Pangkaj *et al.*
Environmental Systems Research (2023) 12:30
https://doi.org/10.1186/s40068-023-00315-6

Environmental Systems Research

RESEARCH

Open Access

Evaluation of the fate of trace organic compounds using the Level III fugacity model: a case study of Rajbandh open dump site in Khulna City of Bangladesh

K. M. Pangkaj[1*], I. M. Rafizul[1], E. Kraft[2] and S. Berner[2]

Abstract

Khulna is the 3rd largest city corporation in Bangladesh that produces 450 tons of Municipal solid waste (MSW) per day and dumps the waste in the Rajbandh open dump site. The main focus of this study is to determine the fate of chemicals in different environmental media at the Rajbandh open dump site. To accomplish the aim Level III fugacity model was evaluated which is subject to steady-state partitioning, reaction, advection, and intercompartmental transfer in an evaluative environment consisting of three compartments landfill gas (LFG), leachate, and waste. In this study, the model was implemented for six chemicals Trichloroethylene, Mono-chlorobenzene, 1,4-dichlorobenzene, 1,2,4-trichlorobenzene, Hexachlorobenzene, and Benzene having different physiochemical properties. The result reveals that Benzene was found with the highest fugacity value of 2.03E + 00 Pa in all compartments while Hexachlorobenzene shows the highest value of concentration 2.67E-01 mol/m^3 in the waste compartment. Regarding mass distribution, all chemical shows a higher mass remaining in the waste compartment in comparison with the other compartment. The result also reveals that the dominating removal process of a chemical from the system is the reaction process. For all the chemicals almost all the mass is removed from the environment by reaction process rather than advection in LFG and leachate. Finally, the estimated behavior of the selected chemical will help to evaluate the health and ecological hazards at the open dump site and take necessary steps to control the emission of such hazardous chemicals from the open dump site by the authority.

Keywords Fugacity, Municipal solid waste, Open dump site

Introduction

At present the world population is increasing at an exponential rate causing a significant amount of household waste. Though the amount of waste increasing day by day waste management becoming a more challenging thing all over the world. Sanitary landfilling is the best option for the final disposal of MSW. Most developed countries prefer Sanitary landfilling for the final disposal of MSW. However, the practice of sanitary landfilling in developing countries all over the world or underdeveloped countries is less than that of developed countries. Municipal solid waste generation in Asia is expected to rise from the predicted 1.2 billion tons produced in 2016 to 1.5 billion tons by 2030 and 1.9 billion tons by 2050. (World Bank 2018, as cited in Hondo, Arthur, Gamaralalage, 2020). Despite this worrying rise, managing municipal solid waste (MSW) continues to be a low priority for most Asian cities, especially when contrasted

*Correspondence:
K. M. Pangkaj
pangkaj1001058@gmail.com
[1] Department of Civil Engineering, Khulna University of Engineering & Technology, Khulna, Bangladesh
[2] Faculty of Civil Engineering, Bauhaus-Universität Weimar (BUW), Weimar, Germany

with investment in fields like infrastructure and transit. As a result of landfills' reduced prices when compared to recycling, incineration, or composting, Asia relies extensively on them for the disposal of municipal solid waste. (Terazono et al. 2005, as cited in Hondo et al. 2020). With only 44% in South Asia and 71% in East Asia and the Pacific, Asia's collection rates are low, except for a few high-income nations like Japan, the Republic of Korea, and Singapore. (World Bank 2018, as cited in Hondo et al. 2020). Thus, open dumping of waste is still the most often used waste management strategy, especially in low- and middle-income cities, including 79% of South Asia, 64% of Southeast Asia, and 51.5% of South and Central Asia. (World Bank 2018, as cited in Hondo et al. 2020). At present, only one active official dumping site is available in Khulna City which is an open dump site. The MSW produced in Khulna city is finally disposed of in an Open dump site known as Rajbandh open dump site. Being an open dump site the connection between all the environmental media is very easy, which is why some problems are introduced by it. Various organic compounds can be produced by a dumpsite. The behavior of those organic compounds is different in nature, their partitioning through different environmental media may be different. Many of them are volatilized, some are absorbed by solid materials and many of them stay in the aqueous phase. The pollutants produced by the open dump site can pollute the surrounding environment very effortlessly. It is quite difficult to figure out the concentration of the different volatile compounds in different environmental media produced in an open dump site. In order to provide a complete picture of the environmental behavior of organic chemicals as they transport away from sources, multimedia environmental fate models can combine information on spatial and temporal emissions with well-known physicochemical properties and climate data (Mackay and Paterson 1981, 1991, Dale et al. 2015a, 2015b, Di Guardo et al. 2018 as cited in Li et al. 2021). These models are used to determine the final destination, provide general estimates of concentrations in ecological compartments, and define important routes of chemical transport across various mediums. (Mackay and Paterson 1991, Wania and Mackay 1995, Zhang et al. 2015 as cited in Li et al. 2021). To indicate the increasing complexity of the equations driving mass balance, fugacity simulations can be performed in both static and dynamic conditions and are categorized as level I, II, III, or IV. (Mackay 2001 as cited in Li et al. 2021). The Level III fugacity model is simpler than Level IV models and more realistic than Level I and II models, Level III fugacity models have been employed more frequently (Li et al. 2021). Simplified equations for the processes of partitioning, transport, and reaction are produced as a result of their application to determining the environmental destiny of hazardous compounds, and these equations are then assembled into a compatible model. The interpretation of the dynamic processes to which the hazardous compounds are exposed is made easier when the distribution of pollutants in the environment is expressed in terms of fugacity rather than concentration. Fugacity, derived from the Latin word fugere- "to flee," may be defined as the escaping tendency of a substance from a phase. It is an expression of "activity" and as such has been applied mainly to thermodynamic problems involving phase equilibria, especially to calculations encountered in chemical separation processes such as liquid extraction, distillation, and absorption. A chemical equilibrium between phases can be constructed using fugacity analysis, and partitioning between various phase compartments can be forecasted. The fugacity approach makes it very simple to monitor a chemical as it transitions from one phase to another since fugacity is continuous between phases (unlike concentration, which discontinues between phases) (Mackay 2001; Stumm and Morgan 1996 as cited in Kilic & Aral 2008). The objective of the study is to evaluate the fate of some toxic compounds produced in an open dump site in Khulna, Bangladesh. This study addresses the existence of contaminants in three different phases through a detailed application of fugacity analysis to the Rajbandh open dump site in Khulna City. Figure 1 also illustrated by Pangkaj (2018) represents the location of the study area.

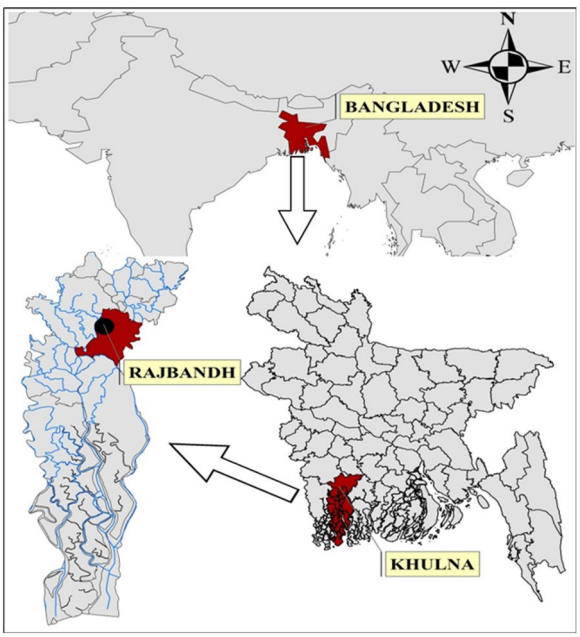

Fig. 1 Rajbandh Open dump site, Khulna, Bangladesh (Pangkaj 2018)

Materials and methods

Study area

Khulna is Bangladesh's third-largest city, after Dhaka and Chittagong. It is in the southwestern part of the country, on the Rupsha and Bhairab Rivers. The city covers an area of 59.57 km^2. The Khulna City Corporation (KCC) covers only 45.65 km^2. Geographically, Khulna City corporation is located between 24°45' and 24°54' north latitudes and between 89°28' and 89°35' east longitudes containing a population of about 1.5 million. KCC used to dump the Municipal Solid Waste (MSW) in an open dump site known as the Rajbandh open dump site.

The open dump site is situated outside the area of KCC near the Khulna-Satkhira highway and the approximate distance from the city center is about 7 km. The latitude and longitude of the Rajbandh open dump site are 22° 47′ 47.87" N and 89° 29′ 57.68" E respectively. The open dump site is now the only active dumpsite for dumping Municipal Solid Waste of KCC. The total area acquired by KCC for dumping waste is approximately 20 acres (80937 m^2). The leachate created in the dumpsite can readily pass through by seepaging because the landfill site's perimeter is made of permeable soil. The barrier is fairly low and very thick. The open dump site's perimeter is easily breached by the leachate during the monsoon. With only a few small patches of vegetation, the site's surroundings are mostly made up of waterbodies.

Fig. 2 Map showing the cell area of the evaluative environment

Table 1 Parameter of the cell considered in this study

Parameters	Unit	Value
Area of the cell	m^2	4.50E+04
Average depth of the cell	m	6
Volume of the cell	m^3	2.70E+05
Volume of pore space of the cell	m^3	8.11E+04
Volume of landfill gas in the pore space	m^3	2.43E+04
Volume of leachate in the Pore Space	m^3	5.67E+04
Volume of waste	m^3	1.89E+05
Density of the waste	Kg/m^3	547

Evaluative environment

The area of the Rajbandh open dump site which is used for dumping MSW was considered an evaluative environment. In this evaluative environment, three phases likely Landfill gas (LFG), Leachate, and solid waste were considered and the phases were denoted as 1, 2, and 3.

Depending on the availability of site-specific information the selection of the environmental compartment was made. The entire area used to dump the waste at the open dump site was considered a unit cell. The area of the considered cell is shown in Fig. 2 and all dimensions are listed in Table 1.

A study by Pamela and Jerome (2020) found the pore space in the waste was 30% of which 30% contained gas and 70% contained leachate. This fraction was also used in this study and the calculated volume of the considered three phases of the evaluative environment was found to be 2.43E+04 m^3 for air, 5.67E+04 m^3 for leachate, and 1.89E+05 m^3 for waste.

Application of Level III fugacity model

This level includes steady-state input, transformation, and intercompartment transfers, and permits the solute to be introduced into one or more compartments at a rate of f, mol/year, and establishes a transfer rate between compartments in terms of an exchange rate constant that is driven by the fugacity difference (Mackay et al. 1979). Fugacity can be defined as the escaping tendency of substances from a phase. The unit of fugacity like the unit of pressure and the concentration of a compound in a phase is a function of fugacity. Mathematically, the concentration of a compound can be defined by Eq. 1.

$$C = Zf \tag{1}$$

where C is the concentration of the selected compound (mol/m^3) Z is the fugacity capacity ($mol/Pa.m^3$) and f is the fugacity (Pa) of the compound in the different compartments. Z depends on temperature, pressure, the nature of the substance, and the medium in which it is present. The Z value for landfill gas is the inverse of a product of absolute temperature and gas constant and it

is independent of the compounds while the Z value of the leachate phase depends on the aqueous solubility and the vapor pressure of the compounds. The equations used to calculate the Z values for landfill gas, leachate, and waste phases are given in the following Eqs. 2, 3, and 4 respectively (Mackay et al. 1985)

$$Z_1 = 1/RT \tag{2}$$

$$Z_2 = C_S/P_S \tag{3}$$

$$Z_3 = 0.411x\rho K_{OW}/H \tag{4}$$

where, R = Molar gas constant (8.314 Pa.m^3/K. mol), T = Absolute temperature (298 K), C_s = Aqueous solubility (mol/m^3), P_s = Vapor pressure (Pa), x = Fraction of organic carbon (0.02), ρ = Density of waste (Kg/L), K_{OW} = Octanol water partition coefficient, H = Henry's law constant (Pa m^3/mol).

In the Level III fugacity approach reaction and advection are considered for the removal of a compound from the selected evaluative system. Advection is considered for landfill gas and leachate and rection is considered for all the compartments of the evaluative system. In the reaction process photolysis, oxidation, hydrolysis, and biodegradation were considered for the removal of the compounds from the evaluative system. For all reactions, first-order reaction expression was considered here, and the first-order reaction rate constant of all compounds was listed in Table 3. Nevertheless, there are numerous circumstances in which a first-order reaction is not the genuine reaction rate. The key idea was that there are other reactants besides pollution, such as the microbial population, sunlight, etc., and that the concentration of the second or third reactant is nearly constant and won't change significantly as the reaction takes place. So, it is often possible to avoid these challenging reaction rate equations by describing them in terms of a pseudo-first-order rate response. The biodegradation reaction was taken into account due to the biological conversion of chemicals in the landfill. The hydrolysis reaction was taken into account since chemical species are subjected to rainwater and in-situ moisture (leachate). Being an open-dumping site, the Rajbandh landfill receives a lot of exposure to the sun and outside air. Due to the possibility of pollutants reacting as a result of exposure to sunlight, ambient oxygen, and aqueous phase oxygen, photolysis, and oxidation processes were taken into consideration. All reaction process is not contextual for all compounds selected in this study for this reason the collective value of the first-order reaction rate was considered in the calculation and the value was obtained by using Eq. 5.

$$K = K_P + K_O + K_H + K_B \tag{5}$$

where, K is the collective first-order reaction rate constant (h^{-1}) and K_P, K_O, K_H, and K_B are the first-order reaction rate constant for photolysis, oxidation, hydrolysis, and biodegradation reaction process respectively (h^{-1}).

Table 2 shows that the first-order reaction rate constant of several compounds for the LFG compartments is zero which implies that the combined reaction rate constant will be zero. In a study by Mackay et al. (1985) the first-order reaction rate constant for the air compartment was considered 1.7E-06 h^{-1} for those compounds which had zero combined reaction rate. In this study, we also considered the same as the study of Mackay et al. (1985). Table 3 shows the value of the collective first-order reaction rate used in this study for the Level III fugacity model.

Table 3 Combined 1st Order Reaction Rate Constant (h^{-1})

Compound	LFG	Leachate	Waste
Trichloroethylene	7.22E-03	9.00E-05	0.00E + 00
Mono-chlorobenzene	2.88E-03	1.88E-04	0.00E + 00
1,4-Dichlorobenzene	9.63E-03	1.09E-02	0.00E + 00
1,2,4-Trichlorobenzene	7.22E-03	1.92E-02	0.00E + 00
Hexachlorobenzene	1.44E-02	0.00E + 00	1.90E-05
Benzene	8.64E-04	4.76E-03	0.00E + 00

Table 2 1st order reaction rate constant (h^{-1}) (Mackay et al. 1985)

Compound	Photolysis		Oxidation		Hydrolysis	Biodegradation	
	LFG	Leachate	LFG	Leachate	Leachate	Leachate	Waste
Trichloroethylene	0.00E + 00	0.00E + 00	7.22E-03	0.00E + 00	9.00E-05	0.00E + 00	0.00E + 00
Mono-chlorobenzene	0.00E + 00	0.00E + 00	2.88E-03	0.00E + 00	0.00E + 00	1.88E-04	0.00E + 00
1,4-Dichlorobenzene	0.00E + 00	0.00E + 00	9.63E-03	0.00E + 00	0.00E + 00	1.09E-02	0.00E + 00
1,2,4-Trichlorobenzene	0.00E + 00	0.00E + 00	7.22E-03	0.00E + 00	0.00E + 00	1.92E-02	0.00E + 00
Hexachlorobenzene	0.00E + 00	0.00E + 00	1.44E-02	0.00E + 00	0.00E + 00	0.00E + 00	1.90E-05
Benzene	8.64E-04	1.80E-04	0.00E + 00	0.00E + 00	0.00E + 00	4.58E-03	0.00E + 00

By advection and reactivity, the pollutant can be eliminated from the various compartments of the evaluation environment. Advection is the controlled movement of chemicals in a flowing media while they are present. The reaction is the process that modifies the solute's chemical composition, and it will exhibit characteristics of intermedia transport (diffusive flux and material flux process) between various landfill compartments. D value, which is also used to calculate the rates of intermedia transport, advection, and reaction individually, is a term that acknowledges advection, reaction, and intermedial transport. The transfer coefficient for the intercompartmental transfer between LFG and leachate, between LFG and waste, and between waste and leachate was calculated by Eqs. 6, 7, and 8 respectively (Mackay et al., 1985)

$$D_{12} = 1/(1/(K_{12}A_{12}Z_1) + 1/(K_{21}A_{12}Z_2)) \quad (6)$$

$$D_{13} = 1/(1/(K_{13}A_{13}Z_1) + Y_3/(B_3A_{13}Z_1)) \quad (7)$$

$$D_{32} = G_W Z_2 + G_S Z_3 \quad (8)$$

where D_{12} = LFG to Leachate phase transfer coefficient (mol/Pa. h); D_{13} = LFG to Waste phase transfer coefficient (mol/Pa. h); D_{32} = Waste to Leachate phase transfer coefficient (mol/Pa. h); K_{12} = Air mass transfer coefficient (m/h); K_{13} = Waste mass transfer coefficient (m/h); K_{21} = Water mass transfer coefficient (m/h); A_{12} = Transfer area of water surface (m^2); A_{13} = Horizontal waste area (m^2); Z_1, Z_2, Z_3 = Fugacity capacity of the compound in LFG, Leachate, and Waste respectively (mol/m^3.Pa); Y_3 = Mean diffusion depth (m); B_3 = Effective diffusivity in the waste LFG; G_w = Water transfer rate (m^3/h); G_s = Waste to leachate transfer rate (m^3/h). The input parameters used to calculate the interphase transfer coefficient are listed in Table 4.

Advection rate is considered for LFG and Leachate compartments. All the reactions are expressed in terms of the first-order reaction rate constant. The rates of reaction and advection are calculated for any environmental compartment by Eqs. 9 and 10 respectively.

Table 4 Intermedia transfer coefficients (Mackay et al. 1985)

Parameters	Unit	Value	Parameters	Unit	Value
K_{12}	m/h	10	G_s	m^3/h	9.60E-02
K_{13}	m/h	10	B_3	m^2/h	1.41E-02
K_{21}	m/h	0.1	Y_3	m	0.075
A_{12}	m^2	4.50E + 04	B_A	m^2/h	0.04
A_{13}	m^2	4.50E + 04	Φ	–	0.5
G_w	m^3/h	9.59E + 00			

$$Reaction\ rate = VKC = VZKf \quad (9)$$

$$Advection\ rate = GC = GZf \quad (10)$$

where V = Volume of the compartment (m^3); G = advection outflow (m^3/h); Z = Fugacity capacity (mol/m^3. Pa); K = Combined First order reaction rate constant (h^{-1}) and f = fugacity of the compartment (Pa).

The mass balance equation for compartment i can be expressed as Eq. 11

$$Emission = Advectiveoutflow + Reactionrate + Transport \quad (11)$$

Mathematically it implies that

$$E_i = G_i Z_i f_i + V_i Z_i K_i f_i + \sum D_{ij}(f_i - f_j) \quad (12)$$

Or

$$-f_i\left(G_i Z_i + V_i Z_i K_i + \sum D_{ij}\right) + \sum D_{ji} f_j = -E_i \quad (13)$$

This gives three linear algebraic equations for the three compartments considered in this study. Thus, the linear algebraic mass balance equation for landfill gas, leachate, and waste is expressed by the Eqs. 14, 15, and 16 respectively

$$-(G_1Z_1 + V_1Z_1K_1 + D_{12} + D_{13})f_1 + D_{12}f_2 + D_{13}f_3 = -E_1 \quad (14)$$

$$D_{12}f_1 - (G_2Z_2 + V_2Z_2K_2 + D_{12} + D_{32})f_2 + D_{32}f_3 = -E_2 \quad (15)$$

$$D_{13}f_1 + D_{32}f_2 - (G_3Z_3 + V_3Z_3K_3 + D_{13} + D_{32})f_3 = -E_3 \quad (16)$$

These three linear equations can be solved readily by a matrix inversion technique such as Gaussian elimination. From the three f values the concentrations, amounts, and process rates can be calculated easily and a behavior profile emerges of where the chemical partitions, reacts, transfers, and how long it persists.

Selection of trace compounds of this study

The landfill produces gas through the degradation of MSW. The dominating gas produced in a landfill is methane, CH_4 (40–70%v/v) and carbon-di-oxide, CO_2 (30–60%v/v) with small amounts of hydrogen (H_2), hydrogen sulfide (H_2S), and other trace components (Shafi et al. 2006). Besides this, there are many low-concentration compounds identified by various researchers that may pose a potential human health risk at the landfill site. Young and Parker (1983), Allen et al. (1997), Eklund et al. (1998), and others that studied the trace composition of LFG found 100–140 trace components of concern that typically made up < 1% v/v of the gas. In the

late 1980s trace components were characterized by the monitoring of three UK-based landfill sites over a period of three years (Dent et al. 1986; Department of Environment 1988). In this monitoring tenor around 136 organic compounds or isomeric groups were evidenced. In 1997 a study was conducted over seven landfill sites in the UK. In the study about 140 trace components were observed of which 90 components were the same in all seven sites (Allen et al. 1997). The volatile organic carbon contents (VOCs) fluctuated with ambient temperature and atmospheric pressure and were tightly connected to methane generation rates. The discovered VOCs included tetrachloroethene, 1,1-dichloroethane, 1,2-dichloroethane, benzene, chlorobenzene, trichloroethylene (TCE), ethylbenzene, xylene, and toluene, among others (Young and Parker 1983; Allen et al. 1997). 550 trace components were found in a similar UK research (Environment Agency 2003a). Pamela and Jerome conducted a study on the phase distribution of trace components observed in a compost mixture in 2020.

In the study, the observed VOCs included Benzene, Chlorobenzene, 1,2-Dichlorobenzene, 1,2,4-Trichlorobenzene, Toluene, nitrobenzene, ethylbenzene, aniline, naphthalene and so on. Atrazine, trichloroethylene, and benzene were considered in a study by Rafi et al., (2020) to evaluate the fate of different environmental media. To fulfill the evaluation of the Level III fugacity model in this study seven trace compounds were selected depending on previous studies by researchers and the selected chemicals were Trichloroethylene, Mono-chlorobenzene, 1,4-Dichlorobenzene, 1,2,4-Trichlorobenzene, Hexachlorobenzene, and Benzene. The physicochemical properties of the selected chemicals are listed in Table 5.

Results and discussion

In this study, total emission in the whole evaluative environment was considered as 1 mol/h. In the analysis, intermedia transfer between landfill gas and leachate, transfer between landfill gas and waste, and transfer between waste and leachate were considered for all the selected compounds. The key findings of the analysis of the Level III fugacity model will be discussed thoroughly in the following segments.

Trichloroethylene

Figure 3 depicts the phase distribution of Trichloroethylene in the different environmental media of the selected evaluated environment of the Rajbandh open dump site. A common organic solvent is trichloroethylene. Due to its high volatility, it typically evaporates, resulting in emissions of 90% into Landfill gas (LFG), 5% into leachate, and 5% into waste. The figure shows that the fugacity in the Landfill gas, leachate, and waste was found as 1.33E + 01 Pa. In a study by Rafi et al. (2020), the fugacity of trichloroethylene in LFG, leachate, and waste was found 1.1E + 01 Pa, 1.1E + 01 Pa, and 9.6E + 00 Pa respectively. The intercompartmental transfer rate between LFG and leachate was found 7.55E-03 mol/h while 3.14E-02 mol/h and 5.00E-02 mol/h were found between LFG and waste, and between waste and leachate respectively (Fig. 3).

Figure 4 illustrates the concentration of Trichloroethylene in the selected evaluative environment. The concentration of Trichloroethylene was found 1.13E-02 mol/m^3, 9.90E-03 mol/m^3, and 5.37E-03 mol/m^3 respectively in leachate, waste, and LFG. The sequence of concentration of Trichloroethylene follows the order of leachate > waste > LFG. The highest concentration was found in the leachate compartment and the LFG compartment shows the lowest concentration of Trichloroethylene. The sequence of concentration in the study of Rafi et al. (2020) was found as waste > leachate > LFG. In the study of Rafi et al. (2020), LFG has revealed the lowest concentration among LFG, leachate, and waste.

Figure 5a illustrates the mass distribution of trichloroethylene in different environmental media. The figure shows that 70.85% of the mass remains in the waste compartment, 24.21% mass remains in the leachate compartment, and about 4.94% mass remains in the LFG compartment. The removal distribution of Trichloroethylene from different environmental media is depicted in Fig. 5b. The figure shows that around 94% of

Table 5 Physicochemical properties of the selected chemicals (Mackay et al. 1985)

Compounds	Molecular weight, MW (gm/mol)	Water solubility C_S (gm/m^3)	Vapor pressure P_S (Pa)	Log K_{OW}	Henry's constant H
Trichloroethylene	131.4	8.37E + 00	9.87E + 03	2.29	1.18E + 03
Mono-chlorobenzene	112.6	4.33E + 00	1.57E + 03	2.86	3.62E + 02
1,4-Dichlorobenzene	147	4.76E-01	4.75E + 01	3.42	9.98E + 01
1,2,4-Trichlorobenzene	181.5	1.38E-01	6.08E + 01	4.04	4.41E + 02
Hexachlorobenzene	284.8	2.11E-05	3.10E-03	5.61	1.47E + 02
Benzene	78.1	2.28E + 01	1.27E + 04	2.13	5.57E + 02

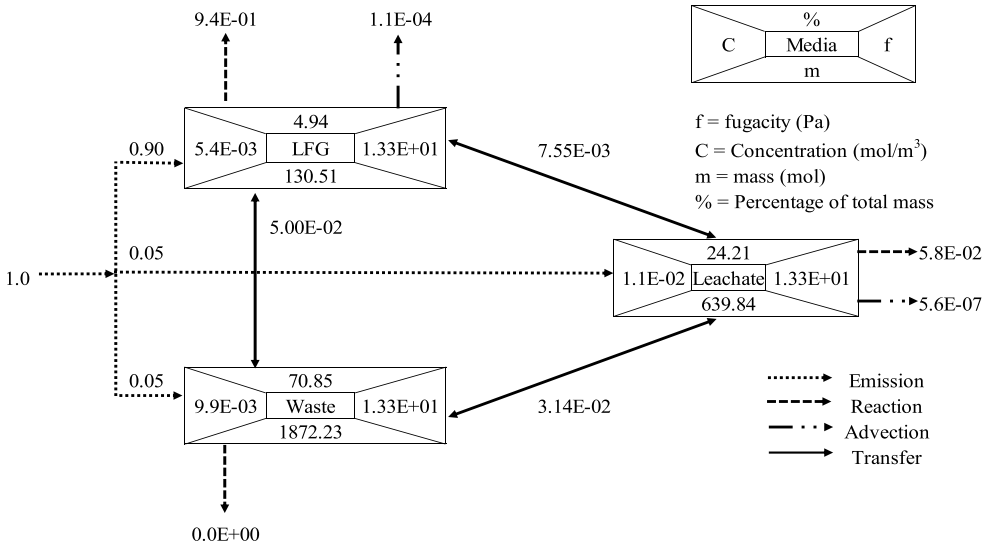

Fig. 3 Phase distribution of Trichloroethylene in the different environmental media

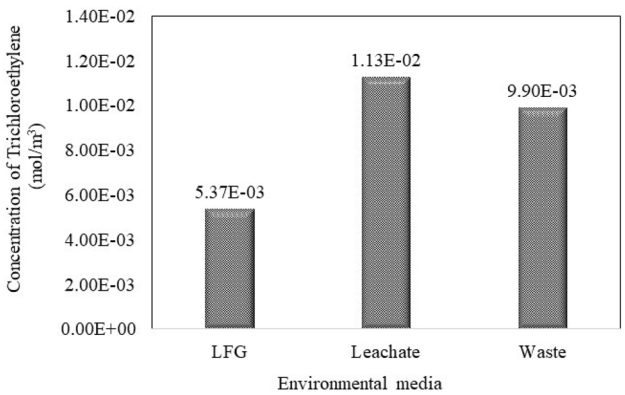

Fig. 4 Concentration Trichloroethylene in different environmental media

inputs volatilize with oxidation while about 6% of inputs undergo hydrolysis process for removal from the system. All the mass is removed from the system by the reaction process rather than the advection of LFG and leachate. Rafi et al. (2020) also identified that the most dominating process for the removal of the mass of trichloroethylene from the system is the reaction process.

1,2,4-Trichlorobenzene

For polyester materials, 1,2,4-trichlorobenzene is employed as a dye carrier. Figure 6 depicts the fugacity distribution of 1,2,4-Trichlorobenzene in the different environmental media of the selected evaluated environment of the Rajbandh open dump site. For level III fugacity calculation the emission of 1,2,4-Trichlorobenzene

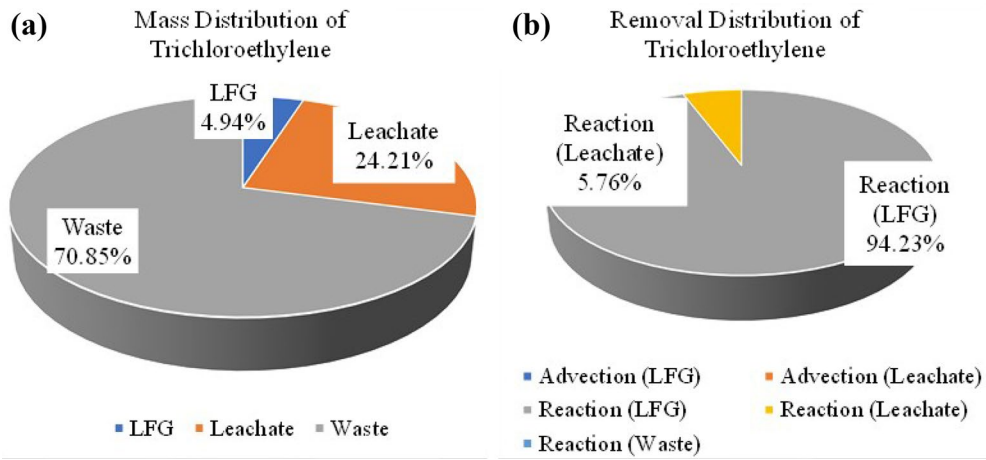

Fig. 5 **a** Mass Distribution **b** Removal distribution of Trichloroethylene in different environment media

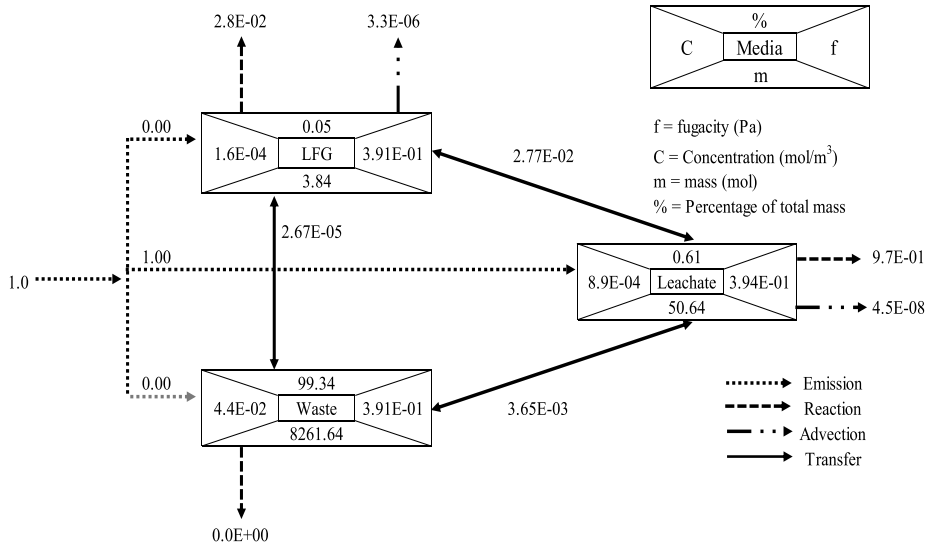

Fig. 6 Phase distribution of 1,2,4-Trichlorobenzene in the different environmental media

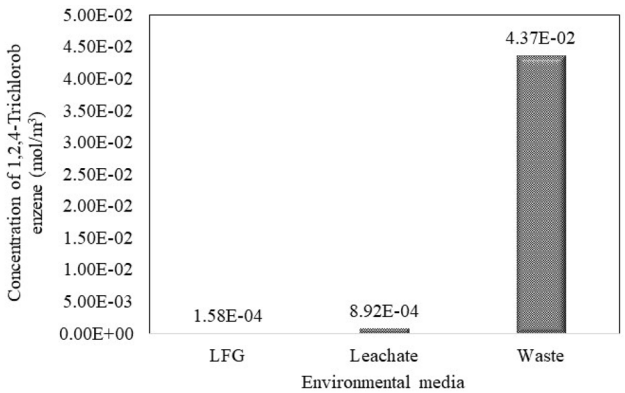

Fig. 7 Concentration of 1,2,4-Trichlorobenzene in different environmental media

was considered 100% in the Leachate. The figure shows that the fugacity in LFG and waste compartments was found at 3.91E-01 Pa while 3.94E-01 Pa was found for the leachate compartment. The intercompartmental transfer rate between LFG and leachate was found 2.77E-02 mol/h while 2.67E-05 mol/h and 3.65E-03 mol/h were found between LFG and waste, and between waste and leachate respectively (Fig. 6).

Figure 7 illustrates the concentration of 1,2,4-Trichlorobenzene in the selected evaluative environment. The concentration of 1,2,4-Trichlorobenzene was found 1.58E-04 mol/m^3, 8.92E-04 mol/m^3, and 4.37E-02 mol/m^3 respectively in LFG, leachate, and waste. The sequence of concentration of 1,2,4-Trichlorobenzene follows the order of waste > leachate > LFG. The highest concentration was found in the waste compartment and the LFG compartment shows the lowest concentration of 1,2,4-Trichlorobenzene.

The mass distribution of 1,2,4-Trichlorobenzene is depicted in Fig. 8a. The figure illustrates that 99.34% of the mass remains in the waste, 0.61% mass remains in the leachate, and about 0.05% of the mass remains in the LFG. The removal distribution of 1,2,4-Trichlorobenzene from different environmental media is depicted in Fig. 8b. The highest contribution to the removal of 1,2,4-Trichlorobenzene from the system comes from the biodegradation in leachate which is about.

97.23% and 2.77% undergoing oxidation in the LFG. All the mass is removed from the system by reaction rather than the advection of LFG and leachate.

Benzene

Due to its wide range of industrial applications and inclusion in fuels, Benzene is frequently found in aquatic environments; as a result, it is presumed that its emission only occurs in leachate. In this study, the emission of Benzene was considered 100% in the Leachate. Figure 9 depicts the fugacity distribution of Benzene in the different environmental media of the selected evaluated environment of the Rajbandh open dump site. The figure shows that the fugacity in all the compartments found was 2.03E+00 Pa. The fugacity of benzene in LFG, leachate, and waste was found respectively 8.9E-01 Pa, 8.1E-01 Pa, and 8.1E-01 Pa in research conducted by Rafi et al. (2020). The intercompartmental transfer rate between LFG and leachate was found 1.72E-02 mol/h while 1.10E-05 mol/h and 1.01E-02 mol/h were found between LFG

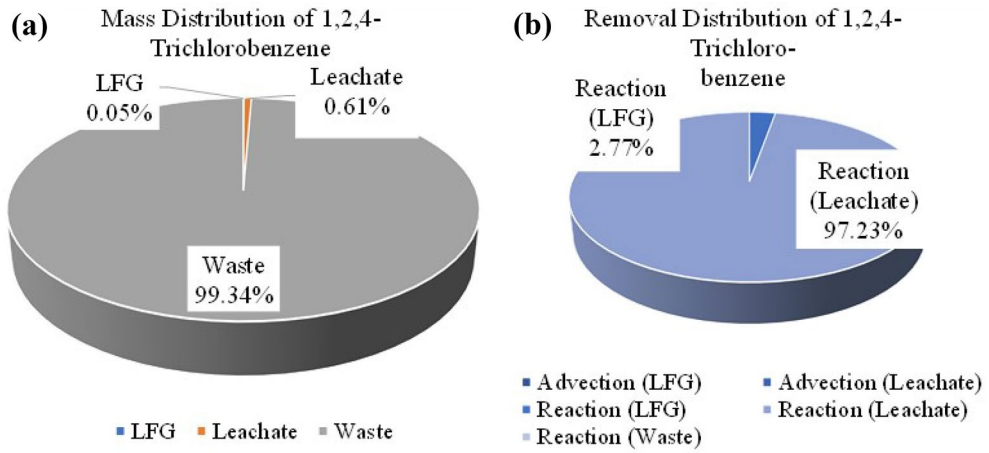

Fig. 8 **a** Mass distribution **b** Removal distribution of 1,2,4-Trichlorobenzene in different compartments

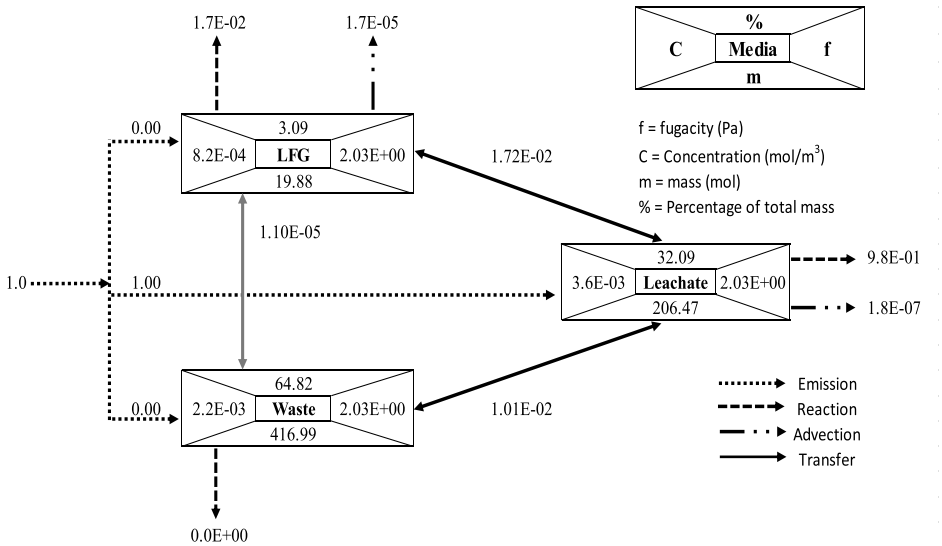

Fig. 9 Phase distribution of Benzene in the different environmental media

and waste, and between waste and leachate respectively (Fig. 9).

Figure 10 illustrates the concentration of Benzene in the selected evaluative environment. The concentration of Benzene was found 2.20E-03 mol/m^3, 3.64E-03 mol/m^3, and 8.17E-04 mol/m^3 respectively in waste, leachate, and LFG. The sequence of concentration of Benzene follows the order of leachate > waste > LFG. The highest concentration was found in the leachate compartment and the LFG compartment shows the lowest concentration of Benzene. Waste > Leachate > LFG was the order of concentration found for benzene in the study by Rafi et al. (2020). For benzene, the LFG compartment shows the lowest concentration among LFG, leachate, and waste as shown for trichloroethylene in the study by Rafi et al. (2020).

The mass distribution of benzene in different environmental compartments is depicted in Fig. 11a. Regarding mass distribution, 64.82% of the mass remains in the waste, 32.09% mass remains in the leachate, and about 3.09% of the mass remains in the LFG.

The removal distribution of Benzene from different environmental media is depicted in Fig. 11b. The highest contribution to the removal of Benzene from the system comes from the leachate reaction which is about 98.28% and 1.72% contributed by the LFG reaction. All the mass is removed from the system by reaction rather than the advection of LFG and leachate. The reaction process was

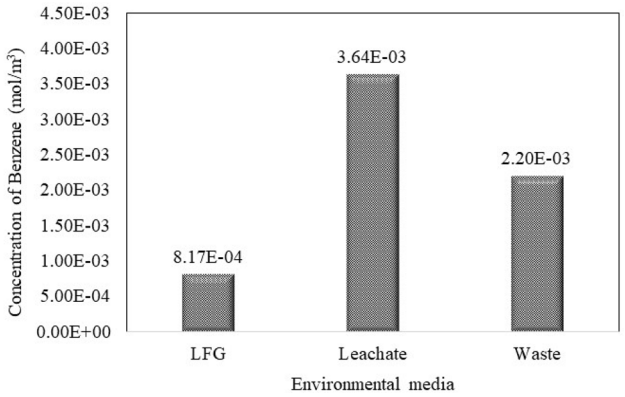

Fig. 10 Concentration of Benzene in different environmental media

found as the most predominating removal process in this study which was also found as the dominating removal process of mass from the system in the study conducted by Rafi et al. (2020).

Table 6 demonstrates the chemical behavior of all the compounds in all the selected environmental media found in the evaluation of the Level III fugacity model at the Rajbandh open dump site in Khulna. From the table, the sequence of fugacity in LFG and leachate compartment was found as the following order of Mono-chlorobenzene > Trichloroethylene > Benzene > 1,2,4-Trichlorobenzene > Hexachlorobenzene > 1,4-Dichlorobenzene while for waste compartment the order was found as follows Mono-chlorobenzene > Trichloroethylene > Benzene > 1,2,4-Trichlorobenzene > 1,4-Dichlorobenzene > Hexachlorobenzene. Mono-chlorobenzene shows the highest fugacity in comparison with all other compounds in all the compartments 1.73E+01 Pa while DDT reveals the lowest fugacity 2.15E-02 Pa in comparison with all the compounds among all compartments. Regarding the concentration of the compounds, the order was found as Mono-chlorobenzene > Trichloroethylene > Benzene > 1,2,4-Trichlorobenzene > Hexachlorobenzene > 1,4-Dichlorobenzene for LFG and leachate compartment the order follows the sequence as Mono-chlorobenzene > Trichloroethylene > Benzene > Hexachlorobenzene > 1,4-Dichlorobenzene > 1,2,4-Trichlorobenzene and for waste compartment, the order was found as Hexachlorobenzene > Mono-chlorobenzene > 1,2,4-Trichlorobenzene > 1,4-Dichlorobenzene > Trichloroethylene > Benzene. Hexachlorobenzene shows the highest value (2.67E-01) and lowest value (1.12E-04) of concentration among all compartments. The concentration of any compound is a product of the fugacity and fugacity capacity of this compound. The result reveals that the fugacity of a compound was nearly the same in all environmental compartments. However, the fugacity capacity varies from one compartment to another compartment which is responsible for the variation in concentration of a compound in all the compartments. Regarding mass distribution for all the compounds the maximum mass remains in the waste compartment and comparatively less mass remains in the LFG compartment. The table also reveals that the removal of compounds from the system is dominated by the reaction process rather than advection.

Figure 12 depicts the concentration of all the compounds in all selected environmental media of the evaluative environment. The figure shows that for Mono-chlorobenzene, 1,4-Dichlorobenzene, 1,2,4-trichlorobenzene, and Hexachlorobenzene the highest concentration was found in the waste compartment while for Trichloroethylene and Benzene the highest concentration was found in leachate compartment (Fig. 12).

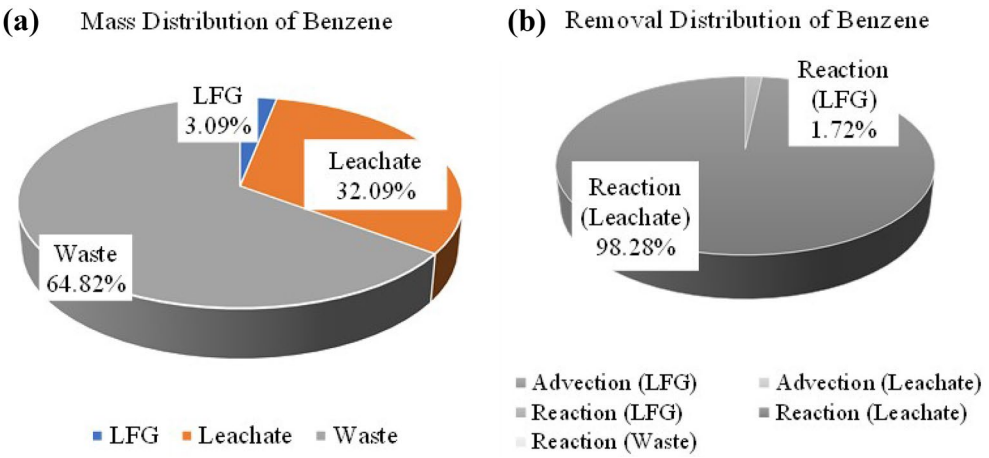

Fig. 11 **a** Mass distribution **b** Removal distribution of Benzene in different compartments

Table 6 All findings of the study

Fugacity, f (Pa)				Fugacity Capacity Z (mol/Pa.m^3)			Concentration, C (mol/m^3)			No. of mole, M=CV (mole)			Mass Distribution %		
Compounds															
	LFG	Leachate	Waste	LFG	Leachate	Waste	LFG	Leachate	Waste	LFG	Leachate	Waste	LFG	Leachate	Waste
Trichloroethylene	1.33E+01	1.33E+01	1.33E+01	4.04E-04	8.48E-04	7.44E-04	5.37E-03	1.13E-02	9.90E-03	1.31E+02	6.40E+02	1.87E+03	4.94	24.21	70.85
Mono-chlorobenzene	1.73E+01	1.73E+01	1.73E+01	4.04E-04	2.76E-03	8.99E-03	6.98E-03	4.79E-02	1.56E-01	1.70E+02	2.72E+03	2.94E+04	0.53	8.41	91.07
1,4-Dichlorobenzene	1.58E-01	1.59E-01	1.58E-01	4.04E-04	1.00E-02	1.19E-01	6.39E-05	1.59E-03	1.88E-02	1.56E+00	9.04E+01	3.55E+03	0.04	2.48	97.48
1,2,4-Trichlorobenzene	3.91E-01	3.94E-01	3.91E-01	4.04E-04	2.27E-03	1.12E-01	1.58E-04	8.92E-04	4.37E-02	3.84E+00	5.06E+01	8.26E+03	0.05	0.61	99.34
Hexachlorobenzene	2.77E-01	3.11E-01	2.15E-02	4.04E-04	6.80E-03	1.24E+01	1.12E-04	2.11E-03	2.67E-01	2.72E+00	1.20E+02	5.06E+04	0.01	0.24	99.76
Benzene	2.03E+00	2.03E+00	2.03E+00	4.04E-04	1.79E-03	1.09E-03	8.17E-04	3.64E-03	2.20E-03	1.99E+01	2.06E+02	4.17E+02			

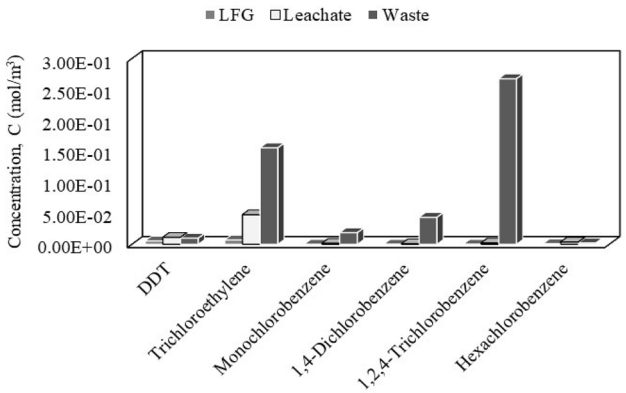

Fig. 12 Concentration of all selected compounds in different compartments

Conclusions

The examination of the Level III fugacity model to assess the chemical fate of an open dump site at Khulna city of Bangladesh in different environmental media has been analyzed. The findings are encouraging as the Level III Fugacity model displays an ability to provide accurate behavior of the profiles of chemicals, even when dealing with compounds that vary significantly in their physical–chemical properties, reactivity, and transport characteristics. This is promising as it suggests that the model could prove to be valuable in predicting the behavior of new or poorly understood chemicals. Combining partitioning, reaction, and transport data is essential when evaluating chemical behavior, and an evaluation model like the Level III fugacity model should be used. The various behaviors displayed by the substances under study emphasize how crucial it is to use a trustworthy model. Visual output representations can be used to communicate results effectively. This model has the benefit of serving as a starting point for the identification of the main compartments and processes of interest, which may then be further investigated using a more accurate and specialized model, perhaps one that is site-specific. It is essential to note that this study underscores the significance of employing sophisticated models to determine the fate of chemicals in the environment accurately. The potential of the Level III fugacity model in providing insights into chemical behavior can be beneficial to environmental scientists and policymakers alike, facilitating informed decision-making regarding chemical management, remediation, and disposal. Overall, the Level III fugacity model's potential to provide valuable insights into the fate of chemicals in the environment suggests a promising future for environmental modeling and risk assessment.

Acknowledgements
The SCIP Plastics project on which this publication is based is funded by the Federal Ministry for the Environment, Nature Conservation, Nuclear Safety, and Consumer Protection under grant no. 67MM0004. Responsibility for the content of this publication lies with the author(s).

Author contributions
The concept was proposed by IMR. KMP did the data acquisition, model analysis, and final draft of the manuscript. EK and SB actively participated in drafting or critically revising the work for important intellectual content and approved the final version for publication.

Funding
The research was conducted under the SCIP Plastics project which is funded by the Federal Ministry for the Environment, Nature Conservation, Nuclear Safety, and Consumer Protection under grant no. 67MM0004.

Availability of data and materials
The data and the supporting information for modeling will be available upon request.

Declarations

Ethics approval and consent to participate
Not applicable.

Consent for publication
Not applicable.

Competing interests
The authors declare that they have no competing interests.

Received: 22 July 2023 Accepted: 23 September 2023
Published online: 03 October 2023

References

Allen MR, Braithwaite A, Hills CC (1997) Trace organic compounds in landfill gas at seven UK waste disposal sites. Environ Sci Technol 31(4):1054–1061
Dale AL, Casman EA, Lowry GV, Lead JR, Viparelli E, Baalousha M (2015a) Modeling nanomaterial environmental fate in aquatic systems. Environ Sci Technol 49:2587–2593. https://doi.org/10.1021/es505076w
Dale AL, Lowry GV, Casman EA (2015b) Stream dynamics and chemical transformations control the environmental fate of silver and zinc oxide nanoparticles in a watershed-scale model. Environ Sci Technol 49:7285–7293. https://doi.org/10.1021/acs.est.5b01205
Dent CG, Scott P, Baldwin G (1986) A Study of Landfill Gas Composition at Three UK Domestic Waste Disposal Sites. In: Proc. Energy from Landfill Gas, Solihull, UK, October 28–31, pp 130–149
Department of Environment (1988) The Composition and Environmental Impact of Household Waste Derived Landfill Gas: Second Report. Environment Agency, Bristol. Research Report CWM 041/88
Di Guardo A, Gouin T, MacLeod M, Scheringer M (2018) Environmental fate and exposure models: advances and challenges in 21st-century chemical risk assessment. Environ Sci-Process Impacts 20, 58e71. https://doi.org/10.1039/c7em00568g
Eklund B, Anderson EP, Walker BL, Burrows DB (1998) Characterization of landfill gas composition at the fresh kills municipal solid waste landfill. Environ Sci Technol 32, 2233–2237
Environment Agency, (2003a). Investigation of the Composition and Emissions of Trace Components in Landfill Gas. Environment Agency, Bristol. <http://publications.environment-agency.gov.uk/pdf/SP1-438-TR-e-p.pdf>. R&D Technical Report P1–438/TR
Hondo D, Arthur L, Gamaralalage PJD (2020) Solid Waste Management in Developing Asia: Prioritizing Waste Separation. ADBI Policy Brief No. 2020–7 (November)

Kilic SG, Aral MM (2008) Probabilistic fugacity analysis of Lake Pontchartrain pollution after Hurricane Katrina. J Environ Manage 88:448–457
Li Y-F, Qin M, Yang P-F, Liu L-Y, Zhou L-J, Liu J-N, Shi L-L, Qiao L-N, Hu P-T, Tian C-G, Nikolaev A, Macdonald R (2021) Treatment of particle/gas partitioning using level III fugacity models in a six-compartment system. Chemosphere 271:129580. https://doi.org/10.1016/j.chemosphere.2021.129580
Mackay D (1979) Finding fugacity feasible. Environ Sci & Technol 13(10):1218–1223
Mackay D (2001) Multimedia Environmental Models - The Fugacity Approach, the second ed. CRC Press LLC, 2000 N.W. Corporate Blvd., Boca Raton, Florida 33431
Mackay D, Paterson S (1981) Calculating fugacity. Environ Sci Technol 15(9):1006–1014. https://doi.org/10.1021/es00091a001
Mackay D, Paterson S, Cheung B, Neely WB (1985) Evaluating the environmental behavior of chemicals with a level III fugacity model. Chemosphere 14(3/4), 335–374
Mackay D, Paterson S (1991) Evaluating the multimedia fate of organic chemicals-a level-III fugacity model. Environ Sci Technol 25:427–436. https://doi.org/10.1021/es00015a008
Pamela LS & Jerome JK (2020) Fugacity Model for Predicting Phase Distribution and Biotreatment Feasibility of Mixed Organic Compounds and Non-Aqueous Phase Liquid. Open access J Envi Soi Sci 4(5). OAJESS MS.ID.000199. https://doi.org/10.32474/OAJESS.2020.04.000199.
Pangkaj KM (2018) Assessment of the potential human health risk of a waste disposal site in Khulna, M.Sc. Engineering thesis, Department of Civil Engineering, Khulna University of Engineering & Technology, Khulna, Bangladesh
Rafi NF, Rafizul IM, Rahman SA (2020) Evaluating fugacity model for organic contaminants in waste deposited in Khulna landfill. J Eng Sci 11(1):67–82
Shafi S, Sweetman A, Houg RL, Smith R, Rosevear A, Pollard SJT (2006) Evaluating fugacity models for trace components in landfill gas. Environ Pollut 144:1013–1023
Stumm W, Morgan JJ (1996) Aquatic chemistry: chemical equilibria and rates in natural waters. Wiley, New York
Terazono A et al. (2005) Waste Management and Recycling in Asia. International Review for Environmental Strategies 5(2):477– 498. https://www.iges.or.jp/en/publication_documents/pub/peer/en/1182/IRES_vol.5-2_477.pdf.
Wania F, Mackay D (1995) A global distribution model for persistent organic chemicals. Sci Total Environ 160:211–232. https://doi.org/10.1016/0048-9697(95)04358-8
World Bank (2018) What a Waste 2.0: A Global Snapshot of Solid Waste Management to 2050. Washington, DC: World Bank
Young PJ, Parker A (1983) The identification and possible environmental impact of trace gases and vapors in landfill gas. Waste Manage Res 1:213–226
Zhang Q-Q, Ying G-G, Chen Z-F, Liu Y-S, Liu W-R, Zhao J-L (2015) Multimedia fate modeling and risk assessment of a commonly used azole fungicide climbazole at the river basin scale in China. Sci Total Environ 520:39–48. https://doi.org/10.1016/j.scitotenv.2015.03.038

Publisher's Note