Minimizing the Exposure Risk from Groundwater Pollution by Optimizing the Extraction Patterns

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Key Points:

- Higher extraction frequencies decrease the above threshold exposure risk to groundwater pollutants

Abstract

Optimization models for minimizing pollutant exposure from groundwater resources require time and resources that many communities might not have ready access to due to their economic conditions. In such cases, it might be useful to develop a "rule of thumb" approach for suggestions in case of uncertainties and inadequate means to address these uncertainties. Monte Carlo analysis was performed for a simplified groundwater system and the effects of extraction patterns, distance to pollution source, dispersivity, pollutant pulse period, pore water velocity and decay were examined for minimizing the high pollutant exposure risk from the extracted groundwater. Results indicate that, in a high uncertainty scenario, the best bet for minimizing the risk of high pollutant exposure would be to adopt a frequent extraction pattern and supply the water as a mixture of extractions from multiple wells spread over an area. These findings can be used as a "rule of thumb" wherever time and resources might be the limiting factors.

1 Introduction

Groundwater is an important freshwater resource for many people, and groundwater contamination is a huge problem in many regions of the world (Syafiuddin et al., 2020).

The role of extraction patterns, as different from extraction rates, has been of interest to researchers for minimizing the exposure of public to pollutants from groundwater (Bagnera et al., 2004; Das & Datta, 2001; Ren et al., 2016). Such research is surprisingly scarce, and usually concludes complex suggestions that require rather detailed data on the state of the groundwater system and pollutants (Bagnera et al., 2004; Das & Datta, 2001; Ren et al., 2016), and proposal of application of intricate extraction patterns that are out of reach of communities with limited resources.

Monte Carlo analysis has been frequently employed for solving problems of uncertainty in groundwater systems (Ren et al., 2016; Ballio & Guadagnini, 2004; Hassan et al., 2009; Jafari et al, 2016; Jiang et al., 2021; Laloy et al. 2013; Mukherjee & Singh, 2022; Neshat et al., 2015; Qiu et al., 2021; Seifi et al., 2020; Soleimani et al., 2022).

Therefore, a "rule of thumb" approach for minimizing the exposure risk to pollutants in groundwater has to be suggested for the communities who lack adequate resources for the application of complex procedures. To the author's best knowledge, such "rule of thumb"

approach has not yet been examined in the scientific literature by using Monte Carlo analysis; this article addresses this existing gap.

2 Materials and Methods

2.1 Model

Pollutant concentrations at extraction point were calculated by using the 1-dimensional advection-dispersion equation for groundwater flow in homogenous porous medium in the case of a confined aquifer. The simplified equation for 1-dimensional groundwater flow in the case of constant velocity, retardation, dispersion and decay rate is given by the following equation (van Genuchten, 1981):

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x} - \alpha RC \quad \text{(i)}$$

where; R is the retardation factor, D is the longitudinal dispersion coefficient, V is the pore water velocity, α is the first-order decay constant, C is the pollutant concentration, x is the distance and t is the time.

For simplicity, groundwater extraction assumed to have no effect on the groundwater velocity or distribution of C in the groundwater; which represents an approximation to cases with relatively lower amounts of local groundwater extraction compared to the local groundwater supply (amount and flow rate).

In equation (i), D is given by the following equation (ii) (Al-Tabbaa et al., 2000):

$$D = \alpha_L V + D^* \quad \text{(ii)}$$

where; α_L is the longitudinal dispersivity and D* is the molecular diffusion coefficient.

D* can be further defined by the following equation (iii) (Murphy, 2015):

$$D^* = \theta D_m\left(\frac{\theta^{7/3}}{\theta_{Eff}{}^2}\right) \quad \text{(iii)}$$

where; θ is the porosity of the medium, D_m is the molecular diffusion coefficient in case of θ=1, and θ_{Eff} is the effective porosity of the medium.

Peclet number for the examination of the contribution of molecular diffusion was calculated by the following equation (iv) (Huysmans & Dassargues 2005):

$$Pe = xV/D^* \quad \text{(iv)}$$

Pollutant source type was assumed to be a step pulse source type, and the solution for this specific case was obtained from Case B1 in van Genuchten's work (van Genuchten, 1981).

Monte-Carlo analysis, with 10,000 runs, was performed for the variables of D, V, α, x, T (step pulse period) and t by using the Microsoft Excel 2016 software. R was ignored, as changing V and D can mimic changes in R (See equation (i)); such as, increasing R would be equivalent to decreasing D and V by the same factor. This can simply be accomplished by changing V, considering that D is directly proportional with V when molecular diffusion is ignored (See equation (ii)).

Matrix multiplication was performed, as in equation (v), to find the total amount of pollutants extracted for each extraction pattern (E). As the total amount of groundwater extracted in a given period of time is expected to be the same regardless of the extraction pattern (by using some sort of storage system as necessary), the results of equation (v) were later calibrated to obtain the total extracted pollutant amounts for a fixed amount of groundwater extracted. As the amount of the extracted groundwater is considered to be fixed for each extraction pattern after this calibration, these calibrated results can be considered as pollutant concentrations in the extracted groundwater.

$$[C]_{D,V,\alpha,x,T,t} \times [Extraction\ amount]_{t,E} = [C]_{D,V,\alpha,x,T,E} \quad \text{(v)}$$

Results were plotted by using the PSPP 1.6.2 statistics software.

2.2 Parameters

Units throughout this article are given in kilograms (kg), meters (m) and days (d).

The scale of the system under examination was determined to be 100 m, as the most reliable data on α_L for porous media in the scientific literature exist for distances shorter than 250 m; and at shorter distances (below 40 m), α_L values are more consistent among themselves (Gelhar et al., 1992). x to α_L ratios (x/α_L) were taken to be 8 and 29 by considering these findings (Gelhar et al., 1992).

The maximum time scale was assumed to be 1000 d. An acceptable time resolution had to be determined with practical limitations in mind; 20 time segments deemed to be suitable for

the purposes of this analysis (leading to 382 extraction patterns and a resolution of 5.3% of the maximum time scale of the study).

Pulse concentration (C_o) was adjusted to give a constant pollutant emission amount under varying pulse period conditions; Example: C_o=100 kg/m^3 when T=1 d, and C_o=1 kg/m^3 when T=100 d.

While determining the range of V, the mentioned system scales had to be taken into account. Very slow and fast velocities were no interest as they are expected to give negligible pollutant extraction; it is obvious that if the pore water velocity is too slow, pollutants will not have time to reach to the extraction well within the time frame of the simulation, and if the pore water velocity is too fast, the pollutants will be mostly washed away from the system without being extracted at the well. Minimum V (1st possible value in Table 1) was determined to be the velocity at which the pore water would travel half the distance (travel 5 m) to the minimum extraction point from the pollution source in 1000 d (maximum time scale). 2nd possible value for V ensured that the pore water would travel to the midpoint of the maximum distance (100 m) and the pollution source within 1000 d. 3rd possible value for V ensured that the pore water would travel twice the maximum distance (travel 200 m) in 1000 d. The rest of the velocities were selected to cover the range of relevant velocities documented in the literature; from 0.09 m/d to 27 m/d (Gelhar et al., 1992).

α was calculated by using the assumed maximum and minimum half-lives, 365,000 d and 1 d, respectively, to cover the extremes of decay.

The range of θ_{Eff} for porous media in the reference study, where the longitudinal dispersivities were obtained from, varied from 0.233 to 0.39 (Gelhar et al., 1992). In the case of sandy media, this range was from 0.33 to 0.39. In this study, θ_{Eff} was taken to be equal to 0.3875 (closer to the upper limit for sandy medium) to ensure that the Peclet number would give conservative results regarding the contribution of the molecular diffusion coefficient. Selection of θ_{Eff} did not play a role in the determination of V, as the values for V were not derived but rather determined from the literature.

Peclet number was calculated to be greater than 20 by using a molecular diffusion coefficient 30 to 50 times greater than the values suggested by Brian L. Murphy (Murphy, 2015); hence the molecular diffusion was ignored.

Table 1 lists the variables and their possible values that were used in the Monte Carlo analysis.

Table 1. Variables and their possible values that were used in the Monte Carlo analysis

		Possible values									
		1	**2**	**3**	**4**	**5**	**6**	**…**	**18**	**19**	**20**
Variable [unit]	**V [m/d]**	0.005	0.05	0.2	3	10	30				
	α [d^{-1}]	1.9E-6	0.693								
	x*V/D [-]	8	29								
	T [d]	1	100								
	x [m]	10	100								
	t [d]	1	53.6	106.2	158.7	211.3	263.9	…	894.8	947.4	1000

Extraction patterns were formed by taking into account different extraction frequencies over 20 time segments. As an example, extraction patterns 1 and 2 have the extraction frequency of 1 d, and extraction patterns 3, 4, 5 and 6 have the extraction frequency of 2 d, and so on. A sample of the 382 extraction patterns can be seen in Table 2.

Table 2. A limited sample of extraction patterns (1 represents uniform extraction and 0 represents no extraction)

		Extraction pattern (E)																	
		1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**…**	**375**	**376**	**377**	**378**	**379**	**380**	**381**	**382**
Time	**1**	1	0	1	1	0	0	1	1	1	…	0	0	0	0	0	0	0	1
	2	0	1	1	0	0	1	1	1	0	…	0	0	0	0	0	0	1	1
	3	1	0	0	0	1	1	1	0	0	…	0	0	0	0	0	1	1	1
	4	0	1	0	1	1	0	0	0	0	…	0	0	0	0	1	1	1	1

	5	1	0	1	1	0	0	0	0	1	…	0	0	0	1	1	1	1	1
	6	0	1	1	0	0	1	0	1	1	…	0	0	1	1	1	1	1	1
	7	1	0	0	0	1	1	1	1	1	…	0	1	1	1	1	1	1	1
	8	0	1	0	1	1	0	1	1	0	…	1	1	1	1	1	1	1	1
	9	1	0	1	1	0	0	1	0	0	…	1	1	1	1	1	1	1	1
	10	0	1	1	0	0	1	0	0	0	…	1	1	1	1	1	1	1	1
	11	1	0	0	0	1	1	0	0	1	…	1	1	1	1	1	1	1	1
	12	0	1	0	1	1	0	0	1	1	…	1	1	1	1	1	1	1	1
	13	1	0	1	1	0	0	1	1	1	…	1	1	1	1	1	1	1	1
	14	0	1	1	0	0	1	1	1	0	…	1	1	1	1	1	1	1	1
	15	1	0	0	0	1	1	1	0	0	…	1	1	1	1	1	1	1	1
	16	0	1	0	1	1	0	0	0	0	…	1	1	1	1	1	1	1	1
	17	1	0	1	1	0	0	0	0	1	…	1	1	1	1	1	1	1	1
	18	0	1	1	0	0	1	0	1	1	…	1	1	1	1	1	1	1	1
	19	1	0	0	0	1	1	1	1	1	…	1	1	1	1	1	1	1	1
	20	0	1	0	1	1	0	1	1	0	…	1	1	1	1	1	1	1	1

4 Results and Discussion

Concentrations of exposure to pollutant found to be negatively correlated with distance (x), decay rate (α) (stronger correlation observed at lower velocities), pulse period (T) (stronger correlation observed at higher velocities), and positively correlated with the pore water velocity (V) within the scale of the model (Table 3).

Table 3. Bivariate correlation of C with other relevant variables

		E	x	T	x/α_L	α	V
Low V	C	-0.004	-0.16	-0.018	0.006	-0.387	0.291
High V	C	0.040	-0.226	-0.217	-0.005	-0.041	0.176

Exposure risk to high concentrations of pollutant (as different from the correlations given in Table 3 for the overall exposure concentrations) found to be also negatively correlated with α_L (dispersion) for low velocities and positively correlated with the extraction pattern (E) (See Figures 1, 2 and 3).

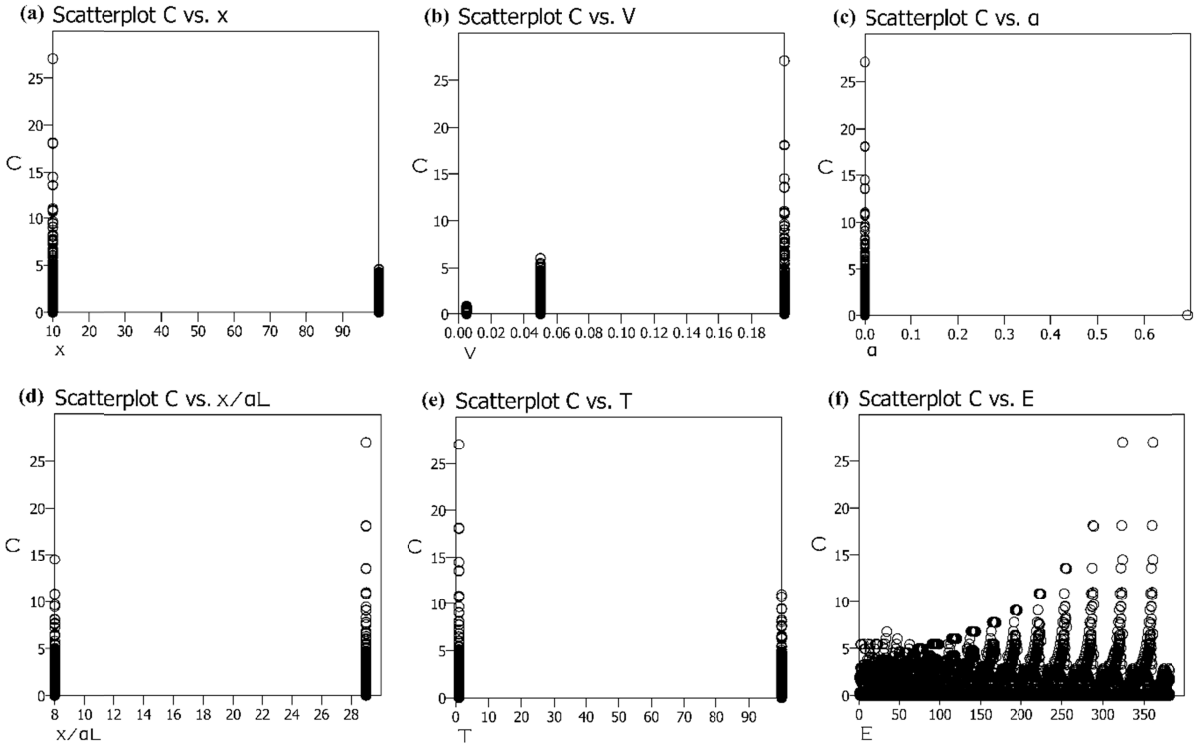
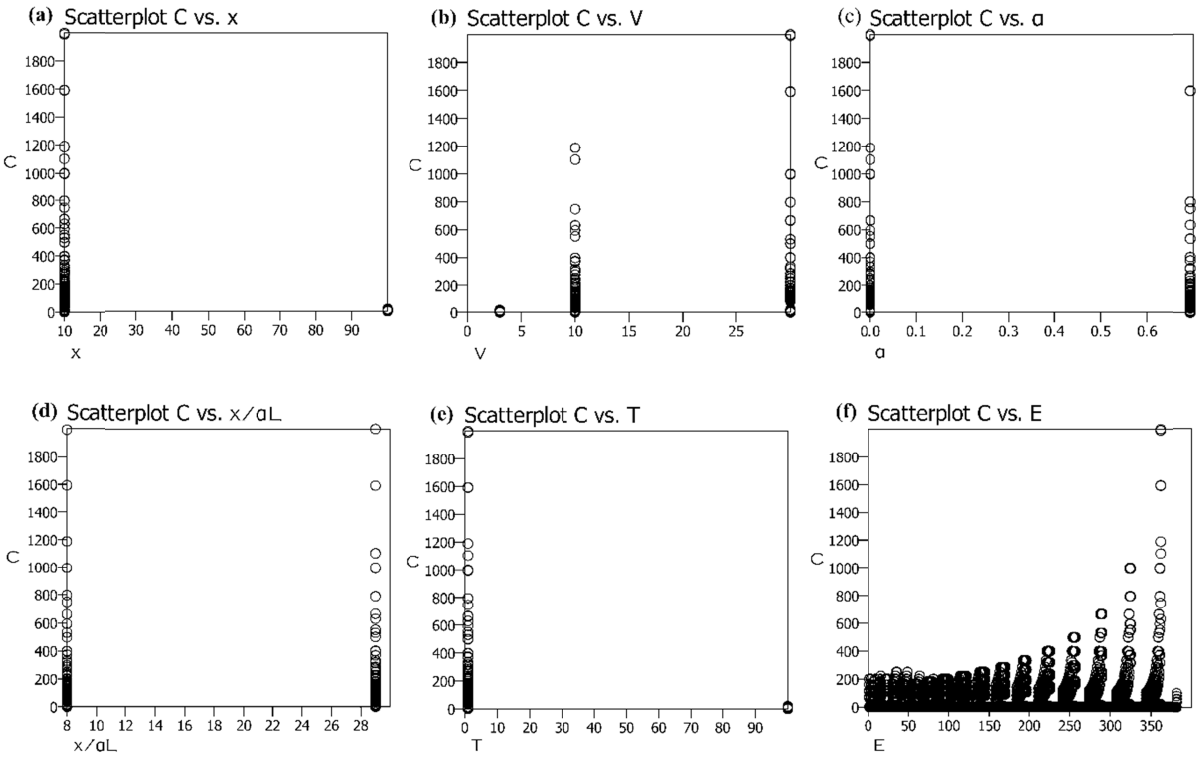


Figure 1. Low pore water velocity condition: (a) Pollutant concentration in the extracted groundwater vs distance from the pollutant source (b) Pollutant concentration in the extracted groundwater vs pore water velocity (c) Pollutant concentration in the extracted groundwater vs first-order decay constant (d) Pollutant concentration in the extracted groundwater vs longitudinal dispersivity (e) Pollutant concentration in the extracted groundwater vs pulse source duration (f) Pollutant concentration in the extracted groundwater vs the extraction patterns



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166 **Figure 2. High pore water velocity condition: (a) Pollutant concentration in the extracted**
167 **groundwater vs distance from the pollutant source (b) Pollutant concentration in the**
168 **extracted groundwater vs pore water velocity (c) Pollutant concentration in the extracted**
169 **groundwater vs first-order decay constant (d) Pollutant concentration in the extracted**
170 **groundwater vs longitudinal dispersivity (e) Pollutant concentration in the extracted**
171 **groundwater vs pulse source duration (f) Pollutant concentration in the extracted**
172 **groundwater vs the extraction patterns**

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175 An exponential curve can be fitted to the maximum exposure amounts in C vs. E graphs,
176 both for low and high V (See Figure 3).

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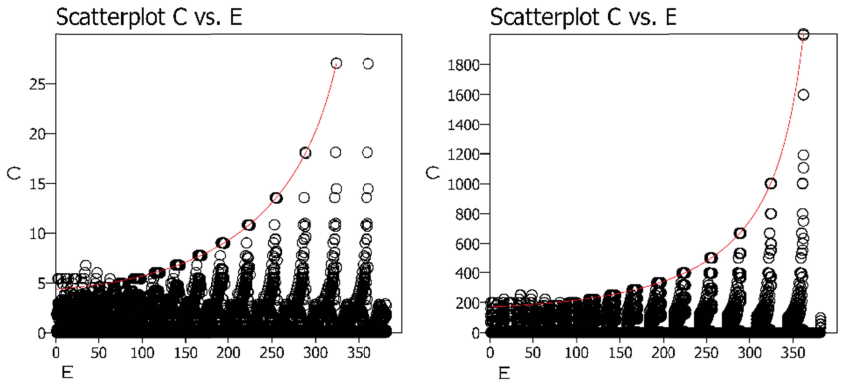


Figure 3. Continuous trend line showing the exponential growth of risk of high pollutant concentration in the extracted groundwater as the frequency of the extraction patterns decrease; low velocity cases (on the left), high velocity cases (on the right)

It can be seen from Figure 3 that as the frequency of extractions decrease, there is an exponentially growing risk of high pollutant extraction from the aquifer both for low and high velocities. It might be possible to tune the timing of extractions to minimize the pollutant extraction from the aquifer if all the variables and the timing of the pollutant emission are known to an adequate certainty. But, in many real world cases these variables are unknown, as in the case of undetected accidental pollutant emissions or the effect of interactions between pollutants on transport and decay processes (Syafiuddin et al., 2020).

Reduction in exposure with increase in x is an intuitive outcome that was also observed in the work of Bagnera et al. (Bagnera et al., 2004). However, in the same study, the results for the correlation of C and E are not clear due to lack of detailed information on the extracted water amounts per well in the Case 1 of the optimization scenario for meeting the water demand (Bagnera et al., 2004).

As this study excludes any removal (either by decay or other means) of pollutants during the storage after extraction, results should be interpreted with caution in case of such removal processes.

Exposure to decay products, if any, was also excluded. However, it should be realized that the decay products that were formed (no matter how complex the dynamics might be) during the transport in the aquifer can be considered as a sum of unsynchronized pulse sources with

unknown origin and timing of emission; which this study showed that the adoption of frequent extraction patterns is the best policy for such situations.

It should be noted that the time scale of the model can affect the findings for x, V and D in certain cases; low D might lead to lower exposure risk when V and the model time scale are small enough; similarly, high V might lead to lower exposure risk when V and the model time scale are large enough, however this was not observed within the scale of the model (100 m, 1000 d).

The finding that a frequent extraction pattern is the best policy in case of uncertainty in variables concerning the pollutant source and transport can be extended beyond the model scale of 100 m by recognizing that the plume of pollutants at around 100 m can be considered as a sum of unsynchronized pulse pollutant sources (just like in the case of decay products). Hence, the best policy at the 200 m distance (or at any other distance as we have just proved) would be, once again, to adopt a frequent extraction policy.

It can also be argued that, for pollutants with toxicity thresholds, in the case in which the pollution source location is uncertain, meeting the water demand by water obtained from multiple wells would further reduce the high exposure risk. In Figures 1 and 2, it is clear that the average concentration of pollutants obtained at x=10 m and x=100 m would be less than the concentration obtained solely from the well at x=10 m.

As the exposure concentrations to pollutant were positively correlated with V, from the previous argument about the reason for the omission of R in the Monte Carlo analysis and considering that x/α_L (or xV/D) is more weakly correlated with C than V is correlated with C (Table 3), it can be argued that R is negatively correlated with C, especially at higher values of V.

5 Conclusions

When the timing of the pollution is not known (such as in the case of undetected accidents or lack of information in which the extraction pattern cannot be adjusted to obtain a minimum exposure), to minimize the exposure risk; the best policy is to maximize distance, maximize decay with considering the decay products if any, maximize dispersion, maximize pulse period, and employ a frequent extraction pattern.

In a situation where all the variables are uncertain or cannot be controlled, which might be the case for communities with limited resources, the best bet for minimizing the risk of high pollutant exposure would be to adopt a frequent extraction pattern such as in the case of extraction patterns 1 or 2, and supply the water as a mixture of extractions from multiple wells spread over an area.

As this study excludes the formation of harmful decay products and removal (either by decay or other means) of pollutants during the storage after extraction, results should be interpreted with caution. Similarly, the findings may not apply to situations that are not covered in this study; such as varying water velocity or non-homogenous or fractured media.

Suggestions for further research might be the examination of the effects of extraction and the effects of storage conditions on exposure risk to pollutants in different extraction pattern scenarios.

Conflict of interest declaration

The author declares no competing financial interest.

Open Research

Monte Carlo simulations can be accessed via 10.6084/m9.figshare.21717482 and 10.6084/m9.figshare.21717479 for low and high pore water velocities, respectively. Listed results of Monte Carlo simulations can be accessed via 10.6084/m9.figshare.21717476.

References

Al-Tabbaa, A., Ayotamuno J.M., & Martin, R.J. (2000). One-dimensional solute transport in stratified sands at short travel distances. *Journal of Hazardous Materials*, 13;73(1), 1-15. doi: 10.1016/s0304-3894(99)00169-7

Bagnera, A., Massabò, M., Minciardi, R., Molini, L., Robba, M., & Sacile, R. (2004). Optimal Groundwater Exploitation and Pollution Control. *International Congress on Environmental Modelling and Software*. 73.

Ballio, F., & Guadagnini, A. (2004). Convergence assessment of numerical Monte Carlo simulations in groundwater hydrology. *Water Resources Research*, 40, W04603. doi: 10.1029/2003WR002876

Das, A., & Datta, B. (2001). Application of optimisation techniques in groundwater quantity and quality management. *Sadhana*, 26, 293-316. doi: 10.1007/BF02703402

Gelhar, L.W., Welty, C., & Rehfeldt, K.R. (1992). A critical review of data on field-scale dispersion in aquifers. *Water Resources Research*, 28(7), 1955-1974. doi: 10.1029/92WR00607

Hassan, A.E., Bekhit, H.M., & Chapman, J.B. (2009). Using Markov Chain Monte Carlo to quantify parameter uncertainty and its effect on predictions of a groundwater flow model. *Environmental Modelling & Software*, 24, 749-763. doi: 10.1016/j.envsoft.2008.11.002

Huysmans, M., & Dassargues, A. (2005). Review of the use of Peclet numbers to determine the relative importance of advection and diffusion in low permeability environments. *Hydrogeology Journal*, 13, 895-904. doi: 10.1007/s10040-004-0387-4

Jafari, F., Javadi, S., Golmohammadi, G., Mohammadi, K., Khodadadi, A., & Mohammadzadeh, M. (2016). Groundwater risk mapping prediction using mathematical modeling and the Monte Carlo technique. *Environmental Earth Sciences*, 75(6), 491. doi: 10.1007/s12665-016-5335-9

Jiang, C., Zhao, Q., Zheng, L., Chen, X., Li, C., & Ren, M. (2021). Distribution, source and health risk assessment based on the Monte Carlo method of heavy metals in shallow groundwater in an area affected by mining activities, China. *Ecotoxicology and Environmental Safety*, 224, 112679. doi: 10.1016/j.ecoenv.2021.112679

Laloy, E., Rogiers, B., Vrugt, J.A., Mallants, D., & Jacques, D. (2013). Efficient posterior exploration of a high-dimensional groundwater model from two-stage Markov chain Monte

Carlo simulation and polynomial chaos expansion. *Water Resources Research*, 49, 2664-2682. doi:10.1002/wrcr.20226

Mukherjee, I., & Singh, U.K. (2022). Exploring a variance decomposition approach integrated with the Monte Carlo method to evaluate groundwater fluoride exposure on the residents of a typical fluorosis endemic semi-arid tract of India. *Environmental Research*, 203, 111697. doi: 10.1016/j.envres.2021.111697

Murphy, B.L. (2015). Chapter 7 - Chemical Partitioning and Transport in the Environment. Introduction to Environmental Forensics (Third Edition), Editor(s): Brian L. Murphy, Robert D. Morrison, *Academic Press*, 165-197. doi: 10.1016/B978-0-12-404696-2.00007-2

Neshat, A., Pradhan, B., & Javadi, S. (2015). Risk assessment of groundwater pollution using Monte Carlo approach in an agricultural region: An example from Kerman Plain, Iran. Computers, *Environment and Urban Systems*, 50, 66-73. doi: 10.1016/j.compenvurbsys.2014.11.004

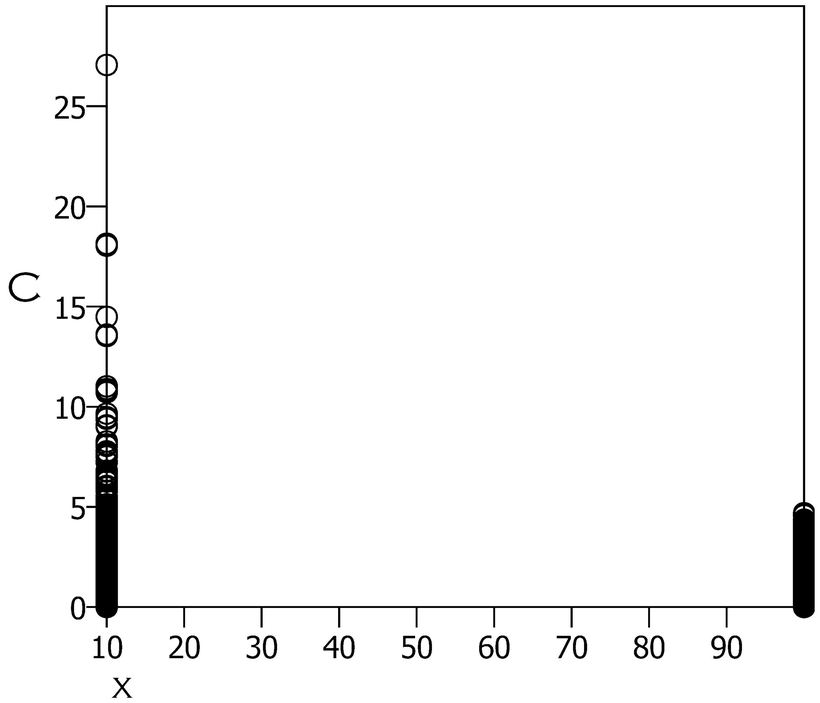
Qiu, H., Gui, H., Fang, P., & Li, G. (2021). Groundwater pollution and human health risk based on Monte Carlo simulation in a typical mining area in Northern Anhui Province, China. *International Journal of Coal Science & Technology*, 8(5), 1118-1129. doi: 10.1007/s40789-021-00446-0

Ren, L., He, L., Lu, H., & Chen, Y. (2016). Monte Carlo-based interval transformation analysis for multi-criteria decision analysis of groundwater management strategies under uncertain naphthalene concentrations and health risks. *Journal of Hydrology*, 539, 468-477. doi: 10.1016/j.jhydrol.2016.05.063

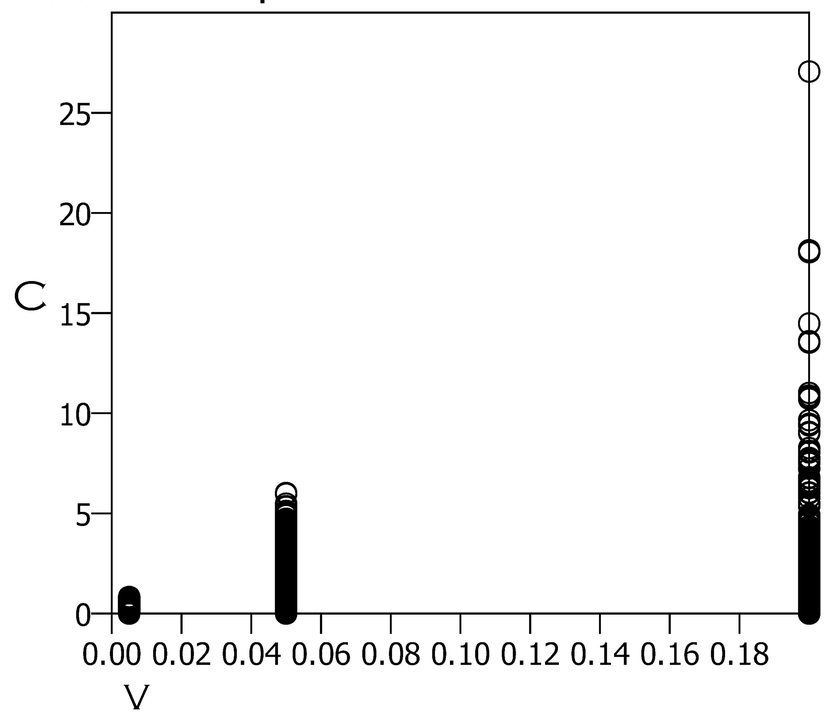
301 Seifi, A., Dehghani, M., & Singh, V.P. (2020). Uncertainty analysis of water quality index
302 (WQI) for groundwater quality evaluation: Application of Monte-Carlo method for weight
303 allocation. *Ecological Indicators*, 117, 106653. doi: 10.1016/j.ecolind.2020.106653
304 Soleimani, H., Nasri, O., Ghoochani, M., Azhdarpoor, A., Dehghani, M., Radfard, M.,
305 Darvishmotevalli, M., Oskoei, V., & Heydari, M. (2022) Groundwater quality evaluation and
306 risk assessment of nitrate using monte carlo simulation and sensitivity analysis in rural areas of
307 Divandarreh County, Kurdistan province, Iran. *International Journal of Environmental*
308 *Analytical Chemistry*, 102(10), 2213-2231. doi: 10.1080/03067319.2020.1751147
309 Syafiuddin, A., Boopathy, R., & Hadibarata, T. (2020). Challenges and Solutions for Sustainable
310 Groundwater Usage: Pollution Control and Integrated Management. *Current Pollution Reports*,
311 6, 310-327. doi: 10.1007/s40726-020-00167-z
312 van Genuchten, M.T. (1981). Analytical solutions for chemical transport with simultaneous
313 adsorption, zero-order production and first-order decay. *Journal of Hydrology*, 49(3-4), 213-233.
314 doi: 10.1016/0022-1694(81)90214-6

Figure 1.

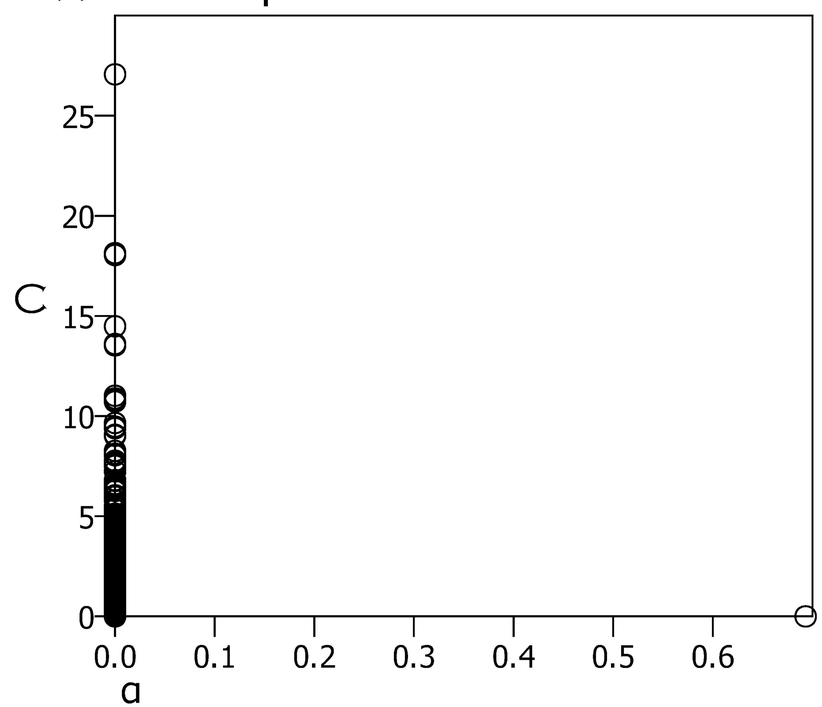
(a) Scatterplot C vs. x



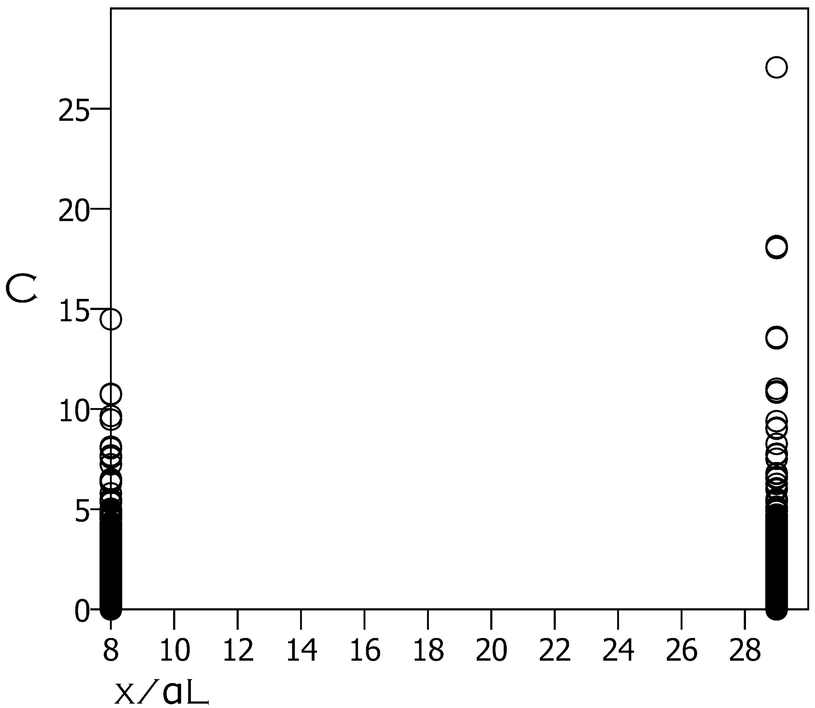
(b) Scatterplot C vs. V



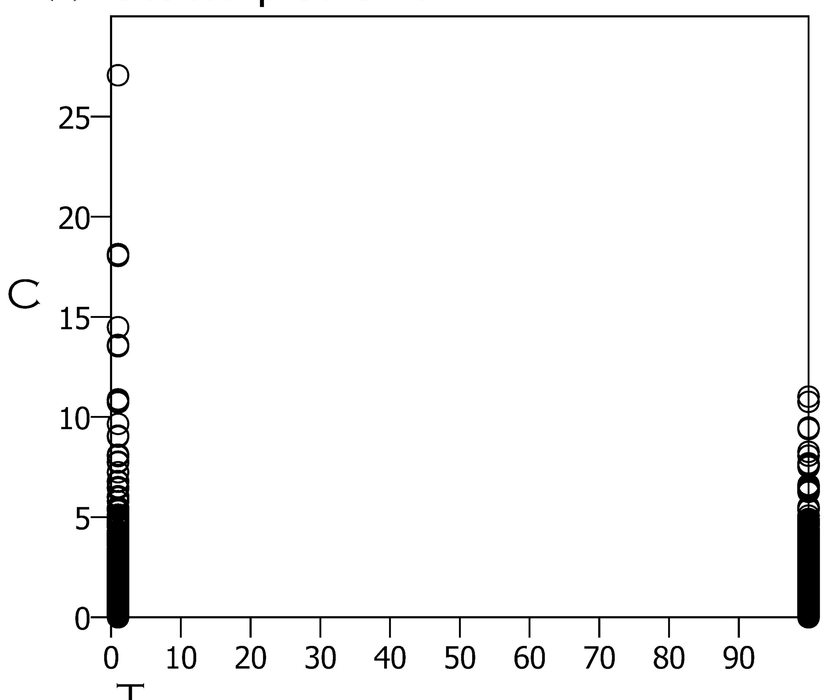
(c) Scatterplot C vs. α



(d) Scatterplot C vs. x/αL



(e) Scatterplot C vs. T



(f) Scatterplot C vs. E

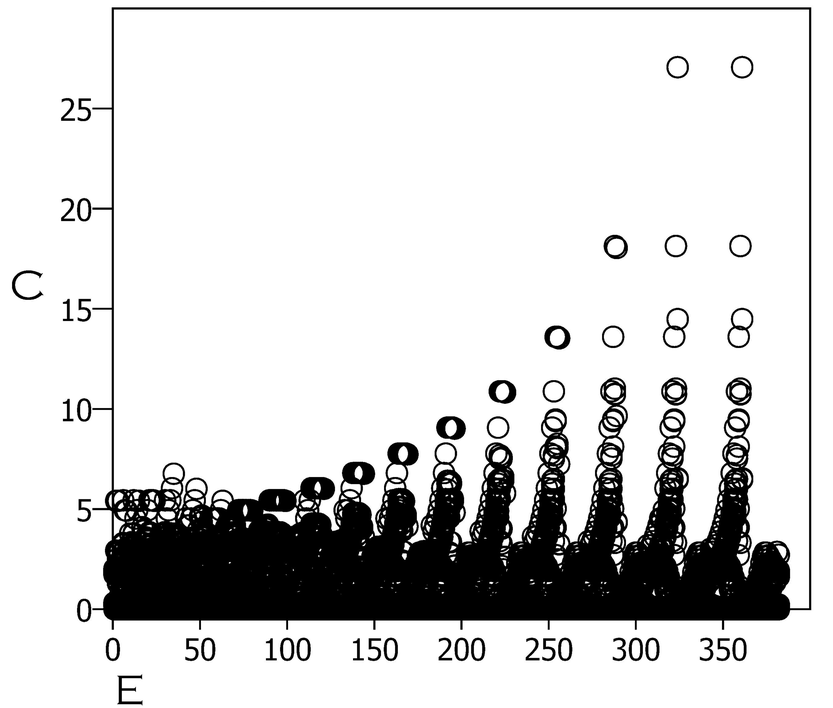


Figure 2.

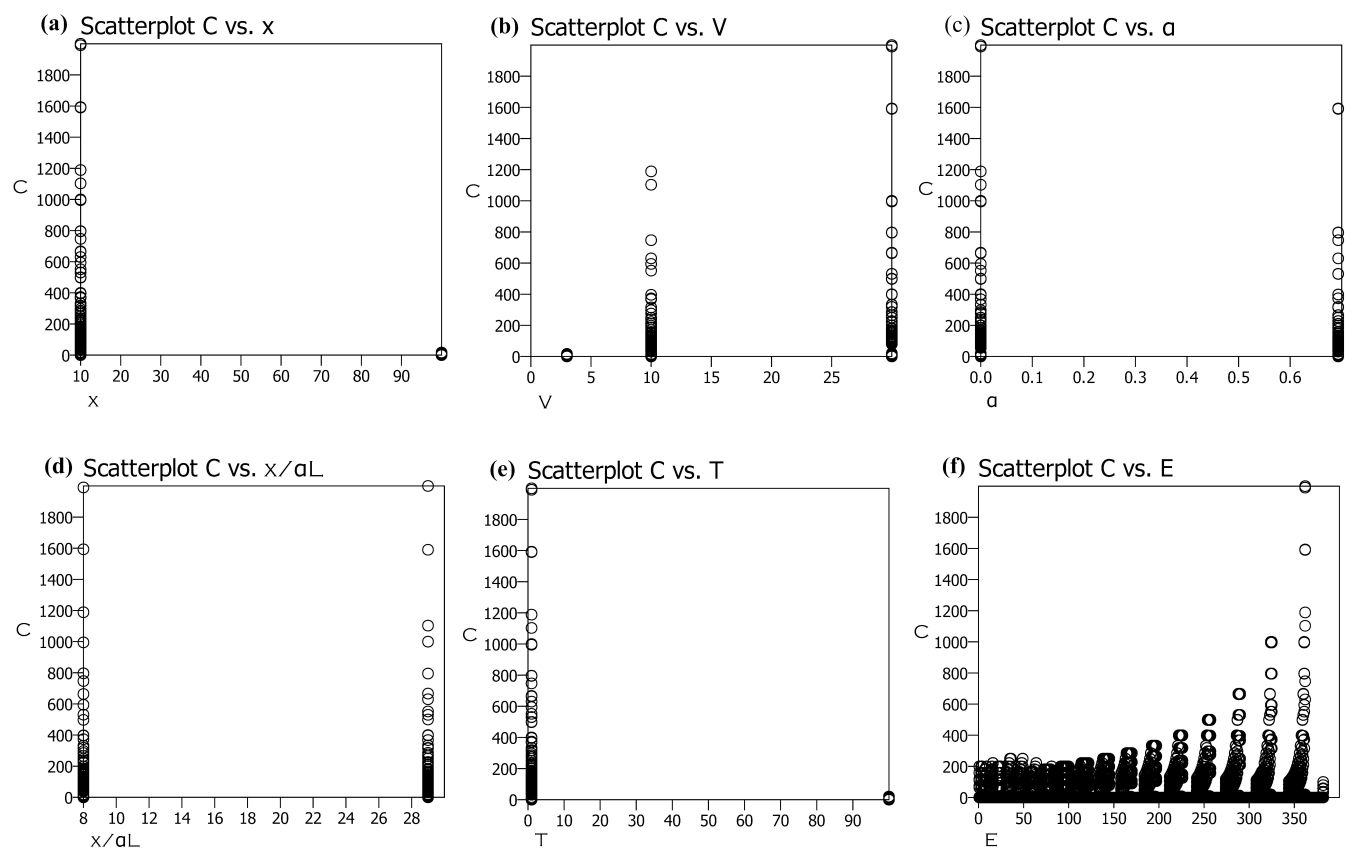
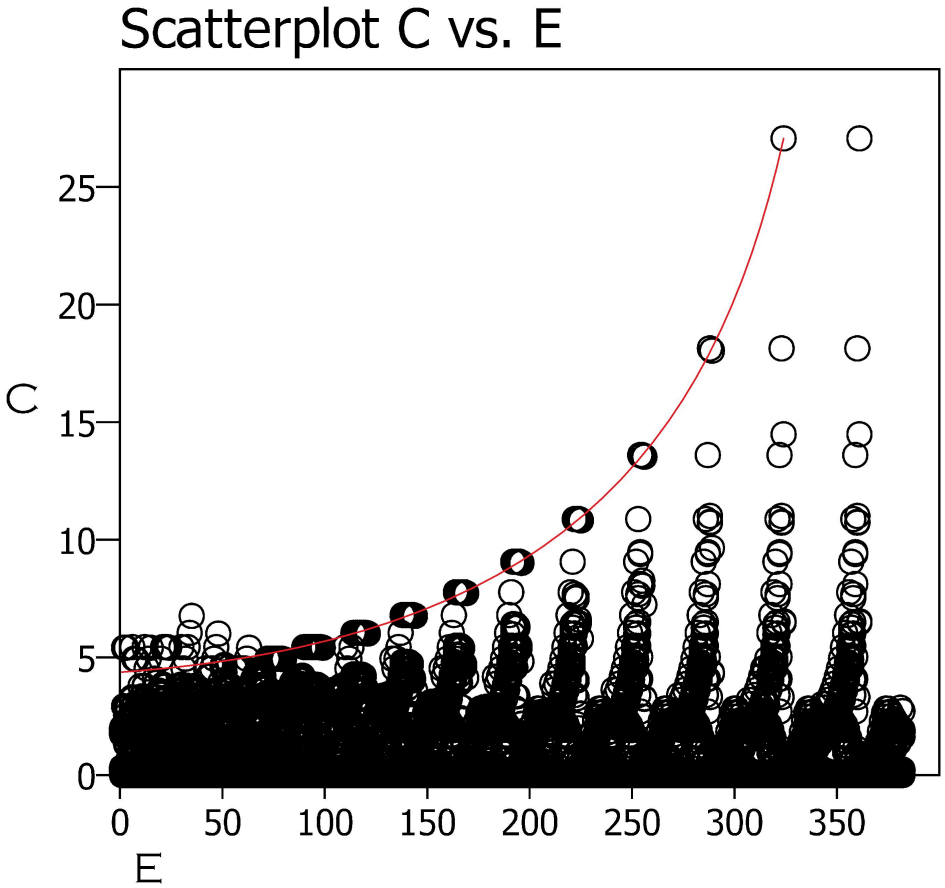
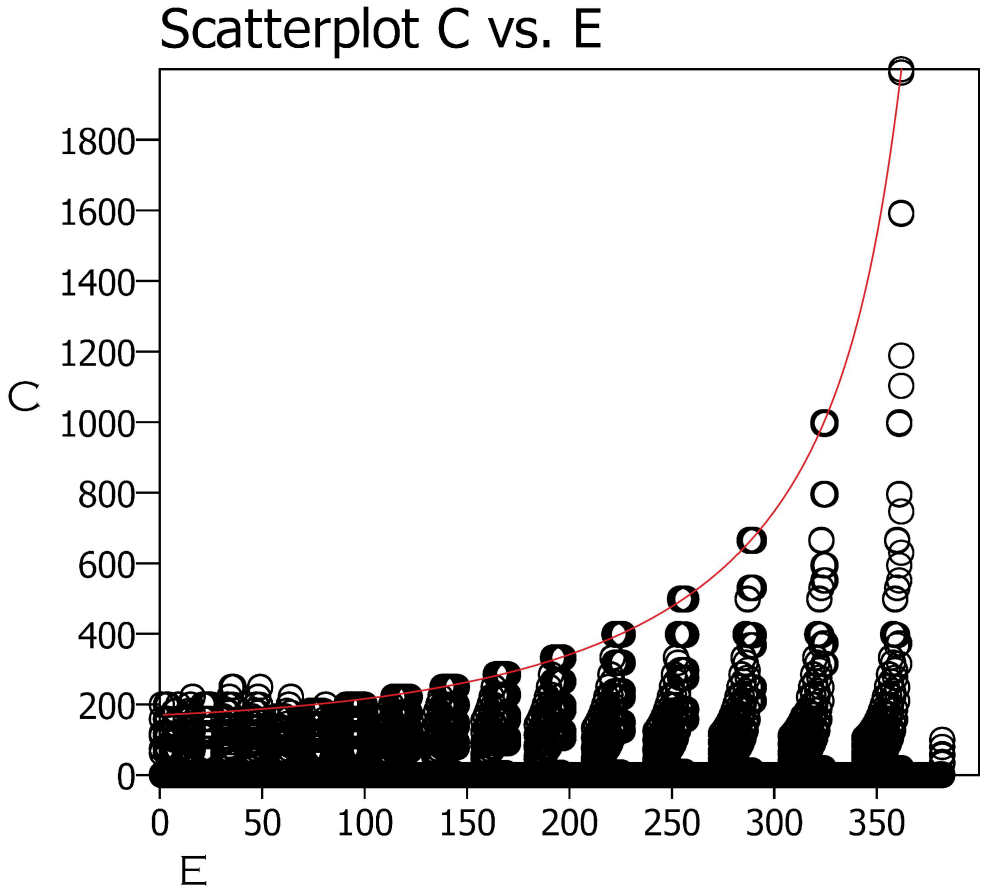

(a) Scatterplot C vs. x
C
x
(b) Scatterplot C vs. V
C
V
(c) Scatterplot C vs. a
C
a
(d) Scatterplot C vs. x/aL
C
x/aL
(e) Scatterplot C vs. T
C
T
(f) Scatterplot C vs. E
C
E

Figure 3.


Scatterplot C vs. E
C
E
0
5
10
15
20
25
0
50
100
150
200
250
300
350


Scatterplot C vs. E
C
E
0
200
400
600
800
1000
1200
1400
1600
1800
0
50
100
150
200
250
300
350