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Empirical Model for Predicting Concentrations of Refractory Hydrophobic Organic Compounds in Digested Sludge from Municipal Wastewater Treatment Plants

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Abstract

An empirical model is presented allowing for the prediction of concentrations of hydrophobic organic compounds (HOCs) prone to accumulate and persist in digested sludge (biosolids) generated during conventional municipal wastewater treatment. The sole input requirements of the model are the concentrations of the individual HOCs entering the wastewater treatment plant in raw sewage, the compound's respective pH-dependent octanol-water partitioning coefficient (D_{OW}), and an empirically determined fitting parameter (p_{fit}) that reflects persistence of compounds in biosolids after accounting for all potential removal mechanisms during wastewater treatment. The accuracy of the model was successfully confirmed at the 99% confidence level in a paired t test that compared predicted concentrations in biosolids to empirical measurements reported in the literature. After successful validation, the resultant model was applied to predict levels of various HOCs for which occurrence data in biosolids thus far are lacking.

Keywords

Biosolids; emerging contaminants; sorption; persistence

Introduction

A large number of hydrophobic organic compounds (HOCs) are used domestically, industrially, and commercially in the United States and, following their intended uses, are discharged into municipal wastewater. Depending on their physicochemical properties, biodegradability and mass loading, they are expected to accumulate in digested sewage sludge (biosolids) to greatly varying degrees.[1,2]

While the treated effluent of municipal wastewater treatment plants (WWTPs) is a commonly scrutinized source of organic wastewater contaminants to aquatic environments, the chemical make-up of biosolids is less frequently investigated and less well understood. Improving the current knowledge of refractory (*i.e.*, difficult to degrade) compounds in biosolids is important, due to the widespread practice of land application of treated sewage sludge for soil conditioning, soil fertilization and as an inexpensive means of disposal of these abundant materials.

The occurrence of organic chemicals in sewage sludge has been reviewed[2-4] and the need for additional analyses pointed out repeatedly. An important step forward was the recent release

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by the U.S. Environmental Protection Agency (EPA) of data from the 2009 Targeted National Sewage Sludge Survey that examined some 145 analytes, including 72 pharmaceuticals and personal care products (PPCPs) by EPA method 1694.[5] Despite the progress made, a more complete characterization of the chemical composition of sludge is desirable. Prior to carrying out targeted chemical analyses of sludge in the laboratory, it can be informative and economically attractive to narrow the number of potentially important analytes by performing qualitative and quantitative modeling in conjunction with risk assessments for susceptible receptor organisms.[2,6-8]

To this end, several models have been developed for predicting the fate of chemicals in sludge, [9-14] all assuming the standard practice of primary treatment of wastewater by sedimentation followed by activated sludge treatment as the secondary, biological stage. These models have been applied to a limited number of chemicals featuring a fairly narrow range of physical-chemical properties. For example, one model was used to predict the fate of consumer product additives in primary and activated sludge processes.[15] It assumed an unlimited availability of both dissolved and sorbed chemical mass for biodegradation, and required as input parameters independently determined values for the distribution coefficient between sludge solids and liquid, the compound's Henry's law constant and its specific rate of biodegradation. [15] This and related models work well in situations where detailed information is available on the efficacy of the treatment process, such as the specific biodegradation rate of a chemical of interest. Since the latter information typically is not readily available, it is desirable to develop simple, yet reliable models that can serve to estimate the concentration of organic wastewater compounds in treated effluent and biosolids using as input parameters more readily available data.

Recently, an empirical model was introduced that can serve to estimate, with reasonable accuracy, the fraction of the total loading of a given HOC that is expected to persist in biosolids after treatment.[16] The model is based on real-world observations made in full-scale WWTPs. It identifies and utilizes hydrophobicity, expressed as the octanol-water partition coefficient (K_{OW}), as a principal parameter governing the fate of HOCs during municipal wastewater treatment and during biological digestion of sequestered compounds in biosolids. Although the model resembles conventional mathematical approaches to assess sorption of chemicals to organic matter, it is not limited to the latter and reflects contaminant attenuation by all relevant removal mechanisms, including biotransformation. Removal mechanisms other than sorption are considered and parameterized in a composite fitting parameter, termed p_{fit} . Thus, the model's only input requirements are the K_{OW} of the contaminant of interest and the empirically determined fitting parameter that reflects the combined effect of all potential removal processes, including sorption as well as aerobic and anaerobic biological digestion during, respectively, activated sludge wastewater treatment and sludge stabilization. The output of this existing model is the fraction, expressed as a percentage, of the mass input that can be expected to persist in sludge after treatment by digestion.[16]

This study aimed to furnish an extended application of the aforementioned model that would be suitable for the quantitative prediction of HOC concentrations in biosolids using as an additional input parameter, i.e., published concentrations of contaminants in either unfiltered or filtered raw sewage.

Results and discussion

The goal of the present study was to extend the applicability of a recently reported empirical model to enable the prediction of concentrations of refractory HOCs in biosolids based on contaminant levels detected in unfiltered or filtered samples of plant influent (see equation 1). An important objective was to arrive at a model that is simple, reasonably accurate, and that

requires as input parameters only readily available information, namely a given compound's respective pH-dependent octanol-water partitioning coefficient (D_{OW}) value, its concentration in raw sewage entering the treatment plant, and a fitting parameter accounting for loss due to all relevant removal mechanisms, including sorption and biotransformation.

A recently proposed empirical model[16] served as the starting point of our investigation. As can be seen from equation 2, the existing model provided an estimate of the relative fraction of the total mass of an organic wastewater contaminant that becomes sequestered in treated biosolids. In order to relate the fraction of the total contaminant mass loading (expressed in %) to a concentration (expressed in units of mass per dry weight biosolids), we used the relationship shown in equation 3. The accuracy of the resultant model was determined by comparing the predicted values to those obtained experimentally for 10 organic wastewater contaminants that previously had been investigated using a mass balance approach (Fig. 1, Table 1). Model input parameters for this initial model validation were taken from a recent review article[16], and included: the total concentration of both dissolved and sorbed mass of chemical n arriving at the plant contained in raw sewage ($C_{T(influent)}$); the compound's D_{OW} value taken from the literature; and the average value of a dimensionless fitting parameter, p_{fit} (1.76×10^{-6}), that captures the typical behavior of HOCs in conventional U.S. WWTP employing activated sludge treatment followed by anaerobic digestion of the resultant biosolids. Also entering into calculations was the average yield of biosolids per volume of treated raw sewage reported in the literature, $1.296 \times 10^{-4} \text{ kg L}^{-1}$ [16]

Measured concentrations in biosolids and those predicted with equation 3 were in good agreement over a range of log D_{OW} values between 2.38 and 6.37 (Fig. 1). The model provided a particularly good fit for more hydrophobic chemicals featuring a log D_{OW} value of ≥ 4.94 . Similar predictive power of the model for compounds with strong sorptive properties (as opposed to those featuring a log D_{OW} value of < 4.94) had been observed previously for the prediction of the fraction of mass input sequestered in sludge.[16] Model predictions clustered around the actual value with no clear trend of over- or underestimation. On average, predictions matched experimental observations within a factor of 1.6-fold (standard deviation of ± 1.7). Results from a paired t -test that compared predicted to calculated values showed the two datasets to be statistically indistinguishable at the 99% confidence level. These initial findings served to validate the appropriateness of equation 3 for predicting with reasonable accuracy, HOC concentrations in biosolids based on influent concentrations. This initial validation was limited to studies performed at specific plants for which both the influent and biosolids concentrations of contaminants had been determined.

Next, the model was applied to studies that reported the contaminant mass in sorbed and dissolved phases (total), as well as in dissolved phase only, i.e., in filtered samples of plant influent (Table 2). Using equation 4, values of $C_{T(influent)}$ were estimated from experimentally determined dissolved concentrations with an implied assumption of equilibrium conditions. The predicted values were found to be reasonably close to contaminant concentrations measured experimentally in composite samples representative of over 70 U.S. sewage treatment plants (Fig. 2). On average, predicted values fell within a factor of 0.16 (standard deviation of ± 0.23) relative to levels measured experimentally in composite samples of digested biosolids from plants from across the U.S. (Table 2). In situations where multiple measurements were available for dissolved contaminant levels in filtered sewage samples (Table 2), each resultant prediction was compared to the corresponding level of contaminant found in composite samples of representative of U.S. biosolids. As observed in the case of plant-specific predictions, estimated values and experimental measurements were statistically indistinguishable at the 99% confidence level.

The ultimate goal of the rearrangement of equations 3 and 4 was to apply the resultant model to compounds for which monitoring information in biosolids is still lacking. This analysis had to be restricted to the log D_{OW} range of 2.0 to 6.0 (Table 3) for which the model had been successfully validated. Predictions were made for 7 compounds, ranging in log D_{OW} values from 2.28 to 6.14. Predicted concentrations in biosolids ranged from <1 to $7745 \mu\text{g kg}^{-1}$ dry weight and tended to be higher for more hydrophobic contaminants (Fig. 3).

Hydrophobic organic compounds predicted to occur in municipal biosolids at concentrations exceeding one part-per-million on a dry weight basis included traseolide ($7700 \mu\text{g kg}^{-1}$). Investigated compounds projected to be of lesser abundance in biosolids included benzophenone ($2 - 55 \mu\text{g kg}^{-1}$), isopropylparaben ($1 - 8 \mu\text{g kg}^{-1}$), oxybenzone ($10 - 76 \mu\text{g kg}^{-1}$), propylparaben ($7 - 19 \mu\text{g kg}^{-1}$) and simazine ($<1 \mu\text{g kg}^{-1}$) (see Table 3 for additional information).

Many studies relevant to this work reported HOC concentrations detectable in the dissolved phase only, typically in filtered samples.[17,28,29,31,32] Direct entry of the dissolved concentrations of contaminants into the model would result in an underestimation of the mass in biosolids, however, because this input parameter neglects to consider the chemical loading contained in raw sewage in the sorbed state adhering to filterable particulates. Use of equation 4 made the findings of these relevant studies accessible to the presented model.

Proper use of the model and its output requires an understanding of the underlying assumptions and its limitations. The assumption of equilibrium between dissolved and sorbed contaminant mass in plant influent likely will be satisfied in most cases. The approximation of the dissolved chemical mass by exclusion of filterable particulates also should be reasonably accurate, although there may be some residual chemical mass in the filtrate that rather than being truly dissolved instead is associated with dissolved organic matter. In contrast, the concentration of suspended solids in sewage may vary significantly from the average literature value used. This could be particularly problematic in situations where a combined sewer system conveys plant influent representing a mixture of domestic sewage and runoff from storm events. Similarly, usage of an average sludge-to-volume ratio as model input introduces a potential source of inaccuracy that varies with treatment plant. All predicted values presented here are based on an average biosolids yield typical of conventional activated sludge WWTPs in the U.S. Yet, specific sludge-to-volume ratios vary from plant to plant. Therefore, biosolids yields (Y values) lower or higher than the average value used would result in over- or underestimation, respectively, of HOC concentrations in biosolids.

In-plant sources of contaminants resulting from the cleavage of conjugated parent compounds represent another potential source of uncertainty.[17] Also, measured concentrations may be the sum of parent and metabolites, whereas the predicted concentration in biosolids is applicable to the parent compound only. In the case of carbamezepine, for example, the empirical concentration reported in biosolids was a composite measure of the parent compound itself and of 5 of its metabolites, whose respective log K_{OW} values range from -0.07 to 2.41 . [18]

Another source of error could arise from those highly polar organic compounds that are charged at ambient pH. The existence of an electrical charge is known to influence the sorption process by triggering electrostatic interactions between both charged organic compounds and sorbent surfaces. If charges are opposite, sorption is enhanced,[33] while similar charges may either increase or decrease sorption through cation bridging and surface complexation mechanisms. [34] Users of the model introduced here should be cognizant of these potential effects and should examine the structure of compounds for which predictions are made for the possibility of the occurrence of such interactions.

Other more comprehensive models that include all removal mechanisms have been proposed to track the fate of organic chemicals in WWTPs.[12,15,35] However, they typically concentrate on the effluent quality, and require plant-specific parameters that are usually difficult to determine. In contrast, the approach taken here is a simple one that is most suited to organic compounds of appreciable hydrophobicity.

Although the present approach is based on a model frequently employed to describe sorption only, the model shown in equation 3 allows for, and actually considers, removal mechanisms other than sorption alone. These additional mechanisms of removal are captured in the fitting parameter (p_{fit}) that reflects a combined measure of all removal processes occurring in the plant, including biodegradation during the activated sludge stage and during several weeks of sludge digestion. A reduction in the bioavailability of organic compounds following sorption has long been known[36,37] and may form the basis for the finding that equation 3 represents the best fit for describing the accumulation of refractory HOCs in biosolids generated during full-scale wastewater treatment.

Conclusions

This work introduced and validated an empirical model suitable for estimating the concentration of hydrophobic organic wastewater contaminants in biosolids. Predictions on average were within about one order of magnitude of empirical measurements. The model's sole input requirements are the D_{OW} value of a given compound and its concentration in WWTP influent reported either as a total concentration or as a dissolved concentration obtained after filtration of samples for removal of particulates. The model can aid in the chemical characterization of municipal biosolids destined for land application by providing order of magnitude estimates of likely levels of refractory compounds persisting in the sludge matrix. Use of the model does not replace actual measurements, however, as its application requires many generalizations that will not always be met for any given chemical, and for the specific location and type of treatment plant considered. The model's principal value thus lies in its use as a prescreening tool to inform the selection of potentially problematic sewage constituents [38] that may enter the environment as a result of recycling of municipal biosolids.

Experimental methods

The concentration of a chemical n in biosolids ($C_{biosolids}$) is a function of its total concentration arriving in influent at the WWTP ($C_{T(influent)}$), the fraction of the total chemical mass of n remaining in biosolids at the end of the treatment process ($f_{biosolids}$), and the yield of biosolids per volume of raw wastewater treated (Y). This relationship is expressed in equation 1:

$$C_{biosolids} = C_{T(influent)} \times f_{biosolids} \times \frac{1}{Y} \quad (1)$$

The fraction of a chemical n persisting in biosolids after treatment can be estimated using a recently proposed empirical model that relates to the theory of sorption but also considers other removal mechanisms including biotransformation:[16]

$$f_{biosolids} = p_{fit} \times \frac{D_{OW}}{1 + p_{fit} \times D_{OW}} \quad (2)$$

where p_{fit} is a dimensionless fitting parameter, and D_{OW} is the compound's octanol-water partition coefficient at pH 7.5, which is the pH of most influent wastewater in the U.S. [39] Substitution of equation 2 into equation 1 yields:

$$C_{\text{biosolids}} = C_{\text{T(influent)}} \times p_{\text{fit}} \times \frac{D_{\text{OW}}}{1 + p_{\text{fit}} \times D_{\text{OW}}} \times \frac{1}{Y} \quad (3)$$

In situations where the published concentration of chemicals in sewage was reported only for filtered samples of influent, the total (dissolved and sorbed) concentration of chemical *n* in raw sewage was calculated from its experimentally determined dissolved concentration in filtered wastewater [39]:

$$C_{\text{T(influent)}} = C_{\text{aq}} (1 + f_{\text{OC}} \times D_{\text{OC}} \times C_{\text{SS}}) \quad (4)$$

where C_{aq} is the dissolved concentration of chemical *n* in influent, f_{OC} is the fraction of organic carbon in particulate, D_{OC} is the organic carbon normalized sorption coefficient, and C_{SS} is the concentration of suspended solids in influent. Application of equation 4 implies an assumption of equilibrium between the dissolved and sorbed state of a chemical. The value of D_{OC} of a chemical *n* was obtained directly from the database, SciFinder® Scholar™, 2004 Edition.

When f_{OC} and C_{SS} were unavailable, published values of 0.43[20,21] and 119 mg L⁻¹ [16] were used, respectively. These values were obtained as averages from a comprehensive literature review. When the plant-specific value of *Y* was unavailable, a literature value of 1.296×10⁻⁴ kg L⁻¹ [16] was used as an approximation for the average biosolid yield for U.S. WWTPs employing secondary treatment by activated sludge processing. The dimensionless fitting parameter, p_{fit} , for conventional U.S. WWTPs previously was estimated to equal 6.51×10⁻⁶. [16] In this study, pH dependence was considered which resulted in a revised value of 1.76×10⁻⁶.

To determine whether the predicted concentrations of HOCs in biosolids were significantly different from empirical measurements published in the literature, a paired *t* test was performed on both datasets.[40] The standard deviation of the ratio of predicted and experimentally determined concentrations also was calculated and used later to indicate as positive error bars the associated average error of predictions made.

Environmental Context

Tens of thousands of manmade chemicals are discharged into municipal wastewaters on a continual basis by consumers around the world but surprisingly little is known about the occurrence and fate of these substances in the environment. The present study furnishes an easily applicable model that can help to predict the presence and concentration of manmade chemicals in digested municipal sludge (biosolids) destined for disposal on land. The new tool can be used to prescreen and identify in chemical databases potential environmental pollutants.

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Figure 1.

Comparison of experimentally measured concentrations (filled symbols) of selected organic wastewater compounds in municipal biosolids with those of model predictions (open symbols) obtained using treatment plant specific input data (C_{SS} , C_{aq}). Multiple symbols of the same colour represent multiple studies or measurements of the same chemical. Numbers next to data points represent references from which data were obtained.

Figure 2.

Comparison of experimentally measured concentrations of selected organic wastewater compounds in composite samples of biosolids from 94 U.S. treatment facilities (filled symbols) with model predictions (open symbols) calculated from influent concentrations published for specific plants. Multiple symbols of the same colour represent multiple studies or measurements performed for one and the same chemical. Numbers next to data points represent references from which data were obtained.

Figure 3.

Predicted concentrations of organic wastewater contaminants in biosolids. Filled symbols indicate predictions obtained for influent concentrations measured at specific plants. Open symbols represent the average value of obtained predictions. The upper error bar indicates the average uncertainty of the prediction (+ 1 standard deviation) determined during the method validation. Numbers next to data points represent references from which data were obtained.

Table 1

Chemical Abstract Service (CAS) registry number, influent concentration and measured as well as predicted contaminant concentrations in biosolids reported on a dry weight basis (Influent and biosolids concentrations were measured at the same plant)

Compound	CAS #	Ref.	Influent (ng L ⁻¹)	Biosolids (μg kg ⁻¹)	
				Measured	Predicted
Clarithromycin	81103-11-9	17	380	0.7	1
Carbamazepine	298-46-4	18	1533	281	10
Estrone	53-16-7	19	65.7	25.2	4
		20,21	54.8	14.3	4
17β-Estradiol	50-28-2	19	15.8	5.10	3
		20,21	22.0	0.57	4
17α-Ethinylestradiol	57-63-6	19	8.2	1.5	4
		20,21	5.0	0.61	2
Triclosan	3380-34-5	22	1200	1200	1200
		23	4700	30 000	4800
Triclocarban	101-20-2	22	6100	51 000	23 100
Nonylphenol	104-40-5	24	6700	24 000	37 800
		24	8400	13 000	47 400
		24	119 000	898 000	671 800
Galaxolide	1222-05-5	25	1941	3068	11 200
		26	390	6788	2300
		27	7240	57615	42 000
Tonalide	21145-77-7	25	583	1525	3600
		26	86	1349	530
		27	1447	7665	9000

Table 2

Chemical Abstract Service (CAS) registry number, influent concentration and (measured and predicted) concentration of selected PPCPs in biosolids reported on a dry weight basis (Influent and biosolids concentrations for specific compounds were measured at different plants)

Compound	CAS #	Ref.	Total Influent (ng L ⁻¹)	Biosolids (µg kg ⁻¹)	
				Measured[30]	Predicted
Erythromycin-H ₂ O	114-07-8	28	3939	82 ± 52	6
Diltiazem	42399-41-7	29	70	45 ± 34	<1
		29	41		<1
Clarithromycin	81103-11-9	17	380	66 ± 26	1
Carbamazepine	298-46-4	18	1533	163 ± 56	10
Triclosan	3380-34-5	22	1200	12 640 ± 3816	1200
		23	4700		4800
Triclocarban	101-20-2	22	6100	36 000 ± 8000	23 100

Table 3

Chemical Abstract Service (CAS) registry number, influent concentration and concentration predicted for biosolids reported on a dry weight basis.

Compound	CAS #	Ref.	Total Influent (ng L ⁻¹)	Predicted Conc. in Biosolids (µg kg ⁻¹)
Simazine	122-34-9	30	5	<1
			10	<1
Propylparaben	94-13-3	30	810	7
			2130	19
Isobutylparaben	4247-02-3	30	93	2
			438	8
Benzophenone	119-61-9	31	72	2
			2686	55
Menthol	89-78-1	30	3628	78
			17 010	365
Oxybenzone	131-57-7	30	367	10
			2812	76
Traseolide	68857-95-4	30	1417	7700