936	14.724	9.494	10.222
W14	49.083	4.076	15.651	2.840
IND	92.199	16.353	13.067	11.328
CHI	93.229	16.426	13.139	11.380
JAP	80.282	16.377	12.785	11.305

TABLE V: THE RELATIVE IMPORTANCE (RI, ARBITRARY UNITS) OF FOUR DIFFERENT INPUT PARAMETERS IN FATE MODEL FOR 17 SUBCONTIENTAL REGIONS; DISSOLUTION RATE OF ENPS IS EQUAL TO 5.0 ·10-7 S-1

Regions	RI(r_{LSP})	RI(ρ_{SNP})	RI(α_2)	RI($Depth_{water}$)
DEFAULT	22.030	3.925	10.679	2.719
W1	22.138	8.534	5.493	5.599
W2	20.857	9.420	5.509	6.146
W3	13.474	2.034	6.065	1.412

W4	19.842	2.304	7.782	1.602
W5	22.471	13.299	0.000	7.516
W6	22.616	13.303	0.000	7.600
W7	20.391	5.976	6.737	4.078
W8	13.574	4.311	4.662	2.929
W9	21.394	11.193	3.510	6.996
W10	22.305	11.268	3.637	7.139
W12	22.533	10.481	4.659	6.440
W13	22.250	9.095	4.722	6.034
W14	18.184	3.500	9.091	2.420
IND	21.925	9.648	5.747	6.327
CHI	21.983	9.674	5.762	6.344
JAP	21.168	9.627	5.601	6.269

TABLE VI: The Relative Importance (RI, Arbitrary Units) of Four Different Input Parameters in Fate Model for 17 Subcontiental Regions; Dissolution Rate of ENPs Is Equal to 1.0 ·10-6 s-1

Regions	RI(r_{LSP})	RI(ρ_{SNP})	RI(α_2)	RI($Depth_{water}$)
DEFAULT	11.269	3.265	6.318	2.230
W1	11.257	5.767	3.008	3.606
W2	10.896	6.063	2.814	3.664
W3	8.509	1.844	4.437	1.272
W4	10.674	2.064	5.345	1.426
W5	11.170	6.596	0.000	3.177
W6	11.218	6.659	0.000	3.252
W7	10.808	4.528	4.058	2.993
W8	8.536	3.502	3.193	2.322
W9	11.001	6.536	1.659	3.664
W10	11.248	6.619	1.737	3.779
W12	11.328	6.445	2.308	3.666
W13	11.278	5.987	2.558	3.717
W14	10.168	2.965	5.707	2.024
IND	11.183	6.172	2.906	3.751
CHI	11.198	6.182	2.909	3.757
JAP	10.978	6.140	2.822	3.696

TABLE VII: The Relative Importance (RI, Arbitrary Units) of Four Different Input Parameters in Fate Model for 17 Subcontiental Regions; Dissolution Rate of ENPs Is Equal to 3.0 ·10-6 s-1

Regions	RI(r_{LSP})	RI(ρ_{SNP})	RI(α_2)	RI($Depth_{water}$)
DEFAULT	3.801	1.900	1.963	1.208
W1	3.752	2.257	0.743	1.181
W2	3.689	2.179	0.628	1.050
W3	3.434	1.328	1.947	0.887
W4	3.741	1.440	2.122	0.962
W5	3.551	1.572	0.000	0.566
W6	3.568	1.613	0.000	0.588
W7	3.729	2.170	1.195	1.258
W8	3.420	1.925	1.166	1.154
W9	3.654	2.005	0.330	0.860
W10	3.691	2.061	0.350	0.903
W12	3.725	2.162	0.491	0.974
W13	3.746	2.243	0.617	1.127
W14	3.668	1.797	1.921	1.149
IND	3.723	2.203	0.641	1.067
CHI	3.725	2.204	0.640	1.066
JAP	3.696	2.176	0.619	1.040

TABLE VIII: The Relative Importance (RI, Arbitrary Units) of Four Different Input Parameters in Fate Model for 17 Subcontiental Regions; Dissolution Rate of ENPs Is Equal to 7.0 ·10-6 s-1

Regions	RI(r_{LSP})	RI(ρ_{SNP})	RI(α_2)	RI($Depth_{water}$)
DEFAULT	1.623	0.967	0.604	0.538
W1	1.572	0.835	0.187	0.354
W2	1.542	0.752	0.150	0.289
W3	1.560	0.828	0.762	0.514
W4	1.621	0.869	0.782	0.537
W5	1.382	0.406	0.000	0.123
W6	1.394	0.421	0.000	0.128
W7	1.593	0.939	0.337	0.451
W8	1.540	0.925	0.375	0.472
W9	1.496	0.614	0.075	0.212
W10	1.510	0.641	0.079	0.225
W12	1.536	0.711	0.114	0.257
W13	1.563	0.803	0.153	0.322
W14	1.599	0.947	0.619	0.535
IND	1.549	0.759	0.152	0.293
CHI	1.549	0.758	0.152	0.292
JAP	1.541	0.743	0.146	0.283

TABLE IX: The Relative Importance (RI, Arbitrary Units) of Four Different Input Parameters in Fate Model for 17 Subcontiental Regions; Dissolution Rate of ENPs Is Equal to 1.0 ·10-5 s-1

Regions	RI(r_{LSP})	RI(ρ_{SNP})	RI(α_2)	RI($Depth_{water}$)
DEFAULT	1.130	0.679	0.344	0.348
W1	1.080	0.513	0.099	0.198
W2	1.054	0.448	0.078	0.158
W3	1.105	0.634	0.475	0.374
W4	1.134	0.656	0.478	0.383
W5	0.905	0.218	0.000	0.063
W6	0.915	0.227	0.000	0.065
W7	1.105	0.615	0.185	0.268
W8	1.084	0.631	0.215	0.295
W9	1.010	0.350	0.038	0.112
W10	1.021	0.367	0.041	0.119
W12	1.045	0.417	0.059	0.138
W13	1.071	0.486	0.081	0.178
W14	1.119	0.674	0.358	0.352
IND	1.058	0.452	0.079	0.160
CHI	1.058	0.452	0.079	0.159
JAP	1.052	0.442	0.076	0.154

TABLE XI: The Values of Fitting Parameters and the Coefficients of Determination (R2) Values for the Four Studied Input Parameters of Fate Model In JAP Region

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	$2.63 \cdot 10^{2}$	19.57	16.99	13.64
B	$-1.08 \cdot 10^{2}$	-8.86	-6.49	-7.53
C	$2.98 \cdot 10^{-7}$	$1.85 \cdot 10^{-6}$	$1.10 \cdot 10^{-6}$	$3.40 \cdot 10^{-7}$
D	$-1.52 \cdot 10^{2}$	-10.22	-10.37	-5.92
E	$3.55 \cdot 10^{-10}$	$3.36 \cdot 10^{-7}$	$2.36 \cdot 10^{-7}$	$1.57 \cdot 10^{-6}$
R^2	0.99885	0.99976	0.99976	0.99986

TABLE XII: The Values of Fitting Parameters and the Coefficients of Determination (R^2) Values for the Four Studied Input Parameters of Fate Model In DEFAULT Region

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	$4.67 \cdot 10^{2}$	4.88	26.10	3.41
B	$-3.35 \cdot 10^{2}$	-1.66	-14.70	-1.21
C	$1.42 \cdot 10^{-35}$	$1.01 \cdot 10^{-6}$	$2.63 \cdot 10^{-7}$	$1.06 \cdot 10^{-6}$
D	$-1.29 \cdot 10^{2}$	-2.83	-10.90	-2.02
E	$2.47 \cdot 10^{-7}$	$4.34 \cdot 10^{-6}$	$1.52 \cdot 10^{-6}$	$4.00 \cdot 10^{-6}$
R^2	0.99957	0.99999	0.99965	0.99999

TABLE XIII: The Values of Fitting Parameters and the Coefficients of Determination (R^2) Values for The Four Studied Input Parameters of Fate Model In W1 Region

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$

A	$5.53 \cdot 10^{2}$	15.20	13.70	10.30
B	$-4.16 \cdot 10^{2}$	-7.29	-5.48	-4.84
C	$9.46 \cdot 10^{-95}$	$2.16 \cdot 10^{-6}$	$1.36 \cdot 10^{-6}$	$1.90 \cdot 10^{-6}$
D	$-1.34 \cdot 10^{2}$	-7.45	-8.08	-5.21
E	$2.96 \cdot 10^{-7}$	$4.14 \cdot 10^{-7}$	$2.96 \cdot 10^{-7}$	$4.37 \cdot 10^{-7}$
R^2	0.99968	0.99982	0.99984	0.99989

TABLE XIV: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R^2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL IN W2 REGION

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	$2.22 \cdot 10^{2}$	18.70	16.10	13.10
B	$-1.01 \cdot 10^{2}$	-9.66	-6.16	-7.13
C	$3.09 \cdot 10^{-7}$	$3.47 \cdot 10^{-7}$	$1.15 \cdot 10^{-6}$	$3.51 \cdot 10^{-7}$
D	$-1.18 \cdot 10^{2}$	-8.57	-9.84	-5.73
E	$8.87 \cdot 10^{-10}$	$1.89 \cdot 10^{-6}$	$2.47 \cdot 10^{-7}$	$1.60 \cdot 10^{-6}$
R^2	0.9985	0.99978	0.99977	0.99987

TABLE XV: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R^2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL IN W3 REGION

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	32.19	2.27	9.16	1.58
B	-12.71	-0.48	-4.60	-0.35
C	$1.72 \cdot 10^{-6}$	$1.68 \cdot 10^{-6}$	$2.80 \cdot 10^{-6}$	$1.78 \cdot 10^{-6}$
D	-18.23	-1.48	-4.19	-1.08
E	$2.49 \cdot 10^{-7}$	$6.62 \cdot 10^{-6}$	$6.17 \cdot 10^{-7}$	$6.32 \cdot 10^{-6}$
R^2	0.99944	1	0.99992	1

TABLE XVI: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R^2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL IN W4 REGION

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	$1.40 \cdot 10^{2}$	2.60	13.32	1.82
B	-56.51	-1.68	-6.39	-1.22
C	$8.51 \cdot 10^{-24}$	$6.12 \cdot 10^{-6}$	$4.55 \cdot 10^{-7}$	$5.85 \cdot 10^{-6}$
D	-80.38	-0.60	-6.49	-0.43
E	$3.47 \cdot 10^{-7}$	$1.53 \cdot 10^{-6}$	$2.26 \cdot 10^{-6}$	$1.63 \cdot 10^{-6}$
R^2	0.99713	1	0.99985	1

TABLE XVII: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R^2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL IN W5 REGION

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	$1.46 \cdot 10^{3}$	60.06	0	41.94
B	$-7.28 \cdot 10^{2}$	-22.66	0	-15.36
C	$3.73 \cdot 10^{-8}$	$7.77 \cdot 10^{-7}$	0	$6.14 \cdot 10^{-7}$
D	$-7.28 \cdot 10^{2}$	-36.83	0	-26.37
E	$3.73 \cdot 10^{-8}$	$1.26 \cdot 10^{-7}$	0	$1.25 \cdot 10^{-7}$
R^2	0.99954	0.99965	0	0.99987

TABLE XVIII: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R^2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL IN W6 REGION

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	$2.3 \cdot 10^{3}$	58.21	0	40.67
B	$-1.15 \cdot 10^{3}$	-35.44	0	-25.24
C	$3.22 \cdot 10^{-8}$	$1.29 \cdot 10^{-7}$	0	$1.28 \cdot 10^{-7}$
D	$-1.15 \cdot 10^{3}$	-22.19	0	-15.22
E	$3.22 \cdot 10^{-8}$	$7.96 \cdot 10^{-7}$	0	$6.27 \cdot 10^{-7}$
R^2	0.99981	0.99962	0	0.99986

TABLE XIX: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R^2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL IN W7 REGION

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	$1.74 \cdot 10^{2}$	8.58	14.20	5.99
B	-90.34	-4.37	-6.31	-2.79
C	$3.26 \cdot 10^{-7}$	$3.18 \cdot 10^{-6}$	$1.63 \cdot 10^{-6}$	$7.07 \cdot 10^{-7}$
D	-81.43	-3.77	-7.67	-3.01
E	$9.55 \cdot 10^{-10}$	$6.85 \cdot 10^{-7}$	$3.49 \cdot 10^{-7}$	$2.82 \cdot 10^{-6}$
R^2	0.99786	0.99994	0.99985	0.99996

TABLE XX: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R^2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL IN W8 REGION

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	32.88	5.54	7.63	3.84
B	-12.92	-2.05	-3.75	-2.14
C	$1.70 \cdot 10^{-6}$	$9.20 \cdot 10^{-7}$	$5.53 \cdot 10^{-7}$	$3.56 \cdot 10^{-6}$
D	-18.72	-3.12	-3.69	-1.53
E	$2.45 \cdot 10^{-7}$	$3.99 \cdot 10^{-6}$	$2.27 \cdot 10^{-6}$	$9.45 \cdot 10^{-7}$
R^2	0.99942	0.99999	0.99992	0.99999

TABLE XXI: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R^2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL IN W9 REGION

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	$3.13 \cdot 10^{2}$	28.67	12.10	19.99
B	$-1.15 \cdot 10^{2}$	-11.79	-7.41	-7.84
C	$2.89 \cdot 10^{-7}$	$1.46 \cdot 10^{-6}$	$2.10 \cdot 10^{-7}$	$1.19 \cdot 10^{-6}$
D	$-1.96 \cdot 10^{2}$	-16.40	-4.60	-11.96
E	$4.65 \cdot 10^{-10}$	$2.45 \cdot 10^{-7}$	$9.28 \cdot 10^{-7}$	$2.44 \cdot 10^{-7}$
R^2	0.99914	0.99959	0.99977	0.99974

TABLE XXII: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R^2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL IN W10 REGION

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	$7.52 \cdot 10^{2}$	28.56	12.22	19.96
B	$-1.42 \cdot 10^{2}$	-11.77	-4.61	-11.89
C	$2.62 \cdot 10^{-7}$	$1.48 \cdot 10^{-6}$	$9.65 \cdot 10^{-7}$	$2.50 \cdot 10^{-7}$
D	$-6.07 \cdot 10^{2}$	-16.30	-7.53	-7.87
E	$2.36 \cdot 10^{-9}$	$2.48 \cdot 10^{-7}$	$2.16 \cdot 10^{-7}$	$1.22 \cdot 10^{-6}$
R^2	0.99982	0.99959	0.99977	0.99974

TABLE XXIII: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R^2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL IN W12 REGION

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	$1.06 \cdot 10^{3}$	23.45	14.47	15.09
B	$-9.11 \cdot 10^{2}$	-12.81	-5.44	-8.59
C	$4.16 \cdot 10^{-32}$	$2.92 \cdot 10^{-7}$	$1.07 \cdot 10^{-6}$	$3.11 \cdot 10^{-7}$
D	$-1.49 \cdot 10^{2}$	-10.15	-8.92	-6.31
E	$2.56 \cdot 10^{-7}$	$1.68 \cdot 10^{-6}$	$2.34 \cdot 10^{-7}$	$1.46 \cdot 10^{-6}$
R^2	0.99991	0.9997	0.99977	0.99983

TABLE XXIV: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R^2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL IN W13 REGION

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	$6.40 \cdot 10^{2}$	17.22	11.90	12.04
B	$-1.38 \cdot 10^{2}$	-8.67	-7.10	-6.36
C	$2.65 \cdot 10^{-7}$	$3.74 \cdot 10^{-7}$	$2.98 \cdot 10^{-7}$	$3.82 \cdot 10^{-7}$
D	$-4.99 \cdot 10^{2}$	-8.05	-4.69	-5.47
E	$8.35 \cdot 10^{-11}$	$2.01 \cdot 10^{-6}$	$1.34 \cdot 10^{-6}$	$1.72 \cdot 10^{-6}$
R^2	0.99976	0.99979	0.99985	0.99988

TABLE XXV: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R^2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL IN W14 REGION

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	85.26	4.25	18.74	2.96
B	-56.97	-2.53	-8.48	-0.98
C	$1.13 \cdot 10^{-7}$	$4.65 \cdot 10^{-6}$	$1.78 \cdot 10^{-6}$	$1.16 \cdot 10^{-6}$
D	-26.49	-1.33	-9.85	-1.81
E	$9.20 \cdot 10^{-7}$	$1.10 \cdot 10^{-6}$	$3.35 \cdot 10^{-7}$	$4.30 \cdot 10^{-6}$
R^2	0.99936	0.99999	0.99979	1

TABLE XXVI: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R^2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL IN IND REGION

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	$4.56 \cdot 10^{2}$	19.51	17.35	13.63
B	$-1.28 \cdot 10^{2}$	-10.16	-6.64	-7.48
C	$2.75 \cdot 10^{-7}$	$3.37 \cdot 10^{-7}$	$1.11 \cdot 10^{-6}$	$3.44 \cdot 10^{-7}$
D	$-3.25 \cdot 10^{2}$	-8.85	-10.56	-5.95
E	$5.75 \cdot 10^{-11}$	$1.86 \cdot 10^{-6}$	$2.36 \cdot 10^{-7}$	$1.58 \cdot 10^{-6}$
R^2	0.99955	0.99976	0.99975	0.99986

TABLE XXVII: THE VALUES OF FITTING PARAMETERS AND THE COEFFICIENTS OF DETERMINATION (R^2) VALUES FOR THE FOUR STUDIED INPUT PARAMETERS OF FATE MODEL IN CHI REGION

Fitting parameters	r_{LSP}	ρ_{SNP}	α_2	$Depth_{water}$
A	$4.82 \cdot 10^{2}$	19.62	17.47	13.70
B	$-1.30 \cdot 10^{2}$	-8.89	-6.69	-7.53
C	$2.73 \cdot 10^{-7}$	$1.86 \cdot 10^{-6}$	$1.10 \cdot 10^{-6}$	$3.42 \cdot 10^{-7}$
D	$-3.49 \cdot 10^{2}$	-10.23	-10.63	-5.98
E	$2.79 \cdot 10^{-11}$	$3.36 \cdot 10^{-7}$	$2.35 \cdot 10^{-7}$	$1.58 \cdot 10^{-6}$
R^2	0.99959	0.99976	0.99975	0.99986

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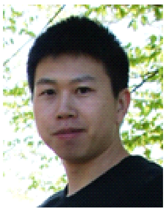

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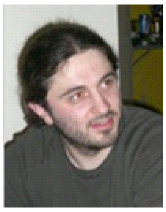

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