IOP Conf. Series: Materials Science and Engineering

Multi-pollutant approach to model contaminants flow in surface and groundwater: A review

S U Wali¹ and N Alias²

^{1,2}Department of Water and Environmental Engineering, School of Civil Engineering, Faculty of Engineering, Universiti Teknologi Malaysia, 81310 UTM Skudai, Johor, Malaysia.

Email: saadu.umar@graduate.utm.my; noraliani@utm.my

Abstract.Pollution of surface and groundwater is largely caused by anthropogenic activities and the natural geogenic processes. Most of the contaminants in surface and groundwater have a common origin. The aim of this review is to highlight the importance of multiapproach modeling of pollutants which is required for various reasons, owing to the availability of different types and sources of water pollutants. We attempted a systematic review to assess the current progress in modeling water pollution using multi-approach methods. Results showed that (9) out of the eleven (11) chosen studies have applied some forms of multi-approach modeling methods to examine pollutants in surface and groundwater. Results also suggest that there is an increased concern on understanding how pollutants are transported from sources to surface water and how impurities are transported to groundwater aquifers by infiltering surface flows. A major limitation of water quality models is that models assumed a uniform environmental setting and can simulate contaminants only in the gas and aqueous states. The rationality of contaminant modeling using multi-pollutant approaches is mostly problematical to validate because suitable field data is wanting for comparison. Therefore, the model output must be scrutinized within the context of the uncertainty of the model inputs, data limitations and consistently essential application of established standards from the literature.

1. Introduction

Contamination of surface and groundwater is largely caused by nutrients, plastics, and chemicals such as pesticides and heavy metals [1-3]. Such contaminants have diverse ecological effects [4]. For example, hypoxia and harmful algal blooms in surface water can be caused by excess nutrients. Chemical derived contamination can have toxic effects on aquatic organisms [5, 6]. Often surface and groundwater aquifers are influenced by the joint impact of various contaminants [4]. Surface and groundwater bodies are chiefly contaminated from human activities, including agriculture, urbanization, industrialization and improper sewage disposal [7, 8]. Contaminants transported to a stream via overland flows can be transported to very far places via river channels and deposited in coastal areas [4]. In places where the streams are in hydraulic conductivity with groundwater aquifers, pollutants can enter groundwater via infiltration or recharge [9, 10].

Most of the contaminants in surface and groundwater have a common origin. For example, nutrients, pesticides, and heavy metals can be derived from agriculture and sewage released from municipal and/or industrial sources [11-13]. Implying that decontamination or treatment measures that were put in place to lessen a contaminant in polluted water perhaps affects interactions between

Sustainable and Integrated Engineering International Co	IOP Publishing	
IOP Conf. Series: Materials Science and Engineering	884 (2020) 012030	doi:10.1088/1757-899X/884/1/012030

other contaminants [4]. How this problem is addressed under field condition present presents a thought-provoking subject. Therefore, in decontamination of polluted water sources, for example, concentrations of most contaminants are reduced while recovering water and nutrients. Effective management of pollution remediation, therefore, requires an account for both the co-benefits as well as the side-effects [14, 15]. In addition, it is important to note that there are regional and/or environmental variations relating to the causes, types, and impacts of water pollution [4].

Water pollution is a global phenomenon as rivers all over the world serve as channels through which pollutants are collected at the basin scale and transported downstream to seas and/or groundwater aquifers [16-18]. In advanced regions of the world, nearly all the causes and types of water pollution are well-known [19]. Yet in some regions (i.e. Africa, South America, and Asia), these causes and/or consequences of water pollution, are either poorly known or not well investigated [20]. In this kind of situation, models can be used [21] to aid understanding of the problem and provide bases for decision making on environmental management and pollution control [4]. The objective of this review is to identify the extent to which surface and groundwater pollution are studied using a multi-pollutant approach method.

1.1. Why a multi-pollutant approach to water quality modeling is essential?

It has been argued that an integrated and more comprehensive multi-approach is required for various reasons [4]: (i) A new and comprehensive model approach is required to clearly address the joint exposure of surface and groundwater bodies to contaminants; (ii) Sound knowledge of the interactions between physical, chemical and biological processes in rivers and groundwater aquifers (Figure 1) is necessary for managing pollution; (iii) A multi-pollutant approach to modeling may well aid to better predict upcoming ecological gravities; and (iv) The future water quality models might be required to account for pollutants build-up in the environment. Generally, a clear multi-pollutant simulation will help to improve understanding of the sources and effects of imminent surface water contamination and prosper promising answers to the entire global water pollution problem. These types of models can be applied to (i) Analyze and quantify both water quality and quantity; (ii) For appraisals of the accessibility of potable water in the future; (iii) Aid in enhancing our awareness of water safety; (iv); Lay the foundation for systematic and management apparatuses that resolve simultaneously various water-related problems; and (v) Empathetic knowledge of how surface water quality disturbs bionetworks and humanity is crucial for human development and wellbeing. Therefore, multi-pollutant water quality models can provide desirable innovative knowledge, and applicable policy funding and consequently underwrite acceptable Sustainable Development Goals by the United Nations [4].

2. Methods

The pollutant source, pathway, and receptor models are widely applied in water and air-related studies [22-24]. The model approach is adopted because hydrochemical transformation in rivers and groundwater aquifers present a thought-provoking topic [25-27], due to difficulties involved in understanding the interaction between surface and groundwater and biogeochemical processes in rivers and groundwater (Figure 1). The main review procedure has been adapted from past studies [24]. The formulated research question directing this review is: "What are the causes, pathways, and the recipient(s) of contaminants in surface and groundwater, and how far has this problem has been studied"? Both Web of Science, Scopus, and other databases were searched on 10th June 2019, with the Source-Pathway-Receptor (SPR) Model adopted from [24], used for search term formulation and literature documentation as shown in Figure 1. The quest was limited to publications in English and available from 1970 to date (Table 1). The Boolean positional operators ("AND00, "OR00, "SAME00, "WITH00, "ADJ00) literature searches were used to suitably filter literature identification. Article inclusion required confirmation of water quality modeling via surface, and/or groundwater of urban and/or industrial sewage, plastics and chemicals (pesticides, heavy metals, etc). Water quality studies, whether surface or groundwater, were considered eligible once a surface or

groundwater source directly polluted by surface filtration (or recharge) was designated as the primary source of contaminant infiltration. A total of 3,502 potentially relevant papers were identified, reducing to 420, based on eligibility (or accessibility) criteria. Eleven(11) articles were finally selected for this review based on the standard summarized in Figure 2.



Figure 1. Potential risks to surface and groundwater pollution. After [24].

	Table 1. Sea	rch terms applied	in searching the data	abase and corresponding	g classification
--	--------------	-------------------	-----------------------	-------------------------	------------------

Term classification	Search terms
Source of pollutant	Landfills, mines, industry, urban sewage, agriculture,
Pathway	Streams/river, shallow well, borehole, mining sites, pit latrines,
	soak ways.
Infiltration	Aquifer, stream, river, pond, lake, sea.
Date	Search was limited to 1970

After completing the process of review, 11 papers were involved in the analysis as shown in Table 2. These studies present modeling approaches applied to both surface and groundwater. Apart from two studies i.e. [28] and [29], all the remaining nine (9) studies evaluated have used some form of multi-pollutant approach to surface-groundwater pollution modeling. This demonstrated that despite the difficulties involved in water pollution modeling, there is an increased concern on understanding how pollutants are transported to groundwater via recharge by infiltering contaminated surface water. However, one study i.e. Appelo and Rolle [30], compared the results of numerical simulations of fluid levels in groundwater bores. Heavy metal modeling was attempted by [31] and [3]. Two studies i.e. [32] and [33] presented a tool for groundwater contamination risk assessment. Similarly, [34] and [35] showed how water contamination from petrochemicals and hydrocarbons can be modeled. Conversely, [36] show how nitrogen (N) and phosphorus (P) retention in surface water can be simulated. Lastly, [29] presented a comparison of two models (NEWS and SPARROW) illustrating how N is transported to coastal areas. A major limitation to water quality models is that they assumed a uniform environment and can simulate pollutant only in the gas and aqueous state.

IOP Conf. Series: Materials Science and Engineering

884 (2020) 012030

doi:10.1088/1757-899X/884/1/012030



Figure 2. A methodical procedure used in the current review including the result of literature documentation, assessment, accessibility, and final study enclosure. After [24].

3. Results

Table 2 presents the major descriptive faces of incorporated studies. The remediation or cleanup of light non-aqueous phase liquid (LNAPL) polluted areas indicates that the systematic models can be applied to improve/refine hypothetical site models and for evaluating possible LNAPL recovery endpoints, particularly in places having fluctuating water levels in wells [30]. Simulation of continental-scale spatiotemporal frameworks of exchanges between surface water and groundwater aquifers can help with water management, recognizing potential sites of heavy nutrient mass loading from the aquifer to streams and ecological evaluation and planning decided on sites of high groundwater release [31]. A Compositional Multiphase Model for Groundwater Pollution (CMGP) is applicable for estimation of oil plume establishment in the unsaturated zone, and solute and vapor movement following the immiscible plume establishment is then established from the general model [34].

The natural decrease of unstable hydrocarbons in the shallow groundwater plumes and unsaturated zone can be estimated using Scenario-specific modeling and laboratory experiments. Groundwater infiltration is an important pollutant path only in soils with high water content [35]. Pollutant fate and movement modeling tool for management and risk evaluation of groundwater contamination by [33], presented a modeling tool comprising of five discrete models, in place of common geological settings, pollutant paths, and transportation processes, which allows for reliable qualitative approximations with wide trends in observations and offer a conservative approximation of pollution. A combined model for evaluating the risk of trichloroethylene (TCE) groundwater pollution, by [3], can be applied to assess the effect of point sources in surface water on human health and groundwater environments. The model results showed that uncertainty calculation discovered hydraulic conductivity to be the most significant site-specific parameter.

Sustainable and Integrated Engineering International Conference 2019 (SIE 2019)

IOP Conf. Series: Materials Science and Engineering

884 (2020) 012030

IOP Publishing

doi:10.1088/1757-899X/884/1/012030

	Table 2. Major descriptive faces of incorporated studies (il=11)				
S/n	Study	Study type	Objectives	Model types	Findings
1	Appelo and Rolle [30]	Comparing results to Numerical Simulation models.	To forecast LNAPL specific volumes and transmissivities from existing fluid level quantities in boreholes and either recorded notable fluid level variations in bores or estimates.	Entrapped, free, and residual LNAPL saturations and the transmissivity of LNAPL	The systematic model can be employed to improve/refine theoretical site models and for evaluating possible LNAPL recovery endpoints, especially in locations with varying water levels in boreholes.
2	Bailey, Wible [31]	Continental-scale spatiotemporal outlines of interactions surface water- groundwater.	Discover the spatiotemporal outlines of groundwater ejection to a stream system in a semi-arid region.	Daily spell phases and coupling.	Results can help with water management, recognizing potential sites of heavy nutrient mass loading from the aquifer to streams and ecological evaluation and planning decided on sites of high groundwater release
3	Corapcioglu [34]	A Compositional Multiphase Model for Groundwater Pollution	To define the fate of hydrocarbon elements of petroleum products present in soil and groundwater.	Molecular changes, microbially arbitrated or abiotic, are combined.	Estimates of two subproblems, oil plume establishment in the unsaturated zone, and solute and vapor movement following the immiscible plume establishment are then established from the general model.
4	Grathwohl [35]	Natural decrease of unstable hydrocarbons in the shallow groundwater plumes and unsaturated zone	To evaluate the diffusive dispersal of unstable fuel elements with and without biodegradation and recharge of groundwater	Scenario-specific modeling and laboratory experiments.	Groundwater infiltration is an important pollutant path only in soils with high water content.
5	Locatelli, Binning [33]	Pollutant fate and movement modeling tool for management and risk evaluation of groundwater contamination.	Assessment of groundwater contamination from polluted locations.	Modeling tool comprising of five discrete models, in place of common geological settings, pollutant paths, and transportation processes.	Approximations are qualitatively reliable with wide trends in observations and offer a conservative approximation of pollution.
6	McKnight, Funder [37]	A combined model for evaluating the risk of TCE groundwater pollution.	Assessing the effect of point sources in surface water on human health and groundwater environments.	Systematic volatilization model	Uncertainty calculation discovered hydraulic conductivity to be the most significant site-specific parameter.
7	Sajil Kumar, Davis Delson [3]	Assessment of Heavy Metals Pollution in Groundwater.	To evaluate Heavy Metal Pollution	Heavy metal Pollution Index Model	Industrialization and indecorous sewage discarding were recognized as the foremost cause for the build- up of metals in the groundwater.
8	Troldborg, Binning [32]	Measuring risk to groundwater of polluted locations.	Developing analytical answers to multiphase transport.	Unsaturated zone discharge models	The models display that both degradation and dispersal are significant tools for the lessening of pollutant absorptions at the water table.
9	Beusen, W [38]	Linking global models for nutrient loading and hydrology.	To simulate N and P holding in surface water.	IMAGE-GNM	Soil N budgets, wastewater and all factors influential litterfall in valleys are significant for N distribution to surface water.
10	Mayorga, Seitzinger [28]	Global N export from Watersheds	Offer a complete model account and present a summary of enhancements to input datasets.	NEWS 2	NEWS 2 can be used as an operative tool to study the effect of policies to lessen coastal eutrophication at local to global scales.
11	McCrackin, Harrison [29]	A comparison of NEWS and SPARROW models	To understand sources of N transported.	NEWS and SPARROW	NEWS and SPARROW both recognized the same single-largest N sources for surface area.

Table 2. Major descriptive faces of incorporated studies (n=11)

Application of the Heavy Metal Pollution Index Model (HMPIM), revealed that industrialization and indecorous sewage disposal were recognized as the foremost cause for the build-up of metals in the groundwater [3]. Measuring risk to groundwater of polluted locations, by the development of analytical answers to multiphase transport revealed that both degradation and dispersal are significant tools for lessening of pollutant absorptions at the water table [32]. Linking global models for nutrient loading and hydrology to simulate N and P holding in surface water indicate that soil N budgets, wastewater and all factors influencing litterfall in valleys are significant for N distribution to surface water [38]. Global N export from watersheds offer a complete model account and present a summary of enhancements to input datasets. The NEWS 2 can be used as an operative tool to study the effect of policies to lessen coastal eutrophication at local to global scales [28]. However, a comparison of NEWS and SPARROW models to understand sources of N transport showed that NEWS and SPARROW both recognized the same single-largest N sources for surface area [29].

4. Conclusion

The literature is almost unanimous on the importance of understanding how contaminants are transported from pollution sources by surface water to groundwater aquifers. Equating studies employed in this review leads to the following remarks:

- 1. The analogy with experimental data at different locations disclosed that the water quality models are capable of simulating the major trends and make available significant information to evaluate the menace modeled by pollutant sources from the surface to groundwater; chiefly, the high concentration, pollutant mass ejection and plume dispersal at the infiltration or recharge point;
- 2. Consequently, there is an increasing application of the multi-pollutant approach to the evaluation of water quality in both the aquifers and surface water;
- 3. Similarly, there is an amplified concern on understanding how contaminants from sources are transported to surface water and/or groundwater aquifers by in filtering surface flows.
- 4. These models allow for reliable qualitative and quantitative approximations with wide trends in observations and offer a conservative approximation of pollution.

However, the rationality of using multi-pollutant approaches is mostly hard to authenticate because suitable field data are lacking for evaluation. So, the model output must be analyzed within the framework of the uncertainty of the model inputs, data constraints and regularly essential application of accepted standards from the literature.

Conflict of Interest

The authors pronounced that, there is no conflict of interest associated with this article.

Acknowledgements

The authors would like to acknowledge the financial support of this research by Universiti TeknologiMalaysia under GUP Tier 1 vote number Q.J130000.2522.20H53. Also, express appreciation to all who are involved either directly or indirectly.

IOP Conf. Series: Materials Science and Engineering 884 (

884 (2020) 012030

References

- [1] Hashim, M.A., et al., *Remediation technologies for heavy metal contaminated groundwater*. J Environ Manage, 2011. **92**(10): p. 2355-88.
- [2] Pal, A., et al., *Emerging contaminants of public health significance as water quality indicator compounds in the urban water cycle*. Environ Int, 2014. **71**: p. 46-62.
- [3] Sajil Kumar, P.J., P. Davis Delson, and P. Thomas Babu, Appraisal of heavy metals in groundwater in Chennai city using a HPI model. Bull Environ Contam Toxicol, 2012.
 89(4): p. 793-8.
- [4] Kroeze, C., et al., *Global modelling of surface water quality: a multi-pollutant approach.* Current Opinion in Environmental Sustainability, 2016. **23**: p. 35-45.
- [5] Brack, W., et al., Towards the review of the European Union Water Framework Directive: Recommendations for more efficient assessment and management of chemical contamination in European surface water resources. Sci Total Environ, 2017. 576: p. 720-737.
- [6] Sánchez-Bayo, F., K. Goka, and D. Hayasaka, Contamination of the Aquatic Environment with Neonicotinoids and its Implication for Ecosystems. Frontiers in Environmental Science, 2016. 4: p. 1-14.
- [7] Srinivasamoorthy, K., et al., Integrated techniques to identify groundwater vulnerability to pollution in a highly industrialized terrain, Tamilnadu, India. Environ Monit Assess, 2011.
 182(1-4): p. 47-60.
- [8] Manoj, K. and P. Padhy, discourse and review of environmental quality of river bodies in India: an appraisal of physico-chemical and biological parameters as indicators of water quality. Current World Environment, 2015. **10**(2): p. 537-571.
- [9] Machiwal, D., et al., Assessment and mapping of groundwater vulnerability to pollution: Current status and challenges. Earth-Science Reviews, 2018. **185**: p. 901-927.
- [10] Liu, Y., et al., Occurrence and spatial distribution of perfluorinated compounds in groundwater receiving reclaimed water through river bank infiltration. Chemosphere, 2018. 211: p. 1203-1211.
- [11] Abdalla, F. and R. Khalil, Potential effects of groundwater and surface water contamination in an urban area, Qus City, Upper Egypt. Journal of African Earth Sciences, 2018. 141: p. 164-178.
- [12] Barletta, M., A.R.A. Lima, and M.F. Costa, Distribution, sources and consequences of nutrients, persistent organic pollutants, metals and microplastics in South American estuaries. Sci Total Environ, 2019. 651(Pt 1): p. 1199-1218.
- [13] Yesmeen, R., et al., Heavy metal and major ionic contamination level in effluents, surface and groundwater of an urban industrialised city: A Case Study of Rangpur City, Bangladesh. Asian Journal of Chemical Sciences, 2018. 5(1): p. 1-16.
- [14] Alves, A., et al., Assessing the Co-Benefits of green-blue-grey infrastructure for sustainable urban flood risk management. J Environ Manage, 2019. 239: p. 244-254.
- [15] Wu, D., X. Ma, and S. Zhang, Integrating synergistic effects of air pollution control technologies: More cost-effective approach in the coal-fired sector in China. Journal of Cleaner Production, 2018. 199: p. 1035-1042.
- [16] Brusseau, M.L., D.B. Walker, and K. Fitzsimmons, *physical-chemical characteristics of water*. 2019: p. 23-45.
- [17] Hoellein, T.J., et al., *Microplastic deposition velocity in streams follows patterns for naturally occurring allochthonous particles.* Sci Rep, 2019. **9**(1): p. 3740.
- [18] Kellner, E. and J.A. Hubbart, *Flow class analyses of suspended sediment concentration and particle size in a mixed-land-use watershed.* Sci Total Environ, 2019. **648**: p. 973-983.
- [19] Tornero, V. and G. Hanke, Chemical contaminants entering the marine environment from seabased sources: A review with a focus on European seas. Mar Pollut Bull, 2016. 112(1-2): p. 17-38.

day I	ot al	First comprehensive	sorooning	of linonhilio	organia	contaminants	;

- [20] Dsikowitzky, L., et al., First comprehensive screening of lipophilic organic contaminants in surface waters of the megacity Jakarta, Indonesia. Mar Pollut Bull, 2016. 110(2): p. 654-64.
- [21] Brack, W., et al., The SOLUTIONS project: challenges and responses for present and future emerging pollutants in land and water resources management. Sci Total Environ, 2015. 503-504: p. 22-31.
- [22] Hopke, P.K., Review of receptor modeling methods for source apportionment. J Air Waste Manag Assoc, 2016. 66(3): p. 237-59.
- Yao, H., et al., Regional risk assessment for point source pollution based on a water quality [23] model of the Taipu River, China. Risk Anal, 2015. 35(2): p. 265-77.
- [24] Andrade, L., et al., Surface water flooding, groundwater contamination, and enteric disease in developed countries: A scoping review of connections and consequences. Environ Pollut, 2018. **236**: p. 540-549.
- [25] Cartwright, I., A.D. Werner, and J.A. Woods, Using geochemistry to discern the patterns and timescales of groundwater recharge and mixing on floodplains in semi-arid regions. Journal of Hydrology, 2019. **570**: p. 612-622.
- [26] Kattan, Z., Using hydrochemistry and environmental isotopes in the assessment of groundwater quality in the Euphrates alluvial aquifer, Syria. Environmental Earth Sciences, 2018. 77(2).
- [27] Szczucińska, A., et al., Hydrochemical Diversity of a large alluvial aquifer in an arid zone (Draa River, S Morocco). Ecological Chemistry and Engineering S, 2019. 26(1): p. 81-100.
- [28] Mayorga, E., et al., Global nutrient export from watersheds 2 (NEWS 2): Model development and implementation. Environmental Modelling & Software, 2010. 25(7): p. 837-853.
- [29] McCrackin, M.L., J.A. Harrison, and J.E. Compton, A comparison of NEWS and SPARROW models to understand sources of nitrogen delivered to US coastal areas. Biogeochemistry, 2013. 114(1-3): p. 281-297.
- Appelo, C.A. and M. Rolle, PHT3D: a reactive multicomponent transport model for saturated [30] porous media. Ground Water, 2010. 48(5): p. 627-32.
- [31] Bailey, R.T., et al., Assessing regional-scale spatio-temporal patterns of groundwater-surface water interactions using a coupled SWAT-MODFLOW model. Hydrological Processes, 2016.
- [32] Troldborg, M., et al., Unsaturated zone leaching models for assessing risk to groundwater of contaminated sites. J Contam Hydrol, 2009. 105(1-2): p. 28-37.
- [33] Locatelli, L., et al., A simple contaminant fate and transport modelling tool for management and risk assessment of groundwater pollution from contaminated sites. J Contam Hydrol, 2019. **221**: p. 35-49.
- [34] Corapcioglu, M.Y., A compositional multiphase model for groundwater contamination by petroleum products 1. Theoretical considerations. Water resources research, 1987. 23(1): p. 191-200.
- [35] Grathwohl, P., Klenk, I.D., Maier, U., Reckhorn, S.B.F., Natural attenuation of volatile hydrocarbons in the unsaturated zone and shallow groundwater plumes: scenario-specific modelling and laboratory experiment. In: Groundwater quality: natural and enhanced restoration of groundwater pollution. Proceedings of the Groundwater Quality 2001 Conference held at Sheffield. UK, June 2001. 2002: p. 7.
- Beusen, et al., Global riverine N and P transport to ocean increased during the 20th century [36] despite increased retention along the aquatic continuum. Biogeosciences, 2016. 13(8): p. 2441-2451.
- [37] McKnight, U.S., et al., An integrated model for assessing the risk of TCE groundwater contamination to human receptors and surface water ecosystems. Ecological Engineering, 2010. **36**(9): p. 1126-1137.

Sustainable and Integrated Engineering International Co.	IOP Publishing	
IOP Conf. Series: Materials Science and Engineering	884 (2020) 012030	doi:10.1088/1757-899X/884/1/012030

[38] Beusen, et al., *Coupling global models for hydrology and nutrient loading to simulate nitrogen and phosphorus retention in surface water – description of IMAGE–GNM and analysis of performance.* Geoscientific Model Development, 2015. **8**(12): p. 4045-4067.