Comparative study of multimedia modeling for dynamic partitioning of fossil fuels-related pollutants

C.R. Hsieh*, J.R. Ouimette

Health, Environment and Safety Group, Chevron Research and Technology Company, Richmond, CA 94804-4054, USA

Abstract

Health-based risk assessments have uncertainties in many areas. These uncertainties necessitate the use of assumptions which are required to err on the side of public health protection. One source of uncertainty in risk assessment is the extent of human exposure to pollutants in various media such as air, water, soil, sediment and biota. The pollutant concentrations in these media can be simulated through multimedia modeling of the complex physical, chemical, and biological processes that govern the fate and transport of the pollutants. By reducing uncertainty (which often leads to conservatism) and providing realistic scenarios, multimedia modeling can help develop operating and control strategies which will minimize expenditures of societal resources without compromising environmental quality and public health.

Multimedia calculations are complex. A variety of methodologies and models have been proposed in the last two decades. However, the task has been made easier in recent years because of the advent in personal computers and the development of PC-based computer software. Two of such softwares are the fugacity models and the spatial multimedia compartmental (SMCM) model. In this paper, these two models were applied to study the dynamic partitioning of several fossil fuels-related pollutants in different locations. The transient behavior of a pollutant resulting from an environmental perturbation was also examined. Finally, the capabilities and limitations of these models were compared from a user's point of view.

1. Introduction

In the 1990 amendments to the Clean Air Act, the focus of regulation on fuels-related pollutants shifted from a risk-based to a technology-based approach. By applying the maximum achievable control technology (MACT), the United States is expected to reduce air toxics by roughly 75–90% from the current levels. Although

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*Corresponding author.

risk assessment can be performed to "delist" a source category, the United States Environmental Protection Agency (EPA) must also determine on a risk basis whether more stringent standards than MACT are required to protect public health with an "ample margin of safety," i.e. a cancer risk that is less than one in one million in a 70 yr lifetime.

In California, the Safe Drinking Water and Toxic Enforcement Act of 1986 (Proposition 65) requires business to give clear and reasonable warning to individuals before knowingly exposing them to certain chemicals. The Air Toxics "Hot Spots" Information and Assessment Act of 1987 (AB2588) and its 1992 modification (SB1731) established a statewide program for the report of air toxics emission inventories from individual facilities and many will need to prepare a multiple pathway health risk assessment. A health risk assessment includes a comprehensive analysis of the dispersion of hazardous substances in the environment, the potential for human exposure, and a quantitative assessment of both individual and population-wide health risks associated with those levels of exposure. If the risks exceed certain levels, public notification of potential health risks is required.

Risk assessment is complex and continues to be conservative in areas where uncertainty is the greatest. These uncertainties necessitate the use of assumptions which are required to err on the side of public health protection. While appropriate in concept, this approach often leads to assessments with considerable conservatism – as much as several orders of magnitude has been estimated in some cases [1]. Because societal resources are finite and the costs for reducing air emissions increase drastically at very low concentration levels, more realistic methodology in risk assessment can greatly reduce the unnecessary expenditures associated with the conservatism.

One source of uncertainty in risk assessment is the extent of human exposure before or after application of regulatory controls. Since many pollutants are eventually distributed among various media such as air, water, soil, sediment and biota, knowledge of their concentrations in these compartments are essential for realistic assessments of human exposure. Field measurements are often expensive and limited by analytical techniques. Projected scenarios are not measurable at all. An alternative is to perform multimedia modeling of the complex physical, chemical, and biological processes that govern the fate and transport of the pollutants. By estimating realistic and technically valid distribution of these pollutants under scenarios which are of interest to the society, multimedia modeling can, in a cost effective manner, be used as a screening tool to help develop operating and control strategies which will minimize societal expenditures while reducing the environmental risks to levels acceptable to the public.

2. Multimedia modeling

A variety of approaches have been taken to model the multimedia fate and transport of pollutants. Depending on the level of complexity, these models differ in

their treatment of spatial and temporal resolution. While the earlier models were developed for applications on mainframe computer, some of the more recent models were designed for the personal computers.

The traditional approach to multimedia modeling is to link together several single medium models to mimic nature's multimedia environmental system. In efforts to retain the spatial and temporal details of the individual medium, these models become highly complex and require a large amount of input data. As a result, feedback transport loops are usually ignored. Examples include the UTM-TOX (Unified Transport Model for TOXicant) [2–4] and TOX-SCREEN [5–7] models developed by the Oak Ridge National Laboratory, and the ALWAS (Air, Land, Water Analysis System) model [8,9] developed by A.D. Little, Inc. The computer programs developed for these models were typically on mainframe computers requiring significant efforts in program installation, data collection and processing. Consequently, these models are not convenient for "what-if" and sensitivity studies.

Another approach is to take into account the interactions among the various media while at the same time simplifying data and computer operation requirements. This is accomplished by taking into consideration a variety of transport processes and chemical reactions while assuming that all the environmental media under considera-tion are well mixed. The concept of fugacity is applied and extended to describe the equilibrium and steady-state distribution of pollutants. Fugacity is a thermodynamic term which is identical to partial pressure in ideal gases and near-linearly related to concentration. The fugacities of a chemical in equilibrium are the same in all compart-ments. By focusing on the relative amounts and concentrations of the pollutants partitioned into each environmental medium, these models require only modest amounts of data input. With the advent in personal computers and the development of PC-based computer software, these models are emerging as useful screening tools. Examples include the Fugacity models [10–12] (Levels I–III) developed by the University of Toronto and MCM (Multimedia Compartmental Models) [13,14] developed by the University of California, Los Angeles. These models, however, do not provide the dynamic nature of the environment.

A third approach, a hybrid of the two, is an attempt to provide a screening-level tool while retaining as much physical realities as possible. In particular, the SMCM (Spatial Multimedia Compartment Model) [15–17] being developed by UCLA rep-resents the state-of-the-art in this effort. The model considers the environment as consisting of both uniform (air, water, biota, and suspended solids) and nonuniform (soil and sediment) compartments. It also incorporates a low-degree spatial resolution which is not found in the compartmental models, but avoids the complexities encoun-tered with the spatial models. Another feature is the extensive use of built-in correla-tions for many of the required parameters and the development of a database which includes the physical and chemical properties of many commonly found air toxics, and the geographical and meteorological data of several regions. This PC-based user-friendly software allows a relatively inexperienced user to start using the software quickly.

3. Level III fugacity and SMCM models

Because of their similarities in many aspects and the availability of PC-based software, we evaluated the Level III fugacity and SMCM models as two likely screening-level tools for studying multimedia partitioning of toxics.

While the Level III fugacity model considers four bulk compartments (air, water, soil, and sediment) in the environment, the SMCM model takes into account two additional compartments (suspended solids and biota) in the bulk calculations. The Level III fugacity model includes suspended solids and biota as subcompartments in the water compartment. The fugacity model considers aerosols as a subcompartment in the air compartment while the SMCM model does not. The Level III fugacity model considers all compartments uniform while the SMCM model treats soil and sediment as nonuniform. Another difference is that while the Level III fugacity model considers only equilibria and steady states, the SMCM model can perform time-dependent dynamic simulation of the environment. Table 1 summarizes the nature of the compartments.

Both models apply the concept of fugacity capacity, which is defined as the proportionality constant of a chemical's concentration to its fugacity. In many cases, the fugacity capacities can be rigorously calculated, as is evident by the same formulas used by the two models. The SMCM model also provides the option of estimating some parameters internally and the flexibility of using partition coefficients. Table 2 compares the fugacity capacities used in the two models.

The transport processes considered by the two models are similar. One difference is that the Level III fugacity model includes deposition and resuspension of sediment in water. This is considered important for hydrophobic chemicals. Table 3 displays the various transport processes in the models. Tables 4 and 5 summarize the default transport and other parameters used. While the Level III fugacity model uses "ball

Table 1
Comparison of compartments

	Fugacity	SMCM
Bulk compartments	Air, water, soil, sediment	Air, water, suspended solids,
Subcompartments in		biota, soil, sediment
each bulk compartment		
Air	Air, aerosols	Air
Water	Water, solids, biota	Water
Solids	N/A	Suspended solids
Biota	N/A	Biota
Soil	Air, water, solids	Air, water, solids
Sediment	Water, solids	Water, solids
Uniform compartments	Air, water, soil, sediment	Air, water, suspended solids, biota
Nonuniform compartments	None	Soil, sediment
Time dependence	Equilibrium, steady state	Dynamic, steady state

Table 2
Comparison of fugacity capacities

Compartment	Fugacity	SMCM
Air	$1/RT$	$1/RT$
Water	$1/H$, C^a/P^a	$1/H$
Solids	$X_{oc}K_{oc}(\rho)/H$	$X_{oc}K_{oc}(\rho)/H$
	$K_{oc} = 0.41K_{ow}$	$K_{oc} = f(K_{ow})$
		$K_{ow} = f(C^a$, type)
Aerosols	$6 \times 10^6/P^aRT$	N/A
Biota	$0.048(\rho)K_{ow}/H$	BCF $= C_b/C_w$,
		BCF $= f(K_{ow})$
Manual override	Software modification	Partition coefficients

R = gas constant, 8.314 Pa $*$ m^3/mol K, T = absolute temperature, K, H = Henry's law constant, Pa m^3/mol, C^a = aqueous solubility, mol/m^3, P^a = vapor pressure, Pa, X_{oc} = fraction of organic carbon, K_{oc} = organic carbon partition coefficient, K_{ow} = octanol–water partition coefficient, ρ = density of solids, kg/l, BCF = bioconcentration factor, C_b = concentration in biota, ng/kg, and C_w = concentration in water, ng/kg.

Table 3
Comparison of transport processes

	Fugacity	SMCM
Air to water	Diffusion, rain, wet deposition, dry deposition	Diffusion, rain, wet deposition, dry deposition
Air to soil	Diffusion, rain, wet deposition, dry deposition	Diffusion, rain, wet deposition, dry deposition
Soil to water	Soil runoff, water runoff	Water runoff
Sediment to water	Diffusion, deposition, resuspension, burial	Diffusion
Reaction	First order	First order
Advection	Bulk phase	Bulk phase

park" numbers for simplicity and allows users to modify the parameters, the SMCM model simplifies the process with many internal correlations which free the users from tedious estimates, but also somewhat restrict their flexibility in using alternate parameters.

Because of the uniformity assumed for the compartments in these models, they are designed to simulate relatively large regions. A recent study, however, demonstrated that the SMCM model can be used in conjunction with an air dispersion model to study the dynamic partitioning of 11 chemicals emitted from an oil refinery [31].

In terms of computer programming specifics, the Level III fugacity model is part of 11 fugacity models written and saved in BASIC language. They can be retrieved, run, and modified using a commonly available BASIC compiler. The programs are fully

Table 4
Comparison of default transport parameters

	Fugacity	SMCM
Mass transfer coefficients, m/h		
Air-side over water	3	Brutsaert [18]
Air-side over soil	1	Fernandez et al. [19]
Water-side over air	0.03	Cohen et al. [20]
Water-side over sediment	0.01	Thibodeaux et al. [21]
Water-side over solids	Not considered	Rowe et al. [22]
Overall Vol water to biota		Cohen et al. [23]
Diffusion coefficients, m^2/h		
In air	0.04	Reid et al. [24]
In water	4.0×10^{-6}	Reid et al. [24]
In soil	Internal calc.	Jury et al. [25], Sallam et al. [26]
In sediment	Internal calc.	Cohen et al. [17]
Manual override	Yes	Yes
Diffusion path length, m		
Soil	0.05	No limit
Sediment	0.005	No limit
Rates, m^3/m^2 h		
Rain	9.7×10^{-5}	User input
Infiltration		Smith [27]
Soil drying		Van Bavel [28]
Water runoff from soil	3.9×10^{-5}	Smith and Cherry [29]
Solids runoff from soil	2.3×10^{-8}	None
Leaching to groundwater	40% of rain	Boundary conditions
Sediment deposition	4.6×10^{-8}	N/A
Sediment resuspension	1.1×10^{-8}	N/A
Sediment burial	3.4×10^{-8}	N/A

commented and forms are provided to help users develop appropriate input data. Using the programs, nevertheless, requires some knowledge of BASIC and a good understanding of the fate and transport processes involved. The SMCM model, on the other hand, is supplied to users in compiled, executable codes. Data input are minimum and there is a growing library of chemicals and geographic locations which greatly simplifies input preparation by the users. The incorporation of a user-friendly interface and the availability of on-line help make the model application almost a turn-key operation. Since the users do not have access to the source codes, they have limited flexibility in modifying the correlations used in estimating the various parameters. Table 6 compares the programming aspect of the two models.

4. Model applications

The Level III fugacity model has been applied by its developers to calculate the steady-state distribution of six chemicals in the region of southern Ontario in Canada.

Table 5
Comparison of other default estimates

	Fugacity	SMCM
Air compartment		
Depth, m	2000	User input
Solids, f	2×10^{-11}	0
Water compartment		
Depth, m	50	User input
Solids, f	5×10^{-6}	User input
Biota, f	1×10^{-6}	User input
Soil compartment		
Depth, m	0.1	User input
Air, f	0.2	1 of 4 choices
Water, f	0.3	1 of 4 choices
Solids, f	0.5	1 of 4 choices
Sediment compartment		
Depth, m	0.01	User input
Water, f	0.7	Internal calc.
Solids, f	0.3	Internal calc.
Densities, kg/m^3		
Air	Calc. from T, P	Calc. from T, P
Water	1000	Internal calc.
Solids	2400	User input
Biota	1000	Not required
Carbon on solids, X_{oc}		
In water, X_{oc}	0.2	User input
In soil	0.02	User input
In sediment	0.04	User input
Velocities, m/h		
To high altitude	0.01	N/A
Dry deposition	10.8	Internal calc.
Meteorological data		
Daily temperature, °C	25	Jamison[30]
Rain distribution	N/A	Internal calc.
Scavaging ratio	200,000	User input

The results suggested that the model may be used to determine the processes that control the environmental fate of chemicals in a region and provide approximate estimates of relative media concentrations [32]. In our evaluation, we studied the impact of location differences by comparing the fate of benzene in southern Ontario to that in the Santa Clara region of California. Table 7 summarizes the parameters used. In addition to geographic, meteorological, and emission data, we also modified the default solid densities and the carbon on solids. Because of the significant differences reported in literature for benzene degradation rate in air, we tested the model using a low rate constant (8.6×10^{-4}/h) suggested by the Level III fugacity and a high rate

Table 6
Comparison of computer programming

	Fugacity	SMCM
Hardware required	PC	PC
Software code	BASIC	Executable
Software modification	Yes, need to know BASIC	No, need to contact developer
Input format	In both input and program	Input screen
Output format	Printed tables	Graphs and ASCII files
Input flexibility	100%	Not available for certain parameters
Ease to use	Need to know BASIC	Almost "turn key"
Library		
Chemicals	Small	Dozens
Locations	1	Several

Table 7
Comparison of parameters used for modeling benzene in Level III fugacity model

	S. Ontario	Santa Clara
Air compartment		
Area, m^2	2.000E + 11	3.457E + 09
Depth, m	2000	760
Water compartment		
Area, m^2	8.000E + 10	1.729E + 07
Depth, m	50	10
Biota fraction	1×10^{-6}	0.5×10^{-6}
Soil compartment		
Area, m^2	1.200E + 11	3.440E + 09
Depth, m	0.1	0.1
Air fraction	0.2	0.34
Water fraction	0.3	0.08
Solids fraction	0.5	0.58
Sediment compartment		
Area, m^2	8.000E + 10	1.729E + 07
Depth, m	0.01	0.01
Benzene		
Reaction K in air, 1/h	8.600E − 04/	8.600E − 04/
	9.300E − 03	9.300E − 03
Reaction K in water, 1/h	4.760E − 03	4.760E − 03
Flow rate in air, m^3/h	3.300E + 12	6.770E + 08
Concentration in air, mol/m^3	3.000E − 08	4.090E − 08
Emission in air, mol/h	10,000	1206
Emission in water, mol/h	80,000	0
Solid densities, kg/m^3	2400	1500
Carbon on solids, X_{oc}		
In water, X_{oc}	0.2	0.04
In soil	0.02	0.04
Daily temperature, °C	25	15.4

Table 8
Mass distribution and concentration results for benzene using Level III fugacity model

	S. Ontario	Santa Clara
Using default rate constant 0.00086 l/h		
Total mass in compartment (% of total)		
Air	46.420	99.874
Water	53.545	0.013
Soil	0.010	0.113
Sediment	0.025	0
Biota	0	0
Suspended solids	0.007	0
Concentration (gmol/m^3 × 10^6)		
Air	0.032 (0.78 ppb)	0.415 (10.15 ppb)
Water	3.707 (289.6 ng/l)	0.849 (66.34 ng/l)
Soil	0.241 (12.54 ng/kg)	3.581 (321.4 ng/kg)
Sediment	8.531 (469.3 ng/kg)	1.442 (97.94 ng/kg)
Biota	24.000 (1875 ng/kg)	5.499 (429.5 ng/kg)
Suspended solids	98.650 (3211 ng/kg)	2.825 (147.1 ng/kg)
Using rate constant 0.0093 l/h suggested by SMCM		
Total mass in compartment (% of total)		
Air	31.097	99.869
Water	68.864	0.013
Soil	0.007	0.117
Sediment	0.032	0
Biota	0	0
Suspended solids	0.009	0
Concentration (gmol/m^3 × 10^6)		
Air	0.017 (0.42 ppb)	0.049 (1.20 ppb)
Water	3.700 (289.0 ng/l)	0.100 (7.85 ng/l)
Soil	0.125 (6.52 ng/kg)	0.440 (36.19 ng/kg)
Sediment	8.514 (468.4 ng/kg)	0.171 (11.58 ng/kg)
Biota	23.950 (1871 ng/kg)	0.650 (50.80 ng/kg)
Suspended solids	98.450 (3204 ng/kg)	0.334 (17.40 ng/kg)

constant (9.3×10^{-4}/h) found in the SMCM model. A recent review indicated that the benzene degradation constant is proportional to the hydroxyl concentration in the atmosphere [33]. At a hydroxyl concentration of 1×10^6 molecules/cm^3, the calculated degradation constant is between the two rate constants assumed (4.4×10^{-3}/h).

The mass distribution and concentrations predicted by the Level III fugacity model are displayed in Table 8. Using the low benzene degradation rate constant, the model predicts that about half of the steady-state benzene is in the water in southern Ontario, while more than 99% of the benzene stays in the air in Santa Clara. This is primarily because water represents about 40% of the southern Ontario region, but only 0.5% of Santa Clara. Another reason is that the emission sources were mostly in the water in southern Ontario, but entirely in the air in Santa Clara (Table 7). While

the emission sources are irrelevant in a closed system which has reached equilibrium, they can affect the partitioning of these emissions in an open system where the emissions are transported between the system and its environment. This difference is also reflected in the benzene concentrations calculated in the media. The predicted concentration in air is low in southern Ontario (0.8 vs. 5.0 ppb) [32], but high in Santa Clara (10 vs. 5 ppb) [15]. This observation suggests that the degradation constant may be different in the two regions. Another observation is that, while they represent only an extremely small fraction of the total mass and their absolute levels are extremely low, the concentrations of benzene in biota and suspended solids are order(s) of magnitude higher than those in air and water. The much higher benzene concentration predicted for the suspended solids in southern Ontario than in Santa Clara results from the 5 time differences assumed for the carbon on solids in the two regions (Table 7). Table 8 also shows that, by assuming a higher degradation rate constant for benzene in the air, the model predicts that more than two-thirds of the total benzene will stay in the water compartment and that the benzene concentration in the Santa Clara air will be almost an order of magnitude lower than that in the previous case.

The SMCM model has been used in several studies and the predicted concentrations were found to be in reasonable agreement with the available field data [17, 31]. In our study, we tested the model by estimating the distribution of benzene and MTBE in the Santa Clara, California region. The benzene in Santa Clara was supplied as an example in version 3.2 of the program. A summary of the geographic and meteorological data relevant to Santa Clara region is presented in Table 9. The physical, chemical, and emission data used in modeling are displayed in Table 10.

Fig. 1 illustrates that the predicted concentrations are very close to steady state about 500 h after a continuous source of air emission starts. The mass distribution and concentrations of benzene and MTBE predicted by the model at 2000 h are summarized in Table 11. The results suggest that a vast majority of the emission remains in the air compartment. The concentration, however, is the lowest in air for both benzene and MTBE. Benzene concentrations are higher in biota and suspended solids while MTBE concentrations are higher in water and biota. Another observation is that, while the water-to-air concentration ratio is about 2 for benzene, it is about 30 for MTBE. This reflects the high solubility of MTBE in water. Finally, this table shows very steep concentration gradients in both soil and sediment because these two compartments are treated as nonuniform in the model and the diffusion is slow.

The dynamic feature of the SMCM model makes it a useful tool to predict the transient behavior of a pollutant resulting from variations in either emission sources or meteorological changes. We simulated a perturbation by assuming that a sudden discharge of benzene in water occurred at 1000 h in Santa Clara. Fig. 2 shows that the concentrations in biota, solids, and sediments almost changed instantaneously, indicating highly effective mass transfer among those media. All of these changes decay back to steady states in about 300 h. The concentrations in air and soil were not significantly affected.

Table 9
Geographic and meteorological data of Santa Clara used in SMCM model

Surface area	1350 miles^2	
Surface slope	2%	
Surface distribution		
Soil	99.5%	
Water	0.5%	
Air height (inversion layer)	760 m	
Water depth	10 m	
Suspended solids		
Diameter	10 μm	
Density	1.5 g/cm^3	
Concentration	5×10^{-4}% of water	
Biota concentration	5×10^{-5}% of water	
Sediment		
Depth	1 m	
Organic carbon fraction	0.04	
Soil		
Depth	8 m	
Air	34%	
Water	8%	
Matrix	58%	
Soil type	Permeable fine sandy	
Ambient temperature (°C) and rainfall (mm)		
January	9.7	76.2
February	11.6	55.6
March	12.6	50.8
April	14.3	27.9
May	16.7	7.6
June	19.0	0
July	20.4	0
August	20.3	0
September	19.9	5.1
October	17.1	15.2
November	12.9	43.2
December	9.8	50.8

Finally, we compared the predictions of the Level III fugacity and the SMCM models for the steady-state distribution of benzene in Santa Clara. The results are summarized in Table 12. The two models agree well in mass distributions and in the concentrations of all uniform compartments. The differences in soil and sediment concentrations are due primarily to the treatment of these two media in the models. The Level III fugacity model assumed uniform soil and sediment media and assigned their default depths 10 and 1 cm, respectively. The calculated concentrations in these two media depend on their assigned depths. The SMCM model, on the other hand, assumed nonuniform soil and sediment media and removed the uncertainty in estimating their depths. In this case, the predicted concentrations depend largely on the diffusion coefficients used in the model. Since the predicted concentrations in these

Table 10
Physical and chemical data used in SMCM model

	Benzene	MTBE
Degradation rate constants (l/h)		
Air	0.0093	0.0165[a]
Water	0.0048	0.0001[b]
Soil	0	0
Sediment	0	0
Biota	0	0
Suspended solids	0	0
Henry's law constant, Pa m^3/gmol	557.3	66.9
Solubility in water, mg/l	1780	43000
Molecular weight, g/mol	78.11	88.15
Boiling point, K	353.25	328.3
Molal volume at b.p., cm^3/gmol	96.5	128.9
Chemical type	Aromatics	Ether
Emission		
Background, ppb	1	1[c]
Compartment	Air	Air
Strength, gmol/h	1206.1	1206.1[c]

[a] Estimation based on hydroxyl reactivity.
[b] Estimation based on Chevron's internal work.
[c] Arbitrarily assumed to be the same as benzene.

compartments are extremely low in either case, the differences are not significant. It is conceivable, however, that these model differences can lead to different conclusions significantly in some other scenarios.

5. Conclusion

A realistic risk assessment requires the use of accurate environmental concentrations of the pollutants being considered. We have evaluated two recently developed computer software – the Level III fugacity and SMCM – which were designed to provide screening-level partitioning and concentrations of various pollutants in the environment through multimedia modeling of the processes that control the fate and transport of the pollutants. The applications of these two PC-based models have illustrated their usefulness in identifying the major differences in either the fate of a pollutant in different regions, or the fate of different pollutants in the same region. In addition, the SMCM model is also suitable for studying the transient behavior of an environmental perturbation. Both software are reasonably documented and easy to use. The execution time is very fast on a typical 486 PC. The SMCM requires an IBM compatible PC/XT with 512 RAM and a math coprocessor. The fugacity model requires a BASIC compiler. The outputs include enough details for the user to interpret most of the results.
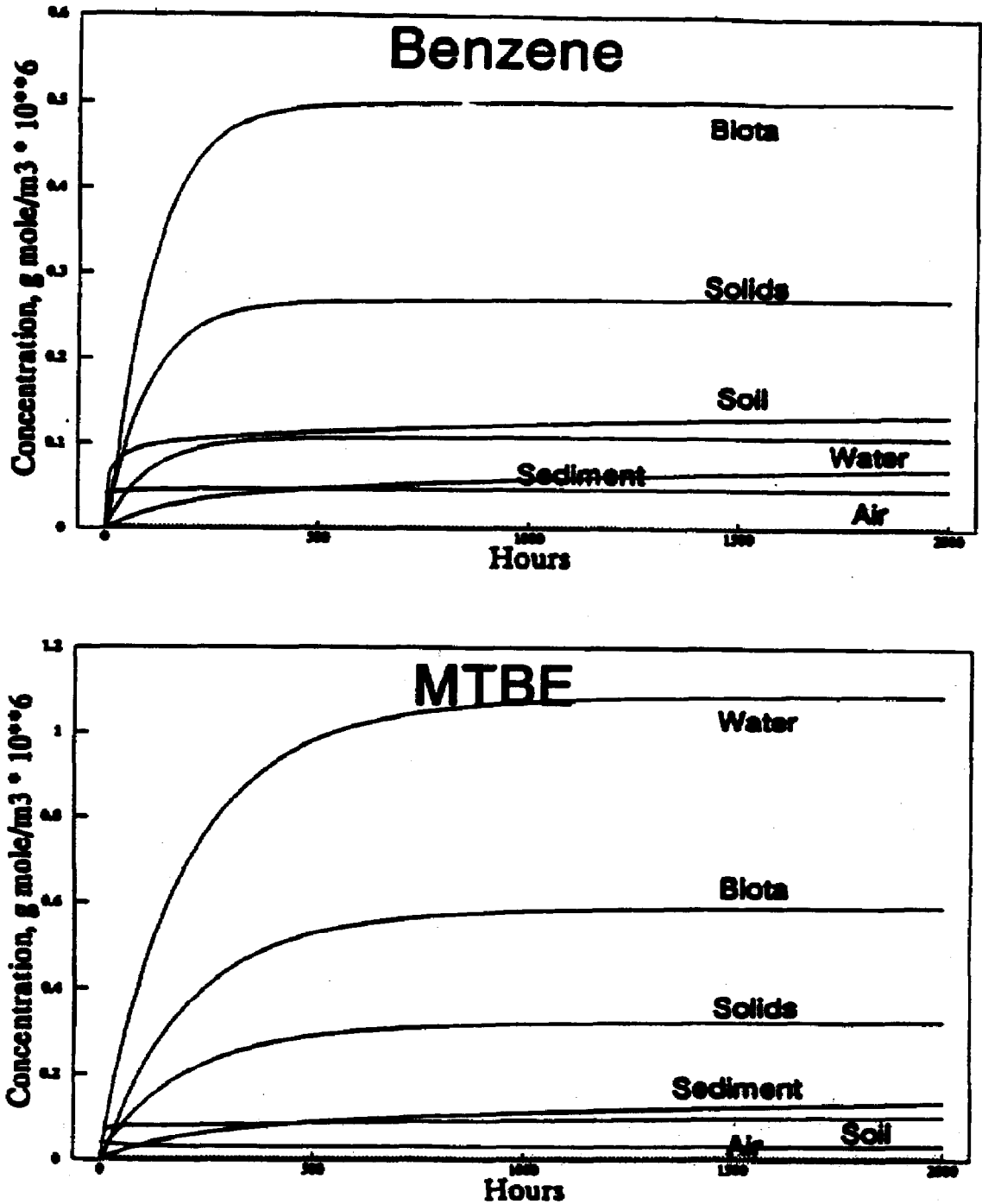
Fig. 1. Simulation with SMCM in Santa Clara.

By estimating realistic and technically valid distribution of emissions under a variety of scenarios, these models are useful screening-level tools which can help both regulatory agencies and industry develop the best operating and control strategies in order to reduce the environmental risks. The friendliness of these models make them

Table 11
Mass distribution and concentrations results using SMCM model 2000 h after emission starts

	Benzene	MTBE
Total mass in compartment (% of total)		
Air	99.756	99.546
Water	0.015	0.228
Soil	0.229	0.226
Sediment	0	0
Biota	0	0
Suspended solids	0	0
Concentration ($gmol/m^3 \times 10^6$)		
Air	0.046 (1.13 ppb)	0.031 (0.77 ppb)
Water	0.108 (8.42 ng/l)	1.090 (95.9 ng/l)
Soil (top 10 cm)	0.133 (6.94 ng/kg)	0.101 (5.92 ng/kg)
Sediment (top 10 cm)	0.071 (3.67 ng/kg)	0.134 (7.88 ng/kg)
Biota	0.503 (39.3 ng/kg)	0.591 (52.1 ng/kg)
Suspended solids	0.270 (14.1 ng/kg)	0.325 (19.1 ng/kg)
Concentration profile in soil ($gmol/m^3 \times 10^6$)		
Centimeters from surface		
0	0.168	0.129
0.8	0.152	0.117
2.4	0.137	0.105
4.8	0.107	0.081
10.4	0.077	0.057
35.2	0.032	0.022
209.6	0.003	0.002
Concentration profile in sediment ($gmol/m^3 \times 10^6$)		
Centimeters from surface		
0	0.209	0.501
1.0	0.124	0.153
2.0	0.051	0.016
3.5	0.016	0.001
5.0	0.003	0.000

convenient tools to study the impact of various physical, chemical, and biological parameters on the distribution and concentrations of pollutants in the various media. However, since these models were not designed to simulate many aspects of human exposure that can be important in risk assessment (e.g., spatial distribution of pollutants in all media, groundwater, indoor environments), more comprehensive models should be used if the screening results suggest that a potential public health risk may exist.
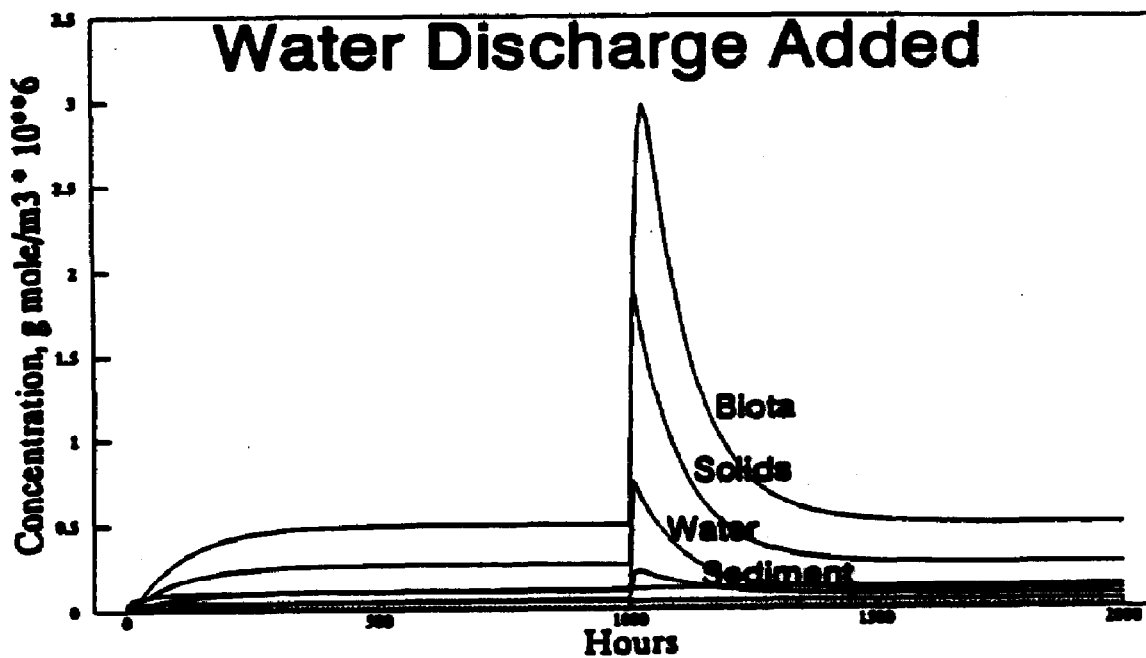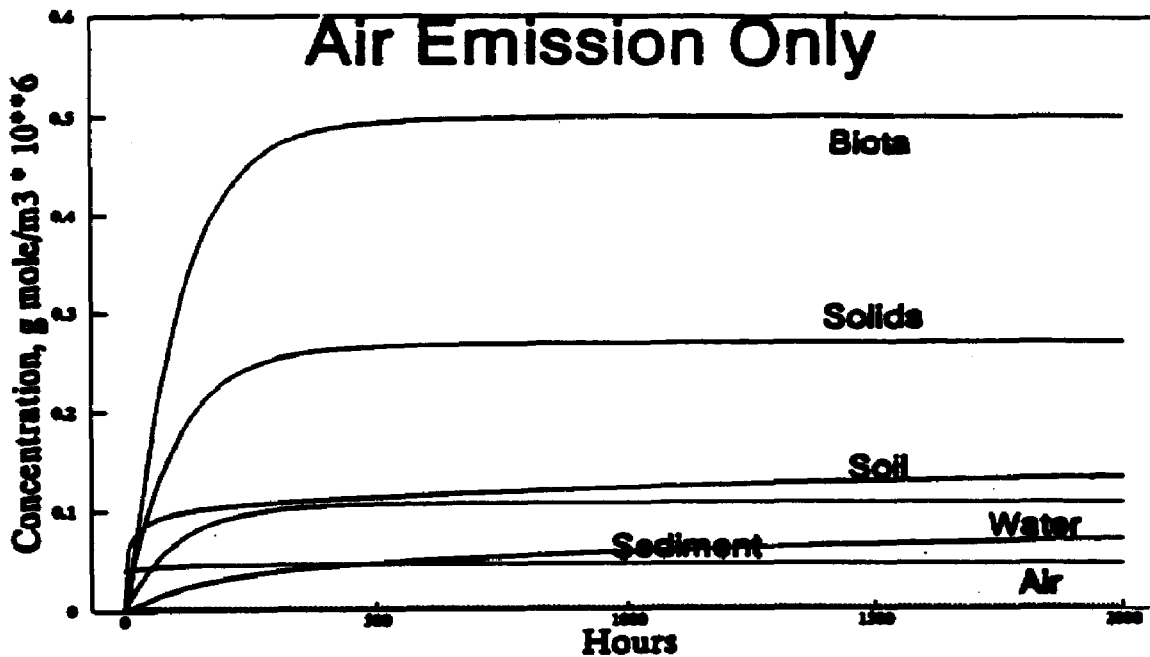
Fig. 2. Simulation of benzene in Santa Clara.

Table 12
Comparison between fugacity and SMCM modeling results for benzene in Santa Clara

	Fugacity	SMCM
Total mass in compartment (% of total)		
Air	99.869	99.756
Water	0.013	0.015
Soil	0.117	0.229
Sediment	0	0
Biota	0	0
Suspended solids	0	0
Concentration (gmol/m$^3 \times 10^6$)		
Air	0.049 (1.20 ppb)	0.046 (1.13 ppb)
Water	0.100 (7.85 ng/l)	0.108 (8.42 ng/l)
Soil	0.440 (36.2 ng/kg)[a]	0.133 (6.94 ng/kg)[b]
Sediment	0.171 (11.6 ng/kg)[a]	0.071 (3.67 ng/kg)[c]
Biota	0.650 (50.8 ng/kg)	0.503 (39.3 ng/kg)
Suspended solids	0.334 (17.4 ng/kg)	0.270 (14.1 ng/kg)

[a] Average of top 10 cm, lower but nonzero concentrations beyond 10 cm.
[b] Uniform in the top 10 cm, zero beyond 10 cm.
[c] Uniform in the top 1 cm, zero beyond 1 cm.

Acknowledgments

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