Journal of
Bioremediation & Biodegradation

Seung Lim, J Bioremediat Biodegrad 2016, 7:3
DOI: 10.4172/2155-6199.1000e171

Editorial Open Access

EPI Suite: A Fascinate Predictive Tool for Estimating the Fates of Organic Contaminants

Seung Lim J*

Research Division for Industry and Environment, Korea Atomic Energy Research Institute, 29 Geumgu, Jeongeup, Jeollabuk-do, 580-185, Republic of Korea

Introduction

EPI Suite was developed by the US EPA, and is based on the BIOWIN and AOPWIN modules to estimate the fates of organic chemicals in the environment. To use EPI Suite, the chemical's Simplified Molecular Input Line Entry System (SMILES) notation is required as input. EPI Suite (ver. 4.11) consists of 13 discrete models as listed below:

- AOPWIN - estimates atmospheric oxidation rates
- BCFBAF - estimates bioconcentration factor (BCF) and biotransformation rate (kM)
- BioHCwin - estimates biodegradation of hydrocarbons
- BIOWIN - estimates biodegradation probability
- ECOSAR - estimates aquatic toxicity (LD50, LC50)
- HENRYWIN - estimates Henry's law constant
- HYDROWIN - estimates aqueous hydrolysis rates (acid-, base-catalyzed)
- KOAWIN - estimates octanol-air partition coefficient
- KOCWIN - estimates soil sorption coefficient (Koc)
- KOWWIN - estimates octanol-water partition coefficient
- MPBPVP - estimates melting point, boiling point, and vapor pressure (also referred to as MPBPWIN)
- WSKOWWIN - estimates water solubility (from log Kow)
- WATERNT - estimates water solubility (using atom-fragment methodology)

It is not necessary that the 13 models be used to estimate the persistence of a chemical. Thus, the user can choose the models used to provide results from 13 discrete EPI Suite models.

BIOWIN

The biodegradation probability program for Microsoft Windows (BIOWIN) models have been developed by the Syracuse Research Corp. (SRC) on behalf of the US EPA since the 1980s. Most BIOWIN models estimate the probability of rapid aerobic biodegradability. BIOWIN7 is the exception as it estimates the probability of rapid anaerobic biodegradability in the presence of heterogeneous microorganisms. Although BIOWIN consists of seven models, EPI Suite uses BIOWIN3 to estimate the fate of a chemical by default. The description of each BIOWIN model is as follows:

- BIOWIN1: linear probability model
- BIOWIN2: nonlinear probability model

The BIOWIN1 and BIOWIN2 models were reviewed in an article by Howard et al. [1]. The linear model (BIOWIN1) and the non-linear model (BIOWIN2) were developed using 264 chemicals.

- BIOWIN3: expert survey ultimate biodegradation model
- BIOWIN4: expert survey primary biodegradation model

BIOWIN3 and BIOWIN4 models were introduced in an article by Boethling et al. [2]. These models are survey models because an expert panel was asked for their response to predicted rates for primary degradation (loss of parent chemical identity) and ultimate degradation (conversion to CO_2 and H_2O) under aerobic conditions.

- BIOWIN5: MITI linear model
- BIOWIN6: MITI nonlinear model

The linear model (BIOWIN5) and non-linear model (BIOWIN6) for assessing organic compounds is based on the Japanese Ministry of International Trade and Industry (MITI) ready biodegradation test.

- BIOWIN7: anaerobic biodegradation model

BIOWIN7 was developed using 169 chemicals and consists of a linear model and a non-linear model to assess the probability of rapid anaerobic biodegradation

There exist so many screening test protocols including the MITI test, Association Française de Normalisation (AFNOR), and the OECD screening test (e.g., BOD tests, activated sludge die-away tests, CO_2 evolution tests, and etc.). Thus, Howard et al. [3] reviewed previous structure/biodegradation test data, collected and evaluated available biodegradation data, and designed and documented the procedures. Using available biodegradation results, Howard et al. [3] assumed that "as the number of consistent test results or test results for which apparent inconsistencies are resolvable increases, the greater is the likelihood that the indication of biodegradability is a property of the chemical rather than of the test system". Evaluation of biodegradability was done with screening tests, biological treatment simulations, grab sample tests, and field studies. The test results were evaluated using the BIODEG model. In order to obtain unacclimated as well as acclimated results, BIODEG used a test time period of 28 days which is the same as used for the OECD-recommended screening tests.

The US EPA reviews thousands of pre-manufacture notices (PMNs; substances not yet in commerce) for potential ecological and human health effects. Under the Toxic Substances Control Act (TSCA), the US EPA regulates chemicals except for pesticides, drugs, and food additives. Boethling and Sabijic [4] surveyed 50 PMN chemicals by an

***Corresponding author:** Seung Lim J, Research Division for Industry and Environment, Korea Atomic Energy Research Institute, 29 Geumgu, Jeongeup, Jeollabuk-do, 580-185, Republic of Korea, Tel: +82-63-570-3357; Fax: +82-63-570-3348; E-mail: seungjoolim@gmail.com

Received March 25, 2016; **Accepted** April 01, 2016; **Published** April 06, 2016

Citation: Seung Lim J (2016) EPI Suite: A Fascinate Predictive Tool for Estimating the Fates of Organic Contaminants. J Bioremediat Biodegrad 7: e171. doi: 10.4172/2155-6199.1000e171

expert panel. Experts were asked to evaluate predicted removal rates in typical wastewater treatment systems (REM) and aerobic ultimate degradation rates in receiving waters (AERUD) for 50 PMN chemicals. Also, AERUD distinguished compounds with high biodegradability rates from compounds with low biodegradability rates using an expert model. Howard et al. [3] developed a linear model and a non-linear model using 264 chemicals. Under aerobic conditions, the accuracy of the results for rapidly degraded compounds was greater than that for the results of slowly degraded compounds because the majority of selected target chemicals were rapidly biodegradable under aerobic conditions. Boethling et al. [4] developed four models. A linear BIODEG model and a non-linear BIODEG model were developed using 295 chemicals where 186 of the chemicals were designated "rapidly biodegradable" and 109 chemicals were designated "does not rapidly biodegradable". These models of Howard and Boethling were on the basis for BIOWIN1 and BIOWIN2. BIOWIN3 and BIOWIN4 (two survey models) were developed for primary degradation and ultimate degradation under aerobic conditions using 200 chemicals. A primary model for the loss of parent chemical identity and an ultimate model for the conversion of CO_2 and H_2O were evaluated by 17 experts. The accuracy of each BIODEG model was approximately 90%, while that of survey models was approximately 83%. Tunkel et al. [5] compared the test results from BIOWIN (ver. 3.63) with those resulted from the MITI-I test using 884 discrete organic chemicals. In the BIOWIN model evaluation, two thirds of the 884 chemicals were used as an evaluation data set, while the remaining one third was used for validation. The compounds used for validation were randomly selected. In the MITI-I test, the OECD pass criterion (inoculum=30 mg sludge solids/L, test period=28 days, ThOD ≥ 60% for pass) was used to discriminate a pass/fail for biodegradation. When using MITI fragments (BIOWIN: training set=884 chemicals, no validation set; MITI-I test=training set: 589 chemicals, validation set=295 chemicals), the accuracies of both a linear model and a non-linear model in MITI-I tests were greater than those of BIOWIN. When, however, BIOWIN used BIOWIN fragments (training set=589 chemicals, validation set=295 chemicals), the accuracies of both a linear model and a non-linear model in MITI-I tests were comparable to those of BIOWIN.

Boethling et al. [6] compared the accuracy of different BIOWIN models (from BIOWIN1 to BIOWIN6) using a total of 944 PMN chemicals. The US EPA used 305 PMN chemicals, 439 chemicals from the MITI databases, and compared 200 PMN chemicals in the expert survey on which the BIOWIN3 and other BIOWIN models were evaluated. The greatest accuracy among BIOWIN models was demonstrated by BIOWIN3 (87%), whereas BIOWIN1 and BIOWIN2 models were deemed not suitable for estimating PMNs [7]. developed the BIOWIN7 model using data from serum bottle tests (incubation period: at least 56 days) using 169 chemicals in the training set and 58 chemicals in two validation sets. The accuracy of the training set was approximately 90% and those of the validation sets were 77% and 91%, respectively.

AOPWIN

The Atmospheric Oxidation Program for Microsoft Windows (AOPWIN) estimates the rate constant between photochemically produced hydroxyl radicals and organic chemicals in air under environmental conditions. AOPWIN also estimates the rate constant between ozone and olefinic compounds. The estimated constants are used to calculate the half-lives of organic compounds in the atmosphere. Since the 1980s, several methods have been developed to estimate hydroxyl radical concentrations in the atmosphere (e.g., utilizing molecular properties of chemicals or ionization energy). However, most of these methods were not based on database molecular properties [8,9]. developed estimation methods using SARs, however the estimations for reactions with fluoresters, ethers, haloalkanes, and haloalkanes containing CF_3 groups were not accurate [10]. updated the AOPWIN model and reported that the accuracy of the hydroxyl radical reaction rate constant was approximately 90% at 25°C. The hydroxyl radical reaction rate constant with organic compounds in AOPWIN model can be calculated as follows:

K_{total}=k(from C – H and O – H)+k(OH addition to >*C*=*C*< and –*C* ≡ *C* – bonds)=k(OH addition to aromatic rings)+k(OH interaction with N–, S–, and P– containing groups)

References

1. Howard PH, Boethling RS, Stiteler WM, Meylan WM, Hueber AE, et al. (1992) Predictive model for aerobic biodegradability developed from a file of evaluated biodegradation data. Environ Toxicol Chem 11: 593-603.
2. Boethling RS, Howard PH, Meylan W, Stiteler W, Beauman J, et al. (1994) Group contribution method for predicting probability and rate of aerobic biodegradation. Environ Sci Technol 28: 459-465.
3. Howard PH, Hueber AE, Boethling RS (1987) Biodegradation data evaluation for structure/biodegradability relations. Environ Toxicol Chem 6: 1-10.
4. Boethling RS, Sabijic A (1989) Screening-level model for aerobic biodegradability based on a survey of expert knowledge. Environ Sci Technol 23: 672-679.
5. Tunkel J, Howard PH, Boethling RS, Stiteler W, Loonen H (2000) Prediction ready biodegradability in the Japanese ministry of international trade and industry test. Environ Toxicol Chem 19: 2478-2485.
6. Boethling RS, Lynch DG, Thom GC (2003) Predicting ready biodegradability of premanufacture notice chemicals. Environ Toxicol Chem 22: 837-844.
7. Meylan W, Boethling R, Aronson D, Howard P, Tunkel J (2007) Chemical structure-based predictive model for methanogenic anaerobic biodegradation potential. Environ Toxicol Chem 26: 1785-1792.
8. Atkinson R (1986) Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds under atmospheric conditions. Chem Rev 86: 69-201.
9. Atkinson R (1987) A structure-activity relationship for the estimation of rate constants for the gas-phase reactions of OH radicals with organic compounds. Int J Chem Kinet 19: 799-828.
10. Kwok ESC, Atkinson R (1995) Estimation of hydroxyl radical reaction rate constants for gas-phase organic compounds using a structure-reactivity relationship: An update. Atmos Emviron 29: 1685-1695.