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Environmental fate of chemicals under reliability tests

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ABSTRACT/RESUME

Abstract: *The aim of this work is to predict biodegradability of complex chemicals pertaining to UVCB(Unknown or Variable composition, i.e. Complex reaction products or Biological materials) used in the oil and gas industry in the Algerian Sahara by internal consistency method to assess the reliability of results. Biodegradability prediction is usually carried out by Quantitative Structure Biodegradability Relationship (QSBR) models. But this method cannot be applied unless molecular structures of chemicals are fully known; this is not the case for UVCB substances. Here we review the clearness that until now, there is uncertainty about the link between biodegradability and the solubility of chemicals. In the present work, we aim to apply reliability test approach to study the existence of a link between these two parameters.The used reliability assessment techniques consist of Split Half Spearman-Brown Prophecy, Split Half Kuder-Richardson KR20 and KR21and Cronbach's Alpha.*

The applied reliability test is a non-biased perfect test since we get the same value for the four tested correlation coefficient with the value of 0.6263.This value in the scale range yields questionable test that can be rejected. Therefore, this analysis confirms the statement of the category of scientists who consider the weak Biodegradability-Solubility relationship.Reliability test techniques can be revolutionary in terms of gaining time when executing biodegradability tests and can also be used while dealing with UVCB substances.This is the first attempt to apply state of art reliability test to study the environmental fate of chemicals in general and UVCB substances in particular.

I. Introduction

Awareness of chemicals' impact on environment, health and flora has urged legislators to toughen environmental protection regulations. The European REACH Directive (Registration, Evaluation, Authorization and Restriction of Chemicals) and the US Toxic Substances Control Act (TSCA) continue to be reviewed and modified. A fundamental analysis that comes up in all legislations is ready biodegradability. The expressions biodegradation and biodegradability are often used as synonyms, though in fact their meanings are different. "Biodegradability is the ability of a substance to undergo microbial attack. Biodegradation is the elimination of an organic compound from an ecosystem by the metabolic activity of the biocenosis actually present in this system [1]. Ultimately, we are interested in a compound's biodegradability, often tacitly assumed

to be a unique property of the compound [2]. These tests of ready biodegradability have very strict conditions (time of analysis, inoculums, substance concentration, etc.). A positive test result means rapid and ultimate substance degradation in all environments [3].
This measure is obtained using one of the OECD screening tests or other international standards such as ISO, AFNOR or ASTM. These experiments have the disadvantage of lacking reproducibility and being very time consuming [4, 5]. The discovery of relationships among different concepts, in particular concepts provided by different scientific fields, represents the most important way to develop new scientific knowledge and transform isolated information into a deeper theoretical knowledge [6]. There is a noticeable activity in developing predictive models for biodegradation with the objective of generating reliable, inexpensive data in the shortest possible time;as a result, there are different mathematical approaches to predict biodegradability in aerobic and anaerobic conditions [7, 2]. Quantitative Structure Biodegradability Relationship (QSBR) models, which are an example of the Quantitative Structure Activity Relationship (QSAR), are the most widely used [8]. The process of modeling starts with a suitable description of molecular structures and ends with some inference, hypothesis, and prediction of the molecules behavior in environmental, biological, and physicochemical systems under analysis [6]. We are faced in the present work with the dilemma of willing to predict biodegradability of chemicals with unknown chemical structures. These substances are known as ''Substances of Unknown or Variable composition, Complex reaction products or Biological materials'' (UVCB). These cannot be sufficiently identified by their chemical composition, because [9]:

- The number of constituents is relatively large, and/or
- The composition is, to a significant part, unknown, and/or
- The variability of composition is relatively large or poorly predictable.

As a result of this compositional variability, the identification of UVCB substances is mostly basedon their generic description. The production source (biological or non-biological), the process of formation (chemical reaction, extraction, fractioning, etc.), the composition of fingerprints (chromatography or spectral information), the physicochemical properties (optical activity, range of variation of boiling point, viscosity, molecular weight, etc.) are used toidentify UVCBsubstancesas indicated by Echa.Europa for UVCB modeling & methodology[10]. The studied substances are: corrosion inhibitors and biocides that are used in oil & gas industry. For these products, we have information about active matter (5 to 30% of the product) but no idea about the chemical structure of the whole product. This is why it is impossible, in this case, to use QSBR concept. Other mathematical concepts are suggested in this article to deal with this special case. We propose through this research work a new way to study biodegradability prediction of UVCB substances based on the physical and chemical properties of chemicals, as well as the behavior of these products towards biodegradability and solubility properties based on the statistical measure of reliability and internal consistency of tests. Internal consistency reliability of the test explains how long experimental measurements remain consistent over repeated tests of the same matter and under identical conditions. Otherwise, the test is considered unpredictable and unreliable. To meet our target and to check the link between biodegradability and the solubility of chemicals, a dichotomous scale with (0, 1) score is imposed. According to L. J, Chronbach (1951), to achieve this result, three techniques are applied in this study to evaluate reliability using: 1). Split half Spearman-Brown Prophecy, 2). Split half Kuder and Richardson Formulas called Formulas 20 and 21, as well as 3). Cronbach's alpha. Since Kuder and Richardson Formulas 20 and 21 are used only with dichotomous scale, and Alpha coefficient with continuous, dichotomous and non-dichotomous scales, thus Alpha coefficient is considered as a good tool to confirm the results obtained from Kuder and Richardson Formulas 20 and 21as described by Chronbach [45]. Our motivation for seeking the link between Biodegradability and Solubility is based on the existence of divergent opinions about the existence of a correlation between these two parameters [11, 12] ; a group of scientists considers that biodegradability increases with a solubility [11] and a more recent trend considers the link between these two parameters is not magical [12,13]. With the proposed statistical approach, we attempt to open a portal for providing clear answers to the above-mentioned problematic.

I.1. Literature Review

In the present work, we are focusing on the relationship between water Solubility and Biodegradability of chemical substances pertaining to UVCB substances family. This information is needed to help predict the chemical behavior once in contact with the environment. On the basis of our literature review, it can be noted that in the eighties and nineties, while biodegradability was studies, all the conclusions were towards the tendancy that biodegradability of chemicals increases with water solubility [14, 15, 16, 17, 18, 19, 20, 21, 22, 23]. For instance, Bartha, (1986), Cerniglia, (1993), and Miller and Bartha, (1989) demonstrated that one of

the main reasons for the prolonged persistence of hydrophobic hydrocarbons in contaminated environments is their low water solubility which increases their sorption to soil particles and limits their availability to biodegrading microorganisms. Hydrophobicity of the organic pollutant is an important parameter when dealing with natural attenuation in the environment [20]. Bioavailability of hydrophobic organic compounds (HOCs) to microorganisms could be a limiting factor during the biodegradation process as highlighted by Mihelcic et al., (1993) and Guha and Jaffe (1996)[21, 22].The aqueous solubility may also be a factor that controls the rate of biodegradation [21] and bioaccumulation processes [24]. For the aromatic compounds, which are known to have a low solubility in water, such as naphthalene, no biodegradation was observed [25]. In the polymer science, to protect the environment, many efforts are made to develop biodegradable water-soluble polymers [19]. PolyVinyl Alcohol (PVA) is a widely used polymer because of its solubility in water, and microorganisms as well as enzymes [18] can easily degrade it. In the structure-biodegradation-activity study conducted in 1996 [24], the authors noticed that water-soluble chemicals are usually more biodegradable than insoluble ones. Many studies aimed at considering the microorganisms' behavior in biodegradability processes and concluded that metabolism was influenced by the solubility [26]. Even more recent studies still consider that biodegradability increases with solubility [11,27, 28]. On the other hand, there are some other scientific works that consider no magical link between Biodegradability and Solubility of chemicals [13]. For example, water-soluble polymers have an extended ability to move rapidly in aqueous media with considerable damage to plants and animals [13]. A chemical that is poorly water-soluble may readily leave aqueous solutions before having the opportunity to biodegrade [29] giving no way to conclude anything about its fate. 1,4-Dioxane (dioxane) is a cyclic ether with a high solubility and low vapor pressure. It is considered to be a problematic water pollutant that has major impacts on human health and the environment.Moreover, it is important to note that until now there has been no testing standard to assess solvent biodegradability [30]. In another study [31], aqueous solubility estimation method for organic compounds based on a group contribution approach has been developed and applied to biodegradation studies, where they concluded that aqueous solubility apparently plays no significant role in the biodegradability of the chain compounds in the studied database of chemicals. Several studies have reported the development of complementary analyses to assess the potential biodegradability of heterogeneous waste [31, 32], of which water extractable dissolved organic carbon (DOC). A recent study [12], investigated complementary approaches to aerobic and anaerobic bio-tests for a swifter evaluation of biodegradability. Their findings showed that the soluble fraction of organic waste was not correlated with biodegradability. They concluded that the analytical parameters commonly used (Organic Mater contents, soluble fractions, leaching behavior…) were not relevant to predict biodegradability because they were not able to provide any information on the structure of the analyzed organic matter, which however controls its bioavailability and thereby its actual biodegradation in the bioassays. These results are confronted to another recent study [11] which reports that the soluble organic matter is an important parameter to consider in biodegradability studies because of its high correlation with biodegradability characteristics.

From these last two recent studies, it can be concluded that the biodegradability link to solubility remains unexplained and as Nendza, in 2004 wrote [33]: "It is necessary to realize that biodegradability is not a well-defined parameter". Moreover, in the real world (environmental) where different processes such as swelling, cracking, creeping, hydrolysis, leaching, and biodegradation can occur simultaneously [34], enzymatic degradation of polymers becomes very complex to predict.

I.2. Theoritical Background

There are mainly two ways to study biodegradability of chemicals, the experimental way and the mathematical way, the latter is developed mainly because experiments lead to lack of reproducibility of results and are very time consuming [4].

I.2.1. Experimental way of studying biodegradability

It uses one of the OECD screening tests or other international standards such as ISO, AFNOR or ASTM standards to determine a chemical potential to undergo biodegradation in the environment. These test were developed as a simple and an inexpensive method to identify those chemicals that are not expected to be of concern in terms of environmental persistence and have found extensive use in hazard and risk assessments worldwide [35].

The choice of the test method depends essentially on three parameters namely: measured parameter,characteristics of the test substance andtest conditions.The most commonly used

standards for aerobic biodegradability measurements in water are those of OECD (301 and 310) for ready biodegradability [35]. According to [36], the biodegradability tests must be carried out according to an analytical strategy, which depends on the objective of the operator. It is necessary to examine: aerobic biodegradability, a simulation test, an inherent biodegradability test may be performed as a complementary or alternative test (aims to study biodegradability under optimized aerobic conditions) and finally, an anaerobic biodegradability test could be considered.This approach is very time-consuming.

In the context of the European REACH Regulation [37], new Enhanced biodegradability tests are developed, where more flexibility is given when assessing biodegradability, particularly while dealing with time of the test and inoculum adaptations.However, these methods are not yet validated and / or standardized and are currently only used in Europe for assessments of the persistence of chemicals in the environment (Persistence Biodegradability Tests PBT and Very Persistent Very Bioaccumulative vPvB assessments) [37].

I.2.2. Mathematical way of studying biodegradability (Predictive Models):

There are different mathematical approaches to predict biodegradability in aerobic and anaerobic conditions [2, 7]. Quantitative Structure Biodegradability Relationship (QSBR) models, which are an example of the Quantitative Structure Activity Relationship (QSAR), are the most widely used. The history of QSAR and molecular descriptors is closely related to the history of what can be considered one of the most important scientific concepts of the last part of the nineteenth century and the whole of twentieth century. That is the concept of molecular structure [6]. QSAR history started a century earlier than the history of molecular descriptors, being closely related to the development of the molecular structure theories. QSAR modeling was born in the toxicology field. In the defense of his thesis entitled 'Action de l'alcohol amylique sur l'organisme' at the Faculty of Medicine, University of Strasbourg, France, on 9 January 1863, Cros noted that a relationship exists between the toxicity of primary aliphatic alcohols and their water solubility. This relationship demonstrates the central axiom of structure–toxicity modeling. That is the toxicity of substances is governed by their properties, which are determined in turn by their chemical structure. Therefore, there are interrelationships among structure, properties, and toxicityas stated by DBSF, Insubria University, Varese, Italy [38].

Crum-Brown, in 1864 [39] and in 1866 [40], and Crum-Brown and Fraser in 1868 [41], proposed the existence of a correlation between the biological activity of different alkaloids and their molecular constitution. More specifically, the physiological action of a substance in a certain biological system (Φ)was defined as a function of its chemical constitution (C):

$$\Phi = f(C).$$

These models can be very useful to predict biodegradability of pure chemical substances with known chemical structure. This can be done by using molecular descriptors, which represent the final result of the logical and mathematical procedure transforming chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment [42].

I.3. Reliability assessment

Reliability assessment demonstrates whether the test designer was correct in expecting a certain collection of items to yield interpretable statements about entity differences. No validity coefficient and no factor analysis can be interpreted without some appropriate estimate of the magnitude of the error of measurement. The preferred way to find out how accurate one's measures are is to make two independent measurements and compare them. The internal consistency method is used to assess the reliability of results across items within a test, and to determine the degree to which all items measure a common property. To evaluate internal consistency, many techniques exist, such as:

*). Split Half (Odd-Even) Pearson's Correlation,
1). Split Half Spearman-Brown Prophecy
**) Split Half Number of Correct and incorrect subjects
2). Split Half Kuder-Richardson KR20 and KR21
3). Cronbach's Alpha

I.3.1. Steps to compute reliability coefficients

To compute these coefficients, the following step-by-step procedure is presented:

I.3.1.1. The mean for the test

The test is split in odd (first column) and even (second column), where the ratio between their sum and the number of items gives the mean of the test:

$$Meanforthetest,\ \mu = \frac{\sum(odd,even)}{n} = \frac{\sum x_i}{n} \qquad (1)$$

I.3.1.2. Standard deviation of the population of the test

The standard deviation σ and the variance of the test σ^2 for a population of sum odd and even is computed as follows:

$$\sigma^2 = \sum_{i=0}^{n-1} \frac{(x_i-\mu)^2}{w} \qquad (2)$$

Where: μ is the mean for the test and, w is equal to n when weighting, is set to population and (n-1) when weighting is set to sample.

I.3.1.3. Split Half (Odd-Even) Pearson's Correlation Coefficient

Generally, it is not always possible to test and retest. The alternative solution is to divide the test into two sequences of questions: one Odd and another Even, and to compare the results by the determination of the linear correlation coefficient between the two sequences. The linear correlation coefficient also is known as the product-moment coefficient of correlation or Pearson's correlation. The following equation describes the linear correlation coefficient:

$$r = \frac{\sum z_x z_y}{n} \quad (3)$$

Where n is the population, z_x and z_y are the standardized z-values of x and y. The standardized z-values indicate how many standard deviations x and y are above or below the mean. ρ the Pearson's product moment correlation coefficient for two variables x and y for a population with discrete or continuous probability density function (pdf) is:

$$\rho = \frac{cov(x,y)}{\sigma_x \sigma_y} = \frac{\sum_{i=1}^{n} x_i x_i - n\bar{x}\bar{y}}{\sqrt{(\sum_{i=1}^{n} {x_i}^2 - n\bar{x}^2)(\sum_{i=1}^{n} {y_i}^2 - n\bar{y}^2)}} \quad (4)$$

The correlation coefficient, r, and Pearson'scorrelation coefficient,ρare always in the interval [–1, 1]. If the correlation coefficient is 1 the x and y have a complete positive correlation. In other words, the data points from the x and y lie on a perfectly straight, positively-sloped line. If the correlation coefficient is –1, the x and y have a complete negative correlation. In other words, the data points from the x and y are inversely proportional and lie on a perfectly straight, negatively-sloped line. If the correlation coefficient is near zero or null, the x and y have no correlation. The adjusted correlation coefficient, r_{adj}, of Pearson's r is:

$$r_{adj} = \sqrt{1 - \frac{(1-r^2)(n-1)}{n-2}} \quad (5)$$

I.3.1.4. Split Half Spearman-Brown Prophecy:

Spearman and Brown have defined the split-half reliability as the correlation between two halves of a test ($r_{1,2}$) corrected to full test length by the Spearman-Brown prophecy (prediction) (r_{sh}) by the following equation:

$$r_{sh} = \frac{2(r_{1,2})}{1+(r_{1,2})} \quad (6)$$

Where $r_{1,2}$ is Pearson's correlation coefficient as defined in Eq.4.

To increase test reliability is to lengthen test items; and by considering that the new items are just like the existing ones. The increasing of the test length by a lot will increase reliability, but not enough to make it worth [43].

I.3.1.5 Split Half Number of Correct and incorrect subjects

We consider with dichotomous choices, subjects that score with 1 pass the test (S_c, correct subject), and that score with 0, will fail (S_w, wrong subjects). Thus, the sum of subjects that fail the query (i) is as follow:

$$\sum S_{wi} = Totalsubjects - \sum S_{ci} \quad (7)$$

The correct proportion P_c, is the sum of correct subjects divided by total subjects:

$$P_{Ci} = \frac{\sum S_{Ci}}{Totalsubjects} \quad (8)$$

The wrong proportion P_w, is the sum of incorrect subjects divided by total subjects:

$$P_{Wi} = \frac{\sum S_{Wi}}{Totalsubjects} = 1 - P_{Ci} \quad (9)$$

The sum of wrong and correct proportions should be equal to one, so that, this rest of proportion $P_{wi,}$is in fact, the difference between 1 and the correct proportion.

I.3.1.6 Split Half Kuder-Richardson KR_{20} and KR_{21}

Kuder-Richardson Formula 20 (K_{20}) is useful for evaluating trueness of the test in only dichotomously scored items with a range of difficulty. It is equivalent to performing the split half methodology on all combinations of queries and is applicable when each query is either right or wrong. A correct query scores 1 and an incorrect query scores 0. Estimated reliability of the full-length test, K_{20}, can be defined as:

$$K_{20} = \frac{n}{n-1}\left(1 - \frac{\sum(P_{Ci} * P_{Wi})}{\sigma^2}\right) \quad (10)$$

(n) is the number of items, P_{Ci} = proportion number passing the test, P_{wi} = proportion number failing the test (P_{wi}=1-P_{Ci}), and σ^2 is the variance of the whole test. K_{20} values range from 0 to 1. A high value indicates reliability; while too high a value (in excess of .90) indicates a homogeneous test.

In case of dichotomously scored items are all about the same difficulty, (i.e. the mean score of each question is approximately equal to the mean score of all the questions), then a simplified version of K_{20} is Kuder-Richardson Formula 21 (K_{21}) defined as follows:

$$K_{21} = \frac{n}{n-1}\left(1 - \frac{\mu(n-\mu)}{n\sigma^2}\right) \quad (11)$$

μ is the mean score on the test. Typically K_{21} underestimates the reliability of a test, compared to K_{20} [44].

I.3.1.7. Cronbach's Alpha

Alpha is a measure of test or scale consistency developed by Cronbach [45]. It is considered as an index of internal consistence measure which describes the relationship between items in a group [46]. It can be calculated only by continued data. It is defined by the function of the number of test items, and the mean of inter-correlation between items:

$$\alpha = \frac{n}{n-1}\left(1 - \frac{\sum {\sigma^2}_j}{{\sigma^2}_{test}}\right) \quad (12)$$

ion, Where n is the number of items, σ^2 is the variance of results on item j, and σ^2_{test} is the total variance of the entire test results. The consistency coefficient demonstrates if the designed test is correct for expending certain collection of items to yield interpretable results based on entity differences [45, 47]. Results obtained from measurement instrument, survey or scales are considered consistent when an item (or a group of items) gives the same result for the entire analysis [48].

Tavakol and Dennick [49] demonstrate that Alpha takes values between 0 and 1. Reported values in the literature [50, 51, 52], are between 0.70 and 0.95. Low values may due to insufficient number of items, to incoherence or to poor correlations between items.

On the other hand, high values of alpha do not always mean high consistency; it may be that the existence of repetition (redundancy) and thus the size, must be corrected by the reduction of items. Field [53], considers that the consistency start from 0.80. The maximum value preferred by Streiner [54] is 0.90, and the rule of thumb, the most accepted for alpha according to George and Mallery [55], is as follow, Fig.1:

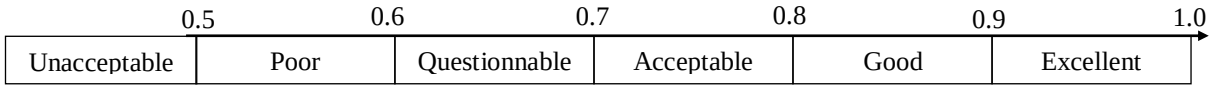

Figure 01. *Reliability scale range*

It is possible to quantify how eachitem contributes to internal consistency reliability, and to take into account the variation of Cronbach's Alpha and the correlation coefficient any time one item is eliminated. If Alpha is increased when the item is discarded, the correlation coefficient also increases. If Alpha still unchanged after item is eliminated, and the correlation coefficient still also unchanged, correlations between the total result and result of the item must be moderate or have tendency to high values. Contrary to that, the result obtained from the scale is considered inconsistent and the relation between items is worst.

In dichotomously scored items (1, 0), Cronbach's Alpha is equal to KR_{20}. However, KR_{21} is generally an under estimate reliability.

II. Materials and methods

A set of thirty seven (37) commercial chemical products are selected from a group of chemicals largely applied in Algerian oil and gas fields mainly at Hassi Messaoud (Table 01) from which a site with GPS coordinates 31°40'14.1"N 6°03'16.5"E. They are corrosion inhibitors, biocides, emulsion breakers etc. Biodegradability test is performedusing the OECD screening test 301 F and solubility phase is taken from their MSDS. The mathematical used method is the reliability test.

II.1. Biodegradability test

The OECD 301 F (respirometry test), from the OCDE guideline [3] (1992), used in our study is equivalent to the international standard ISO 9408 (1999) which aims to measure ready biodegradability of chemicals. Tests are duplicated. This method is chosen because it is applicable for soluble and insoluble products, to thusgenerate reliable results. The Biological Oxygen Demand (DBO) is determined for a period of 28 days using DBO-System with incubator-agitator (WTW OXITOP).

Mineral media are prepared from stock solutions:

- 100 mlof solution A (8.50 g/l KH_2PO_4, 21.75 g/l K_2HPO_4, 33.40 g/l $Na_2HPO_4 \times 2H_2O$, 0.50 g/l NH_4Cl),
- 10 mlof solution B (27.50 g/l $CaCl_2$),
- 10 ml of solution C (22.50 g/l $MgSO_4 \times 7H_2O$), and
- 10 mlof solution D (0.25 g/l $FeCl_3 \times 6H_2O$) are mixed, the volume is adjusted to 10 l with demineralized water, and the pH is adjusted to 7.4.

The used inoculum is brought from an activated sludge collected from the sewage plant or Waste Water Treatment Plant (WWTP) in the city of Boumerdes (36°44'50.83"N, 3°28'4.95"E),Algeria. This plant is dedicated to the treatment of domestic wastewater. The sample is diluted and aerated at room temperature until itis used within 24 hours.
The test material is dispersed directly in the final volume of medium (100 ml) to give a test concentration around 100 mg/l and then it is inoculated in the test flask with 30 mg/l dry weight of sludge. The samples are magnetically stirred and incubated under diffusing light at 22±1°C. On day 28, all barometric data are collected. It is important to indicate that the test duration is extended by two weeks for the chemical products that are not soluble in water as mentioned in the standard method. The automatic barometric device, Oxitop C (WTW, Weilheim) calculates the oxygen consumption. Each sample container is connectedto a barometric system. This system is proportional to the amount of oxygen that is consumed by microorganisms. The percentage of biodegradation is calculated via the OECD 301F guideline (OECD, 1992).

II.2. Reliability Tests

For reliability test, the used products are noted items. The parameters of biodegradability and solubility are questions. If the product is biodegradable or soluble the score is one (1) if not, the score is zero (0). For the statistical analysis we denote the score 1 for a positive test and the score 0 for unsuccessful test.

III. Results And Discussion

The generated data from lab experiments, MSDS and statistical data treatment are presented in the following tables:
The results of solubility and biodegradability test are shown in Table 01. The size of the studied population of subjects is Si = 37 and the size of items is Qi = 2. Reliability is studied using the four coefficients mentioned above, the results are given in tables 2, 3 and 4.

- **Split half Spearman-Brown Prophecy:**

The equation given in subsection 1.3.1.4 to calculate Split Half Spearman-Brown Prophecy coefficient is applied to the results of biodegradability and solubility given in table 01. The results are given in table 02. The applied reliability test expressed by the calculation of split half Spearman-Brown Prophecy correlation coefficient reveals a value of 0.6263. This value yields questionable test in the scale range as indicated in Fig.1 [55].In the following subsection, the test of Split Half Kuder-Richardson KR20 and KR21 is applied to the results of biodegradability and solubility of table 01.

- **Split Half Kuder-Richardson KR20 and KR21:**

The equations given in subsections 1.3.1.5 and 1.3.1.6, to calculate Split Half Kuder-Richardson KR20 and KR21coefficients, are applied to the results of biodegradability and solubility given in table 01. The results are given in table 03. The applied reliability test expressed by the calculation of the two coefficients reveals a value of 0.6263. This value of 0.6263 yields questionable test in the scale range as indicated in Fig.1 [55]. This result confirms the computed result from split half Spearman-Brown Prophecy correlation coefficient.In the following subsection, the test of Cronbach's Alpha is applied to the results of biodegradability and solubility of table 01.

- **Cronbach's Alpha**

The equation given in subsection 1.3.1.7 to calculate Cronbach's Alpha is applied to the results of biodegradability and solubility given in table 01. The results are given in table 04. The applied reliability test expressed by the calculation of Cronbach's Alpha, reveals a value of 0.6263. This value of 0.6263 yields questionable test in the scale range as indicated in Fig.1 [55] and confirms the calculated results from split half Spearman-Brown Prophecy correlation coefficient and Split Half Kuder-Richardson KR20 and KR21coefficients.

Table 01*. Solubility and Biodegradability results with dichotomous score.*

Subject	Chemicalfamily	Solubility phase (S)	Biodegradability B (%)	B Item 1	S Item 2	Score
1	Amine	Oil	85.4	1	0	1
2	Amine	Water	88.98	1	1	2
3	Quaternary Ammonium	Oil	65.71	1	0	1
4	Amine	Oil	54.44	0	0	0
5	Quaternary Ammonium	Oil	73.87	1	0	1
6	Amine	Oil	19.76	0	0	0
7	Amine	Oil	41.19	0	0	0
8	Amine	Oil	86.06	1	0	1
9	Amine	Oil	17.30	0	0	0
10	Amine	Water	36.73	0	1	1
11	Amine	Oil	54.21	0	0	0
12	Quaternary Ammonium	Water	88.98	1	1	2
13	Amine	Water	74.87	1	1	2
14	Quaternary Ammonium	Water	84.97	1	1	2
15	Quaternary Ammonium	Water	72.54	1	1	2
16	Quaternary Ammonium	Water	82.19	1	1	2
17	Quaternary Ammonium	Water	82.62	1	1	2
18	Quaternary Ammonium	Water	76.44	1	1	2
19	Amine	Water	45.58	0	1	1
20	Amine	Oil	23.01	0	0	0
21	Amine	Oil	33.26	0	0	0
22	Amine	Water	14.91	0	1	1
23	GLUTARAldehyde	Water	65.35	1	1	2
24	Quaternary ammonium	Water	64.92	1	1	2
25	Tetrakishydroxymethylphosphonium	Water	20.86	0	1	1
26	Tetrakishydroxymethylphosphonium	Water	92.84	1	1	2
27	PhosphoniumQuaternarysalt	Water	52.23	0	1	1
28	PhosphoniumQuaternarysalt	Water	63.76	1	1	2
29	Sulfonate	Oil	32.96	0	0	0
30	Benzene	Oil	16.23	0	0	0
31	Sulfonate	Oil	55.44	0	0	0
32	Fuel Diesel	Oil	69.27	1	0	1
33	Amine	Water	69.25	1	1	2
34	Heavyaromatics	Oil	33.12	0	0	0
35	Aromatics	Oil	24.81	0	0	0
36	Phosphonates	Water	66.36	1	1	2
37	PhosphoOrganicCompounds	Water	69.84	1	1	2

***Table 02**. Split half Spearman-Brown Prophecy results.*

Mean for the test	1.0811
Standard Deviation for the population of the test	0.8504
Variance for the population of the test	0.7232
Split half Corr. Coeff	0.4559
radj	0.4303
Split half Spearman-Brown Prophecy Corr. Coeff.	**0.6263**

***Table 03**. Split half Kuder-Richardson KR20 and KR21 results.*

Number of correct subjects for Q1	20.0000
Proportion of correct subjects for Q1, Pc1	0.5405
Number of correct subjects for Q2	20.0000
Proportion of correct subjects for Q2, Pc2	0.5405
Number of wrong subjects for Q1	17.0000
Proportion of wrong subjects for Q1, Pw1	0.4595
Number of wrong subjects for Q2	17.0000
Proportion of wrong subjects for Q2, Pw2	0.4595
Pc1*Pw1	0.2484
Pc2*Pw2	0.2484
Sum of Pc*Pw	0.4967

K20	**0.6263**
k21	**0.6263**

***Table 04**. The value of Cronbach's Alpha.*

Standard deviation for Q1	0.4984
Standard deviation for Q2	0.4984
Variance for Q1	0.2484
Variance for Q2	0.2484
Sum of variance for Q1 and Q2	0.4967
Cronbach's Alpha	**0.6263**

The observation of experimental data of table .1 shows no significant link between the solubility phase and the biodegradability of chemicals. Thus, a chemical product can be soluble in the oil phase but biodegradable and vice versa. This reliability coefficient obtained from K20, K21 and Alpha Cronbach gives the value of 0.6263 which yields questionable test in the scale range as indicated in Fig.1. From this scale, the decision can be rejected because Alpha is less than 0.7. Moreover, the same value is found for the three calculated parameters because of the dichotomous scores approach considered in our work. Therefore, this analysis confirms the statement of the category of scientists who consider the weak Biodegradability-Solubility relationship. As mentioned in the literature review, till now there is a divergence amongst scientists about the link that exists between the two considered parameters [11, 12].Thus, our findings from the reliability test are align with what has been found by scientists.From this statement of reliability evaluation of chemical products belonging to the category of UVCB substances, may be promising approach and a breakthrough in the prediction of biodegradability of chemical products of complex and unknown structures, precisely when QSAR Models cannot estimate their impact on the environment.

IV. Conclusion

According to this study, the following conclusions can be put forward:

- This first attempt to use reliability test to study the environmental fate of chemicals is applied under state of art rules. Thus, reliability tests, especially Cronbach's Alpha, can be used to study and confirm the environmental fate of chemicals, especially those of complex structures such as UVCB substances.

- The applied test is a non-biased perfect test since we get the same number of Split half Spearman-Brown Prophecy Correlation Coefficient, Split Half Kuder-Richardson KR20 and KR21, and Cronbach's Alpha with the value of 0.6263. This perfect test is certainly due to dichotomous scores approach. This value in the scale range yields questionable test that can be rejected. Therefore, this analysis confirms the statement of the category of scientists who consider the weak Biodegradability-Solubility relationship.

- Reliability test techniques can be revolutionary in terms of gaining time when executing biodegradability tests. It is worth noting that generating experimental biodegradability data of the 37 products took an appreciable time. Thus, using reliability coefficients is a useful and flexible tool that gives information on environmental fate of chemicals used in industries such as the oil and gas.

- The generated results are to be used with great care since reliability is not a characteristic inherent to the test itself. It is rather an estimate of the consistency of a set of items when they are applied to a particular group of products at a specific time under particular conditions for a specific purpose.

- These test results awake curiosity to test and confirm biodegradability correlations with other physicochemical properties especially, using Cronbach's alpha to test several items at the same time.

- For future work, it will be very useful to consider reliability test applied to a larger number of chemicals pertaining to UVCB substances usually used in the oil and gas sector, to study the possible links between biodegradability and other physicochemical properties or even toxicity with other physicochemical properties. This study could help operators to select more environmentally friendly chemicals for their future operations.

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