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**A Comparison of Overall
Persistence Values and
Atmospheric Travel Distances
Calculated by Various Multi-Media
Fate Models**

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Introduction and Motivation

Recent and ongoing international negotiations to regulate persistent organic pollutants (POPs), sometimes also referred to as persistent, bioaccumulative and toxic substances (PBTs), on the regional and global level have created the need for defining chemicals as persistent and as being subject to long range transport. Simple procedures involving the comparison of a chemical's properties (e.g. degradation half-lives in various environmental media) with a threshold value have been suggested or are already in use. Multimedia models have been identified as potentially useful tools in a screening process for persistence and long range transport (LRT) potential, and several approaches have been suggested (van de Meent et al., 2000). The first part of this report reviews these models and some of the issues associated with their use in the assessment of persistence and LRT potential.

To implement the use of such models in a regulatory context it is imperative to evaluate to what extent various approaches are comparable. Is it feasible and desirable to prescribe the use of a specific modelling approach, or even one specific model? This project set out to compare the values for overall persistence and LRT potential estimated by models developed and used by various research groups. Various groups (see listing at the end of this report) were invited and/or volunteered to participate in this exercise and were given a set of property data for 26 chemicals to be used in the estimation of overall persistence and LRT potential. By using the same chemical dataset, it was assured that any differences revealed in overall persistence and LRT potential are based on the modelling approaches only. It is likely that uncertainty in the chemical input parameters can result in differences which are at least as significant as those caused by differences between models. The differences derived from the chemical input parameters were not the subject of this investigation.

The results from the various models were compared in terms of the absolute scale of the calculated values and the relative ranking of the chemicals according to persistence and LRT potential. Specifically, the comparison was aimed to address the following set of questions:

- Are the absolute values calculated for overall persistence and travel distance calculated by different models comparable? Does it make sense to define absolute threshold values independent of model?
- Is the relative ranking of the chemicals according to persistence and travel distance calculated by different models comparable? Is the "relative difference" between chemicals comparable? Would it thus be possible to use a "benchmark chemical" as a threshold?
- If there is a significant difference in the ranking between different approaches, why is this the case? If there is discrepancy, can we judge one approach as more reliable than the other?
- What are the minimum specifications for a model to reliably assess overall persistence and travel distance?

Following the review of the model approaches and issues, this report will sequentially describe the comparison of overall persistence values and atmospheric transport distance, to finally derive some conclusions and recommendations.

Use of Multi-Media Mass Balance Models in the Screening of Chemicals for Persistence and Long Range Transport Potential: A Review of the Literature and the Issues

What Are Multimedia Mass Balance Models and What Can They Do?

Multimedia mass balance models are relatively simple mathematical descriptions of the natural environment designed to gain a qualitative and quantitative understanding of the environmental behavior of chemicals, which are likely to be found in more than one environmental phase or medium. Such models subdivide the environment into a number of compartments – well-mixed “boxes” which are assumed to have homogeneous environmental characteristics and chemical concentrations. The model then calculates how a chemical is distributed within that simplified system. The distribution, and thus the concentration that is established in each medium, is influenced both by the chemical’s intrinsic properties and emission patterns and the characteristics of the environment into which it is released. The models thus integrate information on multiple and interacting processes of partitioning, transport and transformation into a comprehensive yet readily comprehensible picture of a chemical’s fate in the environment (Mackay, 1991, Cowan et al. 1995, Wania and Mackay, 1999).

These models can be used in two contexts: real and evaluative situations.

Firstly, they can be used to simulate the observed behavior of contaminants in a real situation. A successful simulation, in which there is satisfactory agreement between observations and model results, suggests that the degree of theoretical understanding of the way chemicals partition, move and react is sufficient to explain the observed behavior in that environment. It is then possible, and justifiable, to use the model to derive information not contained in the measured data, such as fluxes between media, future trend predictions, source apportionment and mass budgets. Examples for this mode of use are the description of PCB fate in the Lake Ontario ecosystem (Gobas et al., 1995) or the fate of α -hexachlorocyclohexane in the global environment (Wania et al., 1999).

Secondly, these models can be used to describe the fate of a chemical in a hypothetical or evaluative setting. The objective is not to describe a real situation, but to provide the likely picture of a chemical’s fate in a generic environment for the purpose of assessment and evaluation. This is particularly useful within a regulatory context, e.g. in the registration process for new chemicals, or when the environmental behavior of several chemicals is to be compared. Examples for this mode of model use are the SimpleBox model (Brandes et al., 1996) and the EQC model (Mackay et al., 1996). It is obviously this latter type of application of multimedia mass balance models that is of interest in the context of screening chemicals for persistence and long range transport potential. The entire focus is on the chemicals’ properties and not on how different environments result in differing fate.

Why Use Multimedia Models in the Evaluation of Persistence (P) and Long Range Transport (LRT) Potential?

Some of the approaches that have been suggested, or already are in use, for screening of chemicals for persistence, do not require the use of models, but rely on the comparison of media-specific half-lives with media-specific threshold values. A substance is considered persistent if its half-life in any of the media exceeds the threshold for that medium. Persistence in any one environmental compartment is thus judged sufficient to classify a chemical as persistent in general. Webster et al. (1998) have pointed out the inconsistencies which result

when the effects of partitioning to other media and mode of entry are ignored in developing these criteria half-lives. Because the overall persistence of a chemical in the environment is influenced by its dynamic multimedia distribution, the approach based on individual compartment half-lives is conservative for a chemical which does not partition significantly into a compartment in which it is very persistent, while being easily degraded in other compartments. In colloquial terms it is “wrongly penalized” for being persistent in a place it rarely, if ever, goes. Obviously the amount lost by degradation in a particular medium is determined both by the medium-specific degradation rate constant and the amount present in that medium. It follows, that for persistence in the overall environment, the degradation rate constants which are most important, and must be known most accurately, are for compartments where most of the chemical resides. A screening process should thus weigh the persistence in the various environmental media according to where a chemical is likely to reside. This issue is complicated by the observations that the distribution depends on how the chemical enters the environment as to air or soil.

In the case of screening for LRT potential simple fail/pass criteria based on the degradation half-life in air and/or volatility-related parameters such as vapor pressure or Henry’s law constant have been suggested. Again, a chemical’s ability to be transported over large distances is the result of complex interactions between its environmental phase distribution and persistence in various phases. A criterion based on one or two parameters is very unlikely to capture the complexity and interdependence of processes controlling a chemical’s potential to reach remote regions.

In short, the purpose of using multimedia mass balance models in the screening process is to take into account the influence of a chemical’s environmental phase distribution on its ability to persist and be transported over long distances. The environmental phase distribution is influenced by a large number of factors related to both environmental and chemical characteristics, which is not necessarily intuitive or easily comprehended. A multimedia model provides a tool to take most of these factors into account in a transparent, objective and reproducible manner (van de Meent et al., 1999).

Approaches Using Multimedia Models for the Evaluation of Persistence

The environmental persistence of a chemical τ in the framework of multimedia model calculations is typically defined as the average time a chemical resides in a particular environment before it is degraded, i.e. chemically transformed into another compound:

$$\tau = M_{\text{tot}}/N_{\text{Rtot}}$$

where M_{tot} is the total amount of chemical in the system, and N_{Rtot} is the total loss rate from that system by degradation. If a multimedia mass balance model has n compartments, M_i is the amount of chemical in compartment i , and k_i is the degradation rate in that compartment, the overall persistence τ can be calculated using

$$\tau = \frac{M_{\text{tot}}}{N_{\text{Rtot}}} = \frac{\sum_i^n M_i}{\sum_i^n (M_i \cdot k_i)}$$

Inverting this to obtain the overall rate constant gives:

$$k_{\text{tot}} = \frac{1}{\tau} = \sum_i^n \frac{M_i}{M_{\text{tot}}} \cdot k_i$$

which implies that the overall rate constant is the sum of the rate constants in the individual compartments, weighted by the mass fraction present in each of these media. If all rate constants are assumed to be first order or pseudo-first order, the overall persistence becomes independent of the release rate. Essentially, all existing approaches for calculating an overall persistence using multimedia models adopt this relationship. Differences relate:

1. to the way the weights or mass fractions are derived.
2. to the number and nature of compartments that make up the multimedia model
3. to whether transport processes that result in a permanent and irreversible removal from the sphere accessible to organisms should be included.
4. to whether or how environmental variability is treated.

Approaches to Deriving Environmental Distribution

There are several methods of deriving the proportion of mass in each environmental medium. The most commonly employed in multimedia models assume an equilibrium or steady-state distribution.

Approaches Based on Equilibrium Distribution

The simplest method of estimating the distribution between the model compartments is to assume equilibrium partitioning among the model compartments. This approach is characteristic of Level I and Level II fugacity models (Mackay, 1991). In one of the first approaches to calculate an overall persistence using multimedia models (Müller-Herold et al. 1996, 1997) the weights were derived this way. This approach has the advantage that (1) transport processes do not have to be included in the model, and (2) the calculated persistence is independent of the way the chemical is introduced into the environment. Its limitation is that it is only valid for chemicals for which degradation occurs more slowly than intermedia transport, whereas many organic chemicals have atmospheric degradation half-lives which are shorter than relevant transport processes. A persistence estimation based on equilibrium partitioning may thus severely underestimate the real environmental half-life of a chemical by assuming partitioning into a phase with high degradation half-life, which the chemical cannot reach because of significant intermedia transfer resistances (Wania, 1998a).

Approaches Based on a Steady-State Distribution

The steady-state approach to estimate the distribution in a multimedia environment allows for deviation from equilibrium, yet assumes that the rates of chemical input and loss are equal at all points in time. This is the Level III approach. A steady-state distribution is governed by equilibrium partitioning, intermedia transfer rates and the mode of entry. Webster et al. (1998) assessed an overall chemical persistence using an existing steady-state multimedia model, the generic multimedia model by Mackay et al. (1992), and found the calculated overall reaction time to be clearly dependent on physical-chemical properties and the selected emission scenario, i.e. it is important into which media discharge is assumed to occur. Bennett et al. (1999) calculated and compared an overall persistence for several chemicals using equilibrium, steady-state and transient or dynamic distributions. They concluded that a persistence “based on the steady-state distribution in the environment closely approximates the dynamic

characteristic time for a range of chemicals and can be used in decisions regarding chemical use in the environment". Fenner et al. (2000) recently showed that scenarios involving a steady-state assumption and a pulse release gave the same media distribution, and thus yielded equivalent estimates for persistence and spatial range.

Number and Nature of Compartments

Multimedia models have variable numbers and types of compartments ranging from two to more than a hundred. Several investigators suggest that the minimum number of compartments for a model aimed at estimating an overall persistence is three, namely air, water and soil (Müller-Herold, 1996, Müller-Herold et al., 1997, Wania, 1998a, Bennett et al., 1999, Scheringer, 1996). Webster et al. (1998)'s approach relied on an established model which additionally includes a sediment compartment. In Scheringer's model (Scheringer, 1996), the basic three-compartment block is multiplied to additionally provide the possibility to assess a spatial range parameter (see below).

Loss Processes Other than Degradation

Transfer of chemical to the outside of the modeled region, e.g. by atmospheric transport, does not contribute to the reduction of persistence in the environment. For this reason the multimedia models used in the assessment of overall persistence usually do not include advective transport processes that only contribute to a redistribution of chemical within the environment. Existing models can easily be modified in this respect (Webster et al. 1998). It could be argued that loss processes other than degradation that lead to a permanent and irreversible removal from the biosphere should be included in the estimation of overall persistence to avoid unrealistically high overall persistence values for very slowly degraded chemicals (Wania, 1998a). Examples are the loss to the stratosphere, irreversible sorption to soil solids, transfer to the deep oceans, and burial in deep sediments. This issue remains a topic of debate.

Influence of Environmental Variability on Environmental Persistence

Environmental persistence is dependent on environmental properties, especially climate. Simple approaches as described above rely on the use of a "typical" environment, as reflected in the selected environmental parameters (i.e. parameters used to describe the dimensions and composition of the compartments, as well as those describing intermedia transport). These typical environments tend to reflect temperate climatic conditions, because that is where most of the knowledge and understanding of chemical fate and behavior has been gained. The shortcoming of this approach is that chemicals may behave quite differently in other climatic or zonal circumstances. An example that has gained prominence is the increased persistence of chemicals in the Arctic environment. Similarly, chemicals can be expected to behave quite differently in subtropical deserts or tropical rain forests. This could be addressed by a variety of approaches:

Approaches Using Regional Environments

It is possible to adapt the evaluative models to a variety of regional conditions by adjusting the environmental input parameters. For example, the overall persistence could be estimated using the same model and different temperature conditions or dimensions of the compartments. The regionalisation of multi-media models for assessing persistence and LRT potential was proposed and discussed in more detail during a recent UNEP workshop on a regionally based assessment of persistent toxic chemicals in Geneva (UNEP, 1999).

Approaches that Describe the Entire Global Environment

Another option is to describe the entire global environment in a model that accounts for the zonal variability of persistence. Such a model has been developed by Wania and Mackay (1993, 1995). Klein (1999) developed a steady-state version of that model with the objective of explicitly estimating global persistence values. Using a variety of hypothetical emission scenarios, he found a strong dependence of the calculated overall persistence on the zones and compartments of chemical release. Wania et al. (1999), using the original non-steady state global distribution model and historic emission estimate, calculated overall persistence for α -HCH. These calculations revealed the temporal variability of the overall global persistence, both on a seasonal and a long term time scale.

Any approach taking into account environmental variability suffers from two problems.

- There is a lack of basic and especially quantitative understanding of chemical behavior in conditions other than temperate climatic conditions. For example, it is not at all clear how degradation rates and intermedia transfer rates are influenced by zonal environmental conditions.
- There are greatly enhanced data requirements, in particular environmental parameters, and global emission scenarios.

Approaches Using Multimedia Models in the Evaluation of LRT potential

Multimedia model based approaches for assessing the potential of a chemical to undergo long range transport, usually take the form of calculating a chemical's characteristic distance or spatial range. A chemical with a large spatial range has high LRT potential. Often it is assumed that long range transport occurs only in the atmosphere. It is increasingly obvious, however, that water can be a medium of long range transport for some chemicals, both in the form of rivers and ocean currents. In some cases LRT by migrating organisms can be of importance by "focusing" the contaminant to a vulnerable receptor (Wania, 1998c).

Van Pul et al. (1998) suggested the calculation of a spatial range in air using a one-compartmental modelling approach for the atmosphere, avoiding the need to describe surface compartments by using net deposition velocities. Using a multimedia approach, Bennett et al. (1998) calculated a travel distance in air using a model involving a Lagrangian cell of air passing over a stationary soil/plant surface in a one dimensional system, such that the stationary terrestrial phase in contact with the air cell is at steady-state with respect to the air concentration. Beyer et al. (2000) extended these studies and showed that existing multimedia models, such as the EQC-model (Mackay et al., 1996), can be used directly to calculate travel distances in air and water. If emission is assumed to occur into a mobile phase, the travel distance in that mobile phase M can be calculated using:

$$L_M = \frac{u \cdot M_M}{N_{R_{tot}}} = \frac{u}{\sum_i^n \frac{M_i}{M_M} \cdot k_i} = \frac{u}{k_{eff}}$$

where u is the advective velocity of the mobile phase, M_M is the amount in the mobile phase and $N_{R_{tot}}$ and k_i are defined as above. This equation does not apply if emission occurs to a medium other than the mobile phase or to more than just the mobile phase. The denominator in above equation has been termed an effective loss rate constant, k_{eff} (Bennett et al. 1998). In the case of emissions into the mobile phase only, spatial range and overall persistence are then related with this simple relationship:

$$L_M = u \cdot \frac{M_M}{M_{\text{tot}}} \cdot \tau$$

The travel distance is an expression of how far the chemical can be transported within the average life-time τ it has available for transport. This is controlled by the speed of phase movement u and the fraction of the chemical in the transport medium M_M/M_{tot} . As is the case in the overall persistence calculation, a multimedia model can be used to derive these compartmental mass fractions.

Scheringer (1996, 1997) employed a somewhat different approach to derive a spatial range, based on a circular multimedia model involving many interconnected three compartment units. For each of the three compartments a spatial range can be calculated from the spatial distribution among the various units. The rationale is that on the global scale chemical dispersion is more appropriately described with a macrodiffusive approach than the one-dimensional advective approach described above. This latter approach is more suited for describing atmospheric transport on a smaller scale. A more thorough discussion of this issue and a comparison of advective and diffusive model types can be found in Scheringer et al. (2000).

A similar macrodiffusive approach is adopted in the global distribution model by Wania and Mackay (1995) or the steady-state version of that model by Klein (1999). Such models could be used to assess the LRT potential of organic chemicals, e.g. by computing the fraction of chemical emitted into the global environment in a certain way that reaches the Arctic model compartment (Wania, 1998b).

Much of what is discussed above concerning various approaches to derive mass proportions based on equilibrium and steady-state distributions, the number and types of compartments and the influence of environmental variability applies equally to the assessment of spatial range.

Approaches to reduce input data requirements for the multimedia model based evaluation.

The approaches discussed require usually a minimum of chemical specific-data, namely (1) degradation rates in each of the various model compartments, and (2) physical-chemical partitioning data (vapor pressure, solubility in water and solubility in organic matter or octanol; alternatively the air-water and the octanol-water partition coefficient). If the mass proportions are to be calculated using a non-equilibrium distribution, information is also needed on the mode of entry into the environment for the assessment of overall persistence. For some chemicals, this information, in particular the media-specific degradation half-lives and the mode-of-entry may not be readily obtained. For this reason several suggestions have been made to reduce the input data requirement in the assessment.

One such method suggests identifying those chemicals among the large population of substances to be screened which, based on their physical-chemical properties, will partition almost exclusively into a single environmental medium. This identification could be based on compartmental distributions calculated using multimedia models. No actual modeling is required if tables or graphs are used to display which combination of physical-chemical properties results in single-media distributions (Gouin et al., 2000). If, for such chemicals, the degradation half-life in the medium of predominance is lower than the critical threshold for the overall persistence, the chemical could be classified as non-persistent without information on the degradation rate in the remaining compartments. It is possible to devise a simple graphical method by which a

chemical is located on one or more two-dimensional surfaces, and a decision made on the basis of location (Gouin et al., 2000).

An intriguing approach suggested by Bennet et al. (2000a and b) is to run a number of chemicals through a multimedia model and determine their persistence. A Classification and Regression Tree (CART) analysis is then done to identify the key input properties which can control persistence in the form of a decision tree. The tree can be used for other chemicals not in the “training set”. There may be errors in the evaluation but they are predictable in magnitude.

Another approach which reduces the number of required input parameters has been suggested by Pennington (1999b). It consists of several guidelines which determine the pertinence of a degradation half-life in the calculation of overall persistence. These guidelines are based on either mass fractions estimated using an equilibrium model, thus resembling the approach by Gouin et al., 2000), or directly on the underlying partition coefficients, most notably the Henry's law constant. The error associated with eliminating the use of a particular degradation half-life relative to using all degradation data can be estimated. This so-called heuristic approach was included in the model comparison to follow.

It seems likely that for initial screening purposes, simple computer software can be developed which will accept the minimal data input and rapidly produce a result. It is clear that increasing effort is being devoted to the evaluation of persistence and long range transport potential by a number of groups worldwide. This is viewed as a healthy situation since it is likely that one or more approaches will emerge as the most economic and reliable. The emergence of such an approach will be facilitated by regular comparison of approaches. It would be regrettable if a number of competing and different national approaches were to develop since this could impede international regulatory harmonization.

It is likely that a tiered approach will emerge in which there are increasing demands for more accurate data and the use of more complex models as the chemical is increasingly scrutinized for having potentially problematic persistence and long range transport characteristics. Each tier may have its own procedure or model.

Regardless of the final outcome there is a compelling case that the procedure be totally transparent and that the model(s) used be based on the latest scientific understanding of chemical behaviour in the environment. Given the complexity of the environment, and the extreme variability in chemical properties, it seems inevitable that mass balance models of some form will be used to support the decision process.

Selection of Chemicals and Chemical Properties for the Model Comparison

A set of property profiles for 26 chemicals, listed in Table 1, was made available to participants interested in the model comparison. These data were taken from the compilation of physical-chemical property and environmental fate data by Mackay et al. (1992-98). Given are the octanol-water partition coefficient K_{OW} , the vapour pressure p_L in Pascals and the solubility in water C_L in mol/m^3 . The latter two properties refer to the liquid or supercooled liquid state. The data compilation also lists air-water partition coefficients K_{AW} and H in $\text{Pa}\cdot\text{m}^3/\text{mol}$, which were derived from p_L and C_L , and octanol-air-partition coefficients K_{OA} , which were calculated from K_{OW} and K_{AW} . Finally, first order degradation half-lives in air, water, soil and sediment are supplied in units of hours.

The 26 chemicals span an enormous range of physical-chemical properties. Vapour pressure ranges over ten, solubility in water over eight, and K_{OW} over six orders of magnitude. Chemicals with extreme partitioning behaviour within this set are:

- 1,3-butadiene, which is very volatile and thus has a very low K_{OA} and a very high K_{AW} .
- Benzo[k]fluoranthene, which is very involatile and thus has a very high K_{OA} .
- 2,3,7,8-TetraCDD, which is very sparingly soluble in water and thus has a very high K_{OW} .
- Dalapon, which is relatively involatile and has a very high water solubility. It thus has an extremely low K_{AW} and a very high K_{OA} .

Degradation half lives in air range from 5 hours to 2 years, and in water from 170 to 55000 hours. In soil and sediments the range is 550 to 550000 hours. 550000 hours or 6.3 years is the longest degradation half life assigned to a chemical by Mackay et al. (1992-1998). Whereas hexachlorobenzene is the chemical with the highest degradation half-lives, those of 1,3-butadiene and styrene are the shortest.

Whether these chemical properties are reasonable or even “correct”, is of relatively little importance to this model comparison. It could have been conducted with entirely hypothetical chemical property combinations. The advantage of using real chemicals is that it allows a judgement on the reasonability of a chemical being labelled as persistent and having LRT potential based on knowledge of the observed environmental behaviour of these chemicals. For example, independent of the regulatory context no environmental chemists would seriously doubt that HCHs are subject to long range transport, and PCBs are persistent.

A word of caution is in order at this point. All models participating in this comparison rely in one form or the other on empirical relationships that relate chemical partitioning between water or air and various environmental phases – most notably the organic phases found in aerosols, soils, sediments and suspended solids – with that between water or air and n-octanol (Karickhoff, 1981; Seth et al., 1999; Finizio et al., 1997). Some models use similar empirical relationships with a chemical's vapour pressure to describe partitioning into aerosols (Pankow, 1987). These empirical relationships tend to be derived from chemical data sets which span much smaller ranges of physical-chemical properties than those of our test data set. Specifically, the observational datasets tend to be biased towards less polar chemicals, reflecting the chemical characteristics of the most troublesome, highly bioaccumulative organic pollutants. For example, the widely used Junge-Pankow relationship to describe partitioning on to aerosols is almost exclusively based on observations involving polycyclic aromatic hydrocarbons and chlorinated hydrocarbons.

It should thus be kept in mind that there may be significant limitations in the applicability of the models to organic chemicals with physical-chemical characteristics different from those chemicals which were used to derive the empirical partitioning relationships. In the context of identifying persistent organic pollutants this limitation may be acceptable, because the models are likely to be most appropriate for those type of chemicals the model-based screening process is intended to identify.

Comparison of Overall Persistence Values

Models Included in the Comparison of Overall Persistence

Results from twelve models were included in the comparison of estimated overall persistence. Some research groups used several different models, or modifications of the same model, to derive overall persistence values. Four letter acronyms are used to identify these models.

1. **SCHE**: The circular model as developed and described by Scheringer (1996; 1997).
2. **HELD**: A three dimensional version of the SCHE-model developed by Held (2000). In that model the ring of the SCHE-model is replaced by a sphere, which makes the approach somewhat more realistic.
3. **BENN**: The three-compartment (air, water, soil) multimedia model described in Bennett et al. (1999).

PENX: Two models were used by Pennington (1999a):

4. **PEN1** a standard steady-state multi-media model with four compartments (air, water, soil, sediment) and no advective removal derived from the EQC model by Mackay et al. (1996), but formulated in terms of concentration. This model has been used by the US Environmental Protection Agency and is described in Pennington and Ralston (1999).
5. **PEN2** a heuristic-based approach, which enables the identification of key degradation parameters using physical-chemical properties and results in a reduction of required data by about 50% (Pennington, 1999b).

WANX: The persistence criterion model by Wania (1998a), which is a level III fugacity model with three compartments (air, water, soil).

6. **WAN1** includes advective loss processes on a global scale, whereas
7. **WAN2** does not include advection.
8. **TAPL**: The TAPL3 model by Mackay and co-workers (Webster et al., 1998; Beyer et al., 2000), which in turn is based on the generic model (Mackay et al., 1992).

VDMX: van de Meent et al. (1999) used four approaches to calculate overall persistence based on various modifications of the SIMPLEBOX models (Brandes et al., 1996; van de Meent, 1993), namely:

9. **VDM1**: nested two-scale model; SimpleBox 2.1 with regional, arctic and tropic scales set to negligible small dimensions, continental scale set to regional dimensions (200 km^2), global scale set to N-hemispheric dimensions ($255 \cdot 10^6 \text{ km}^2$), advection between inner and outer scale. Emissions to inner scale only.
10. **VDM2**: nested multi-scale model; SimpleBox 2.1 at standard settings. Emissions to regional scale.
11. **VDM3**: closed "unit world" model; SimpleBox 1.1 with global dimensions ($5 \cdot 10^8 \text{ km}^2$, 70 % water, 1000 m water depth, no advection)
12. **VDM4**: closed "regional" model; SimpleBox 1.1. with regional dimensions (37975 km^2 , 12.5 % water, 3 m water depth, no advection)

It should be noted that all models are quite similar. Essentially all are tracing their origin to the multimedia modelling approach by Mackay (1991) and are using very similar, if not identical

expressions to describe environmental partitioning, interphase transfer and degradation (Cowan et al. 1994). Foremost among the similarities is that all participating models were level III, i.e. assumed a steady-state, non-equilibrium distribution of the chemical in the environment. This probably reflects an emerging consensus among multimedia modelling groups that this level of model complexity is both necessary and sufficient to derive reasonable estimates of overall persistence in a multimedia environment. This was also concluded from studies by Wania (1998a) and Bennett et al. (1999).

The most notable differences between the models are due to:

- a variable number of environmental phases, specifically whether a sediment compartment is deemed necessary or not,
- the size of the environment being described by the model (global vs. regional), and
- the complexity of the model structure (unit world type approaches ignoring spatial variability vs. approaches that allow for some form of variability (SCHE, VDMX).

It is well established, that in level III-based assessments of overall persistence, the “mode-of-entry”, i.e. the way the chemicals is discharged into the multimedia environment is of vital importance (Webster et al., 1998, Scheringer et al., 2000). Four emission scenarios or “mode-of-entries” were considered: (1) emission into air only, (2) emission into water only, (3) emission into soil only, and (4) emission into air, water and soil in equal proportions. However, not all models were used for all emission scenarios.

Table 1 Chemical property values used in the model comparison

Name	MW g/mol	P _L Pa	C _L Mol/m ³	log K _{OW}	H Pa·m ³ /mol	log K _{AW}	log K _{OA}	HL _{air} hours	HL _{water} hours	HL _{soil} hours	HL _{sediment} hours
benzene	78.11	12700	22.788	2.13	557	-0.65	2.78	17	170	550	1700
hexachlorobenzene	284.8	0.2447	0.00187	5.5	131	-1.28	6.78	17000	55000	55000	55000
2,3,7,8-TetraCDD	322	0.000118	3.52E-05	6.8	3.337	-2.87	9.67	170	550	17000	55000
1,3-butadiene	54.09	281000	13.5885	1.99	20679	0.92	1.07	5	170	550	1700
styrene	104.14	800	2.8807	3.05	305.48	-0.91	3.96	5	170	550	1700
toluene	92.13	3800	5.59	2.69	680	-0.56	3.25	17	550	1700	5500
acenaphthylene	150.2	4.14	0.49297	4	8.4	-2.47	6.47	55	550	5500	17000
pyrene	202.3	0.0119	0.01289	5.18	0.92	-3.43	8.61	170	1700	17000	55000
fluoranthene	202.3	0.00872	0.00841	5.22	1.037	-3.38	8.60	170	1700	17000	55000
chrysene	228.3	0.000107	0.001649	5.86	0.065	-4.58	10.44	170	1700	17000	55000
benz[a]anthracene	228.3	0.000606	0.001045	5.91	0.581	-3.63	9.54	170	1700	17000	55000
benzo[a]pyrene	252.3	2.13E-05	0.000459	6.04	0.046	-4.73	10.77	170	1700	17000	55000
perylene	252.32	4.36E-06	0.000493	6.25	0.003	-5.92	12.17	170	1700	17000	55000
benzo[k]fluoranthene	252.32	4.12E-06	0.000252	6	0.016	-5.19	11.19	170	1700	17000	55000
pentachlorophenol	266.34	0.12	1.565	5.05	0.079	-4.50	9.55	550	550	1700	5500
diethylphthalate (DEP)	222.26	0.05	4.859	2.47	0.01	-5.39	7.86	170	170	550	1700
dibutylphthalate (DBP)	278.35	0.002	0.04	4.72	0.05	-4.70	9.42	55	170	550	1700
carbon tetrachloride (CCl ₄)	153.82	15250	5.2	2.64	2932	0.07	2.57	17000	1700	5500	17000
Aldrin	364.93	0.0302	0.000331	3.01	91.23	-1.43	4.44	5	17000	17000	55000
Chlordane	409.8	0.0029	0.000869	6	0.302	-3.91	9.91	55	17000	17000	55000
γ-HCH (lindane)	290.85	0.0274	0.184	3.7	0.149	-4.22	7.92	170	17000	17000	55000
Heptachlor	373.4	0.267	0.000756	5.27	353.4	-0.85	6.12	55	550	1700	5500
Methoxychlor	345.7	0.000546	0.000547	5.08	0.999	-3.39	8.47	17	170	1700	5500
Atrazine	215.68	0.00119	4.14	2.75	2.88E-04	-6.93	9.68	5	17000	1700	1700
Dalapon	143	0.00001	3510	0.78	2.85E-09	-11.94	12.72	550	1700	1700	1700
α-HCH	290.85	0.1	0.115	3.81	0.870	-3.45	7.26	170	17000	17000	55000

Results of the Comparison of Overall Persistence Values

The results of the model calculations are shown in a series of 20 tables:

Four tables show the calculated **overall persistence values** calculated by the various models for the 26 chemicals assuming various modes of entry:

Table 2: emission to the atmosphere only.

Table 7: emission to the water only.

Table 12: emission to the soil only.

Table 17: emission to the atmosphere, water and soil in equal proportions.

These tables also contain the arithmetic and geometric mean, the median, the minimum, the maximum and various percentiles of the persistence values calculated by one model for the 26 chemicals.

Four tables show the **correlation coefficients between the results for overall persistence** of the various models.

Table 3: emission to the atmosphere only.

Table 8: emission to the water only.

Table 13: emission to the soil only.

Table 18: emission to the atmosphere, water and soil in equal proportions.

The persistence values calculated for the 26 chemicals by each model have been ranked and each chemical assigned a rank between 1 and 26 (1: most persistent chemical, 26: least persistent chemical). Four tables show these **persistence rankings** for all models:

Table 4: emission to the atmosphere only.

Table 9: emission to the water only.

Table 14: emission to the soil only.

Table 19: emission to the atmosphere, water and soil in equal proportions.

Again, the **correlation among the rankings** calculated by various models is shown in additional tables:

Table 5: emission to the atmosphere only.

Table 10: emission to the water only.

Table 15: emission to the soil only.

Table 20: emission to the atmosphere, water and soil in equal proportions.

For each mode of entry, a number of **statistical parameters**, namely the maximum, the minimum, the ratio between maximum and minimum, the geometric mean, the median, and the average (i.e. arithmetic mean) and standard deviation (absolute and as percent of average) of the overall persistence values calculated for one chemical were determined and are listed in four tables:

Table 6: emission to the atmosphere only.

Table 11: emission to the water only.

Table 16: emission to the soil only.

Table 21: emission to the atmosphere, water and soil in equal proportions.

Similarly, the maximum, minimum, range, geometric mean, median and arithmetic mean of the rankings calculated for each of the chemical are included in these tables.

Table 2 Overall persistence in hours as calculated by various models for 26 chemicals assuming emission to air.

Model	SCHE	HELD	BENN	TAPL	WAN1	WAN2	PEN1	PEN2	VDM1	VDM2	VDM3	VDM4
benzene	1.0	1.0	1.0	1.5	1.0	1.0	0.7	0.7	1.1	1.1	1.1	1.0
HCB	1057	1056	1246	3516	1182	1239	1505	2140	2951	2987	3111	1967
2,3,7,8-TCDD	12	12	51	1390	234	235	611	897	424	577	373	893
1,3-butadiene	0.3	0.3	0.3	0.4	0.3	0.3	0.2	0.2	0.3	0.3	0.3	0.3
styrene	0.3	0.3	0.3	0.4	0.3	0.3	0.2	0.2	0.3	0.3	0.4	0.3
toluene	1.0	1.0	1.0	1.5	1.0	1.0	0.7	0.7	1.2	1.1	1.3	1.0
acenaphthylene	3.7	3.7	4.0	9.4	3.7	3.7	3.7	3.8	8.7	9.6	17	5.6
pyrene	19	19	35	460	54	54	145	212	103	151	103	362
fluoranthene	19	19	37	494	52	52	156	229	113	163	105	366
chrysene	61	61	69	1444	454	460	642	1014	460	609	307	944
B[a]A	22	22	58	1235	206	207	484	879	326	472	221	782
B[a]P	76	76	100	1507	497	504	689	1195	516	693	394	976
perylene	286	283	279	1540	542	551	715	1588	542	757	471	992
B[k]F	146	146	150	1510	528	537	695	1169	524	693	403	983
PCP	38	38	45	132	68	68	58	104	35	44	40	132
DEP	13	13	13	40	19	19	19	332	20	19	14	25
DBP	3.8	3.8	4.1	22.7	5.1	5.1	8.0	11.6	8.7	10.0	8.4	14.0
CCl ₄	1014	1014	1014	1443	979	1019	698	710	530	461	440	1015
aldrin	0.3	0.3	0.3	0.7	0.3	0.3	0.3	0.3	152	37.8	4.6	0.4
chlordane	24	25	18	428	133	133	186	2191	352	450	634	190
γ-HCH	108	110	79	755	59	59	263	272	686	688	753	340
heptachlor	3.3	3.3	3.5	5.7	3.4	3.4	2.5	3.4	6.0	5.9	5.2	3.8
methoxychlor	1.1	1.1	1.2	29.9	1.4	1.4	8.7	10.7	11.0	10.8	5.0	11.9
atrazine	392	398	355	374	46	46	153	1325	502	514	624	145
dalapon	102	102	102	147	100	102	71	108	86	86	93	76
α-HCH	38	39	32	270	21	21	88	91	584	578	707	97
average	132	133	142	645	200	205	277	557	344	385	340	397
geomean	17	17	19	95	27	28	39	68	63	68	53	58
maximum	1057	1056	1246	3516	1182	1239	1505	2191	2951	2987	3111	1967
95 percentile	859	860	849	1533	870	902	711	2002	660	741	741	1009
75 percentile	96	96	95	1351	227	228	579	985	513	577	431	865
median	21	21	36	322	53	53	117	221	132	157	104	138
25 percentile	3.4	3.4	3.6	12.7	3.4	3.4	4.7	5.6	9.3	10.2	6.0	7.2
5 percentile	0.3	0.3	0.3	0.5	0.3	0.3	0.2	0.2	0.5	0.5	0.6	0.3
minimum	0.3	0.3	0.3	0.4	0.3	0.3	0.2	0.2	0.3	0.3	0.3	0.3

Table 3 Correlation between the calculated overall persistence values listed in Table 2

	SCHE	HELD	BENN	TAPL	WAN1	WAN2	PEN1	PEN2	VMD1	VDM2	VDM3	VDM4
SCHE	1	1	0.99	0.70	0.86	0.86	0.72	0.52	0.76	0.72	0.73	0.69
HELD	1	1	0.99	0.70	0.86	0.86	0.72	0.52	0.76	0.72	0.73	0.68
BENN	0.99	0.99	1	0.75	0.88	0.88	0.76	0.53	0.80	0.77	0.78	0.73
TAPL	0.70	0.70	0.75	1	0.91	0.91	1	0.76	0.87	0.91	0.80	0.99
WAN1	0.86	0.86	0.88	0.91	1	1	0.93	0.68	0.78	0.80	0.71	0.92
WAN2	0.86	0.86	0.88	0.91	1	1	0.93	0.67	0.78	0.80	0.72	0.92
PEN1	0.72	0.72	0.76	1	0.93	0.93	1	0.77	0.85	0.89	0.78	0.99
PEN2	0.52	0.52	0.53	0.76	0.68	0.67	0.77	1	0.67	0.73	0.67	0.73
VMD1	0.76	0.76	0.80	0.87	0.78	0.78	0.85	0.67	1	0.99	0.99	0.80
VDM2	0.72	0.72	0.77	0.91	0.80	0.80	0.89	0.73	0.99	1	0.97	0.85
VDM3	0.73	0.73	0.78	0.80	0.71	0.72	0.78	0.67	0.99	0.97	1	0.73
VDM4	0.69	0.68	0.73	0.99	0.92	0.92	0.99	0.73	0.80	0.85	0.73	1
average	0.80	0.79	0.82	0.86	0.86	0.86	0.86	0.69	0.84	0.84	0.80	0.84

Table 4 Overall persistence rank among the 26 chemical as calculated by various models assuming emission to air.

Model	SCHE	HELD	BENN	TAPL	WAN1	WAN2	PEN1	PEN2	VDM1	VDM2	VDM3	VDM4
benzene	23	23	23	23	23	23	23	23	24	24	24	23
HCB	1	1	1	1	1	1	1	2	1	1	1	1
2,3,7,8-TCDD	17	17	11	7	7	7	7	8	10	8	10	7
1,3-butadiene	26	26	26	26	26	26	26	26	26	26	26	26
styrene	25	25	25	25	25	25	25	25	25	25	25	25
toluene	22	22	22	22	22	22	22	22	23	23	23	22
acenaphthylene	19	19	19	20	19	19	20	20	21	21	17	20
pyrene	14	14	14	11	13	13	13	14	15	14	14	10
fluoranthene	15	15	13	10	14	14	11	13	14	13	13	9
chrysene	9	9	9	5	6	6	6	7	9	6	11	6
B[a]A	13	13	10	8	8	8	8	9	12	10	12	8
B[a]P	8	8	7	4	5	5	5	5	7	3	9	5
perylene	4	4	4	2	3	3	2	3	4	2	6	3
B[k]F	5	5	5	3	4	4	4	6	6	4	8	4
PCP	11	11	12	16	11	11	16	16	17	16	16	14
DEP	16	16	17	17	17	17	17	11	18	18	18	17
DBP	18	18	18	19	18	18	19	18	20	20	19	18
CCl ₄	2	2	2	6	2	2	3	10	5	11	7	2
aldrin	24	24	24	24	24	24	24	24	13	17	22	24
chlordane	12	12	16	12	9	9	10	1	11	12	4	12
γ-HCH	6	6	8	9	12	12	9	12	2	5	2	11
heptachlor	20	20	20	21	20	20	21	21	22	22	20	21
methoxychlor	21	21	21	18	21	21	18	19	19	19	21	19
atrazine	3	3	3	13	15	15	12	4	8	9	5	13
dalapon	7	7	6	15	10	10	14	17	16	15	15	16
α-HCH	10	10	15	14	16	16	15	15	3	7	3	15

Table 5 Correlation between the calculated overall persistence rankings listed in Table 4

	SCHE	HELD	BENN	TAPL	WAN1	PEN1	PEN2	VMD1	VDM2	VDM3	VDM4
SCHE	1	1	0.97	0.85	0.87	0.87	0.82	0.86	0.86	0.89	0.85
HELD	1	1	0.97	0.85	0.87	0.87	0.82	0.86	0.86	0.89	0.85
BENN	0.97	0.97	1	0.89	0.91	0.91	0.83	0.82	0.86	0.83	0.90
TAPL	0.85	0.85	0.89	1	0.96	0.99	0.90	0.86	0.94	0.84	0.99
WAN1	0.87	0.87	0.91	0.96	1	0.97	0.87	0.80	0.87	0.80	0.97
PEN1	0.87	0.87	0.91	0.99	0.97	1	0.91	0.86	0.92	0.86	0.99
PEN2	0.82	0.82	0.83	0.90	0.87	0.91	1	0.80	0.87	0.86	0.88
VMD1	0.86	0.86	0.82	0.86	0.80	0.86	0.80	1	0.96	0.94	0.83
VDM2	0.86	0.86	0.86	0.94	0.87	0.92	0.87	0.96	1	0.91	0.90
VDM3	0.89	0.89	0.83	0.84	0.80	0.86	0.86	0.94	0.91	1	0.82
VDM4	0.85	0.85	0.90	0.99	0.97	0.99	0.88	0.83	0.90	0.82	1
average	0.89	0.89	0.90	0.91	0.90	0.92	0.87	0.87	0.90	0.88	0.91

Table 6 Summary statistics on the overall persistence comparison assuming emission to air

ID	absolute value								rank					
	max	min	max/min	geomean	median	average	stdev	%stdev	max	min	range	geomean	median	average
benzene	1.5	0.7	2	1.0	1.0	1.0	0.2	19	24	23	1	23.2	23.0	23.3
HCB	3516	1056	3	1811	1736	1996	918	46	2	1	1	1.1	1.0	1.1
2,3,7,8-TCDD	1390	12	112	234	399	476	422	89	17	7	10	9.1	8.0	9.7
1,3-butadiene	0.4	0.2	2	0.3	0.3	0.3	0.1	19	26	26	0	26.0	26.0	26.0
styrene	0.4	0.2	2	0.3	0.3	0.3	0.1	20	25	25	0	25.0	25.0	25.0
Toluene	1.5	0.7	2	1.0	1.0	1.1	0.2	20	23	22	1	22.2	22.0	22.3
acenaphthylene	17	3.7	5	5.5	3.9	6.3	4.0	63	21	17	4	19.5	19.5	19.5
pyrene	460	19	24	91	103	143	140	98	15	10	5	13.2	14.0	13.3
Fluoranthene	494	19	26	93	109	150	148	99	15	9	6	12.7	13.0	12.8
chrysene	1444	61	24	356	460	544	424	78	11	5	6	7.2	6.5	7.4
B[a]A	1235	22	57	225	273	410	381	93	13	8	5	9.7	9.5	9.9
B[a]P	1507	76	20	413	510	602	448	74	9	3	6	5.7	5.0	5.9
Perylene	1588	279	6	602	547	712	450	63	6	2	4	3.2	3.0	3.3
B[k]F	1510	146	10	483	532	624	424	68	8	3	5	4.7	4.5	4.8
PCP	132	35	4	59	52	67	36	54	17	11	6	13.7	15.0	13.9
DEP	332	13	25	23	19	45	91	199	18	11	7	16.5	17.0	16.6
DBP	23	3.8	6	7.5	8.2	8.8	5.5	62	20	18	2	18.6	18.0	18.6
CCl ₄	1443	440	3	811	996	861	297	34	11	2	9	3.6	2.5	4.5
aldrin	152	0.3	533	1.0	0.3	16	44	267	24	13	11	22.0	24.0	22.3
chlordane	2191	18	121	171	188	397	598	151	16	1	15	8.5	11.5	10.0
γ-HCH	755	59	13	229	267	348	290	83	12	2	10	6.7	8.5	7.8
heptachlor	6.0	2.5	2	4.0	3.4	4.1	1.2	29	22	20	2	20.7	20.5	20.7
methoxychlor	30	1.1	26	4.5	6.9	7.9	8.3	106	21	18	3	19.8	20.0	19.8
atrazine	1325	46	29	278	383	406	345	85	15	3	12	7.1	8.5	8.6
dalapon	147	71	2	96	101	98	19	20	17	6	11	11.6	14.5	12.3
α-HCH	707	21	34	100	89	214	258	120	16	3	13	10.1	14.5	11.6

Table 7 Overall persistence in hours as calculated by various models for 26 chemicals assuming emission to water.

Model	BENN	TAPL	WAN1	WAN2	PEN1	PEN2	VDM1	VDM2	VDM3	VDM4
benzene	6.4	8.7	9.4	9.4	4.7	13	2.2	2.2	9.8	1.6
HCB	1263	3678	1659	3249	1627	2802	2774	2780	3156	1984
2,3,7,8-TCDD	35	2680	33	33	1255	4401	1334	1366	339	2124
1,3-butadiene	6.4	8.0	8.8	8.8	4.5	12	1.3	1.3	9.8	0.9
styrene	6.7	8.5	8.9	8.9	4.7	13	1.8	1.9	9.8	1.1
toluene	12	14	26	26	8.4	13	2.7	2.8	29	1.8
acenaphthylene	27	47	32	32	23	29	20	33	33	14
pyrene	98	1398	99	102	623	1266	694	842	126	937
fluoranthene	97	1467	99	102	654	1358	784	865	128	941
chrysene	102	2980	99	102	1381	5399	1508	1425	214	2144
B[a]A	99	3004	99	102	1394	5465	1441	1413	227	1957
B[a]P	102	3260	99	102	1524	7092	1555	1491	270	2210
perylene	102	3508	99	102	1651	9262	1586	1546	367	2262
B[k]F	102	3207	99	102	1496	6728	1551	1479	255	2209
PCP	33	146	33	33	60	359	113	191	36	222
DEP	10	15	10	10	7.1	7.2	11	11	10	11
DBP	10	24	10	10	10	81	54	44	11	44
CCl ₄	894	1310	101	104	609	722	521	454	205	1008
aldrin	56	24	71	72	15	15	1012	58	246	2
chlordane	932	3791	765	1007	2160	46949	1461	1605	1626	1456
γ-HCH	958	1454	793	1013	680	744	1061	1030	1022	598
heptachlor	19	75	30	31	36	352	103	77	34	27
methoxychlor	10	55	10	10	22	117	145	118	11	110
atrazine	1022	1352	798	1022	659	721	888	980	1020	615
dalapon	102	147	99	102	71	71	102	102	102	102
α-HCH	730	769	769	975	358	390	857	866	994	175
average	263	1324	229	326	628	3630	753	722	404	814
geomean	70	294	70	75	142	382	194	178	113	137
maximum	1263	3791	1659	3249	2160	46949	2774	2780	3156	2262
95 percentile	1006	3635	797	1020	1645	8719	1578	1590	1475	2210
75 percentile	102	2905	99	102	1350	4001	1414	1402	322	1832
median	97	1039	99	102	484	555	739	648	167	410
25 percentile	13	30	27	27	17	39	66	48	30	18
5 percentile	6.5	8.6	9.0	9.0	4.7	12.1	1.9	2.0	9.8	1.2
minimum	6.4	8.0	8.8	8.8	4.5	7.2	1.3	1.3	9.8	0.9

Table 8 Correlation between the calculated overall persistence values listed in Table 7.

	BENN	TAPL	WAN1	WAN2	PEN1	PEN2	VMD1	VDM2	VDM3	VDM4
BENN	1	0.39	0.89	0.82	0.41	0.31	0.51	0.54	0.84	0.21
TAPL	0.39	1	0.43	0.42	0.99	0.58	0.91	0.95	0.54	0.96
WAN1	0.89	0.43	1	0.98	0.43	0.26	0.62	0.65	0.97	0.24
WAN2	0.82	0.42	0.98	1	0.41	0.20	0.63	0.66	0.98	0.25
PEN1	0.41	0.99	0.43	0.41	1	0.67	0.89	0.92	0.54	0.93
PEN2	0.31	0.58	0.26	0.20	0.67	1	0.40	0.44	0.38	0.41
VMD1	0.51	0.91	0.62	0.63	0.89	0.40	1	0.96	0.71	0.86
VDM2	0.54	0.95	0.65	0.66	0.92	0.44	0.96	1	0.73	0.88
VDM3	0.84	0.54	0.97	0.98	0.54	0.38	0.71	0.73	1	0.36
VDM4	0.21	0.96	0.24	0.25	0.93	0.41	0.86	0.88	0.36	1
average	0.59	0.72	0.65	0.63	0.72	0.46	0.75	0.77	0.70	0.61

Table 9 Overall persistence rank among the 26 chemical as calculated by various models assuming emission to water.

Model	BENN	TAPL	WAN1	WAN2	PEN1	PEN2	VDM1	VDM2	VDM3	VDM4
benzene	25	24	24	24	24	24	24	24	24	24
HCB	1	2	1	1	3	8	1	1	1	6
2,3,7,8-TCDD	16	8	16	16	8	7	8	8	7	5
1,3-butadiene	26	26	26	26	26	25	26	26	26	26
styrene	24	25	25	25	25	22	25	25	25	25
toluene	20	23	20	20	22	23	23	23	20	22
acenaphthylene	18	19	18	18	18	20	21	21	19	20
pyrene	13	11	10	13	12	10	14	13	15	11
fluoranthene	14	9	12	14	11	9	13	12	14	10
chrysene	11	7	9	8	7	6	5	6	12	4
B[a]A	12	6	8	7	6	5	7	7	11	7
B[a]P	10	4	11	9	4	3	3	4	8	2
perylene	8	3	14	11	2	2	2	3	6	1
B[k]F	7	5	13	10	5	4	4	5	9	3
PCP	17	16	17	17	16	15	17	15	17	14
DEP	21	22	21	21	23	26	22	22	23	21
DBP	22	20	22	22	21	18	20	20	22	18
CCl ₄	5	13	6	6	13	12	15	14	13	9
aldrin	15	21	15	15	20	21	10	19	10	23
chlordane	4	1	5	4	1	1	6	2	2	8
γ-HCH	3	10	3	3	9	11	9	9	3	13
heptachlor	19	17	19	19	17	16	18	18	18	19
methoxychlor	23	18	23	23	19	17	16	16	21	16
atrazine	2	12	2	2	10	13	11	10	4	12
dalapon	9	15	7	12	15	19	19	17	16	17
α-HCH	6	14	4	5	14	14	12	11	5	15

Table 10 Correlation between the calculated overall persistence rankings listed in Table 9.

	BENN	TAPL	WAN1	WAN2	PEN1	PEN2	VMD1	VDM2	VDM3	VDM4
BENN	1	0.79	0.96	0.98	0.82	0.70	0.77	0.81	0.91	0.69
TAPL	0.79	1	0.73	0.80	0.99	0.97	0.93	0.98	0.84	0.95
WAN1	0.96	0.73	1	0.98	0.75	0.63	0.70	0.75	0.86	0.62
WAN2	0.98	0.80	0.98	1	0.82	0.71	0.79	0.83	0.91	0.70
PEN1	0.82	0.99	0.75	0.82	1	0.96	0.93	0.98	0.87	0.94
PEN2	0.70	0.97	0.63	0.71	0.96	1	0.90	0.95	0.77	0.95
VMD1	0.77	0.93	0.70	0.79	0.93	0.90	1	0.96	0.88	0.89
VDM2	0.81	0.98	0.75	0.83	0.98	0.95	0.96	1	0.88	0.94
VDM3	0.91	0.84	0.86	0.91	0.87	0.77	0.88	0.88	1	0.73
VDM4	0.69	0.95	0.62	0.70	0.94	0.95	0.89	0.94	0.73	1
average	0.84	0.90	0.80	0.85	0.91	0.85	0.87	0.91	0.87	0.84

Table 11 Summary statistics on the overall persistence comparison assuming emission to water.

ID	absolute value								rank					
	max	min	max/min	geomean	median	average	stdev	%stdev	max	min	range	geomean	median	average
benzene	13	1.6	8	5.5	7.6	6.8	3.9	58	25	24	1	24.1	24.0	24.1
HCB	3678	1263	3	2367	2777	2497	809	32	8	1	7	1.8	1.0	2.5
2,3,7,8-TCDD	4401	33	134	487	1295	1360	1411	104	16	5	11	9.1	8.0	9.9
1,3-butadiene	12	0.9	12	4.5	7.2	6.2	3.9	64	26	25	1	25.9	26.0	25.9
styrene	13	1.1	12	5.0	7.6	6.5	4.0	62	25	22	3	24.6	25.0	24.6
Toluene	29	1.8	16	9.3	12	13	10	76	23	20	3	21.6	22.0	21.6
acenaphthylene	47	14	3	28	30	29	9.0	31	21	18	3	19.2	19.0	19.2
pyrene	1398	98	14	387	659	618	498	81	15	10	5	12.1	12.5	12.2
Fluoranthene	1467	97	15	400	719	649	527	81	14	9	5	11.6	12.0	11.8
chrysene	5399	99	54	685	1403	1535	1678	109	12	4	8	7.1	7.0	7.5
B[a]A	5465	99	55	679	1404	1520	1690	111	12	5	7	7.3	7.0	7.6
B[a]P	7092	99	72	742	1507	1771	2148	121	11	2	9	5.0	4.0	5.8
perylene	9262	99	94	804	1566	2048	2770	135	14	1	13	3.7	3.0	5.2
B[k]F	6728	99	68	730	1488	1723	2046	119	13	3	10	5.9	5.0	6.5
PCP	359	33	11	85	87	123	109	89	17	14	3	16.1	16.5	16.1
DEP	15	7.1	2	10	10	10	2.1	21	26	21	5	22.2	22.0	22.2
DBP	81	10	8	22	18	30	25	83	22	18	4	20.4	20.5	20.5
CCl ₄	1310	101	13	439	565	593	402	68	15	5	10	9.9	12.5	10.6
aldrin	1012	1.7	592	46	57	157	308	196	23	10	13	16.3	17.0	16.9
chlordane	46949	765	61	2082	1533	6175	14352	232	8	1	7	2.6	3.0	3.4
γ-HCH	1454	598	2	907	986	935	246	26	13	3	10	6.2	9.0	7.3
heptachlor	352	19	19	51	35	78	100	127	19	16	3	18.0	18.0	18.0
methoxychlor	145	10	14	35	39	61	55	91	23	16	7	19.0	18.5	19.2
atrazine	1352	615	2	884	934	908	220	24	13	2	11	6.1	10.0	7.8
dalapon	147	71	2	98	102	100	21	21	19	7	12	14.0	15.5	14.6
α-HCH	994	175	6	614	769	688	281	41	15	4	11	8.9	11.5	10.0

Table 12 Overall persistence in hours as calculated by various models for 26 chemicals assuming emission to soil.

Model	BENN	TAPL	WAN1	WAN2	PEN1	PEN2	VDM1	VDM2	VDM3	VDM4
benzene	1.1	5.1	1.6	1.6	2.6	3.0	16	18	10	10
HCB	1289	4581	3028	3304	2191	2280	3300	3301	3293	3262
2,3,7,8-TCDD	986	1476	992	1020	710	718	1022	1022	1012	1023
1,3-butadiene	0.4	0.6	0.3	0.3	0.3	0.3	1.7	1.0	0.6	0.5
styrene	0.4	25	4.0	4.0	12	12	30	31	28	28
toluene	1.1	11	2.6	2.6	5.8	6.2	44	54	28	27
acenaphthylene	44	448	296	299	218	219	327	329	326	328
pyrene	909	1469	987	1015	707	711	1021	1022	1009	1021
fluoranthene	898	1470	988	1016	707	712	1021	1022	1009	1021
chrysene	1000	1479	992	1020	711	724	1022	1022	1011	1023
B[a]A	981	1479	992	1020	710	724	1022	1022	1011	1023
B[a]P	1001	1479	993	1020	711	728	1022	1022	1011	1024
perylene	1002	1480	993	1021	711	732	1022	1022	1013	1024
B[k]F	1002	1479	992	1020	711	727	1022	1022	1011	1024
PCP	102	147	102	102	71	71	102	102	102	102
DEP	31	45	28	29	22	372	33	33	33	33
DBP	33	48	33	33	23	23	33	33	33	33
CCl ₄	1014	1438	665	684	695	711	518	452	437	999
aldrin	1.8	129	13	13	69	69	989	632	354	348
chlordane	1018	1481	994	1022	713	850	1022	1022	1030	1022
γ-HCH	809	1447	985	1019	695	702	1015	1015	1011	1005
heptachlor	46	144	98	98	70	70	102	102	102	102
methoxychlor	101	147	102	102	71	71	102	102	102	102
atrazine	217	306	122	123	127	1392	106	107	111	106
dalapon	102	147	100	102	71	112	80	80	80	80
α-HCH	446	1345	978	1010	660	663	1015	1015	1012	1002
average	501	912	595	619	438	515	654	639	622	645
geomean	107	284	151	154	138	176	251	244	220	227
maximum	1289	4581	3028	3304	2191	2280	3300	3301	3293	3262
95 percentile	1017	1481	994	1022	712	1257	1022	1022	1026	1024
75 percentile	997	1478	992	1020	710	724	1022	1022	1011	1023
median	331	896	481	491	439	683	753	542	396	673
25 percentile	36	132	49	49	69	70	86	86	86	86
5 percentile	0.6	6.6	1.9	1.9	3.4	3.8	20	21	14	14
minimum	0.4	0.6	0.3	0.3	0.3	0.3	1.7	1.0	0.6	0.5

Table 13 Correlation between the calculated overall persistence values listed in Table 12

	BENN	TAPL	WAN1	WAN2	PEN1	PEN2	VMD1	VDM2	VDM3	VDM4
BENN	1	0.86	0.85	0.84	0.86	0.75	0.78	0.80	0.81	0.84
TAPL	0.86	1	1	1	1	0.88	0.96	0.97	0.98	1
WAN1	0.85	1	1	1	1	0.87	0.96	0.98	0.99	0.99
WAN2	0.84	1	1	1	1	0.87	0.96	0.98	0.99	0.99
PEN1	0.86	1	1	1	1	0.88	0.96	0.97	0.98	1
PEN2	0.75	0.88	0.87	0.87	0.88	1	0.82	0.84	0.85	0.86
VMD1	0.78	0.96	0.96	0.96	0.96	0.82	1	1	0.98	0.97
VDM2	0.80	0.97	0.98	0.98	0.97	0.84	1	1	1	0.98
VDM3	0.81	0.98	0.99	0.99	0.98	0.85	0.98	1	1	0.99
VDM4	0.84	1	0.99	0.99	1	0.86	0.97	0.98	0.99	1
average	0.84	0.96	0.96	0.96	0.96	0.86	0.94	0.95	0.96	0.96

Table 14 Overall persistence rank among the 26 chemical as calculated by various models assuming emission to soil.

Model	BENN	TAPL	WAN1	WAN2	PEN1	PEN2	VDM1	VDM2	VDM3	VDM4
benzene	24	25	25	25	25	25	25	25	25	25
HCB	1	1	1	1	1	1	1	1	1	1
2,3,7,8-TCDD	8	8	6	6	8	9	8	7	4	6
1,3-butadiene	26	26	26	26	26	26	26	26	26	26
styrene	25	23	23	23	23	23	24	24	23	23
toluene	23	24	24	24	24	24	21	21	24	24
acenaphthylene	19	14	14	14	14	16	15	15	15	15
pyrene	10	10	10	11	10	12	10	10	12	10
fluoranthene	11	9	9	10	9	10	9	9	11	9
chrysene	7	6	8	8	6	7	5	6	10	5
B[a]A	9	7	7	7	7	8	6	8	9	7
B[a]P	6	4	4	4	4	5	3	4	6	3
perylene	4	3	3	3	3	4	2	3	3	2
B[k]F	5	5	5	5	5	6	4	5	7	4
PCP	16	17	16	17	17	18	18	17	17	17
DEP	21	22	21	21	22	15	23	23	22	22
DBP	20	21	20	20	21	22	22	22	21	21
CCl ₄	3	12	13	13	11	11	14	14	13	13
aldrin	22	20	22	22	20	21	13	13	14	14
chlordane	2	2	2	2	2	3	7	2	2	8
γ-HCH	12	11	11	9	12	13	12	12	8	11
heptachlor	18	19	19	19	19	20	19	19	19	19
methoxychlor	17	18	17	18	18	19	17	18	18	18
atrazine	14	15	15	15	15	2	16	16	16	16
dalapon	15	16	18	16	16	17	20	20	20	20
α-HCH	13	13	12	12	13	14	11	11	5	12

Table 15 Correlation between the calculated overall persistence rankings listed in Table 14.

	BENN	TAPL	WAN1	WAN2	PEN1	PEN2	VMD1	VDM2	VDM3	VDM4
BENN	1	0.95	0.94	0.94	0.96	0.90	0.89	0.90	0.89	0.90
TAPL	0.95	1	0.99	0.99	1	0.92	0.96	0.97	0.94	0.97
WAN1	0.94	0.99	1	1	0.99	0.91	0.95	0.96	0.95	0.96
WAN2	0.94	0.99	1	1	0.99	0.91	0.94	0.95	0.95	0.95
PEN1	0.96	1	0.99	0.99	1	0.92	0.96	0.97	0.94	0.96
PEN2	0.90	0.92	0.91	0.91	0.92	1	0.86	0.87	0.84	0.87
VMD1	0.89	0.96	0.95	0.94	0.96	0.86	1	0.99	0.94	0.99
VDM2	0.90	0.97	0.96	0.95	0.97	0.87	0.99	1	0.96	0.98
VDM3	0.89	0.94	0.95	0.95	0.94	0.84	0.94	0.96	1	0.95
VDM4	0.90	0.97	0.96	0.95	0.96	0.87	0.99	0.98	0.95	1
average	0.93	0.97	0.96	0.96	0.97	0.90	0.95	0.96	0.93	0.95

Table 16 Summary statistics on the overall persistence comparison assuming emission to soil.

ID	absolute value								rank					
	max	min	max/min	geomean	median	average	stdev	%stdev	max	min	range	geomean	median	average
benzene	18	1.1	17	4.5	4.0	6.9	6.3	91	25	24	1	24.9	25.0	24.9
HCB	4581	1289	3.6	2843	3278	2983	884	30	1	1	0	1.0	1.0	1.0
2,3,7,8-TCDD	1476	710	2.1	979	1016	998	209	21	9	4	5	6.8	7.5	7.0
1,3-butadiene	1.7	0.3	5.6	0.5	0.5	0.6	0.4	73	26	26	0	26.0	26.0	26.0
styrene	31	0.4	76	11	19	18	12	69	25	23	2	23.4	23.0	23.4
toluene	54	1.1	49	9.3	8.6	18	19	104	24	21	3	23.3	24.0	23.3
acenaphthylene	448	44	10	250	313	283	106	37	19	14	5	15.0	15.0	15.1
pyrene	1469	707	2.1	968	1012	987	210	21	12	10	2	10.5	10.0	10.5
fluoranthene	1470	707	2.1	967	1012	986	211	21	11	9	2	9.6	9.0	9.6
chrysene	1479	711	2.1	982	1015	1000	209	21	10	5	5	6.7	6.5	6.8
B[a]A	1479	710	2.1	980	1015	998	209	21	9	6	3	7.4	7.0	7.5
B[a]P	1479	711	2.1	983	1016	1001	208	21	6	3	3	4.2	4.0	4.3
perylene	1480	711	2.1	984	1017	1002	208	21	4	2	2	2.9	3.0	3.0
B[k]F	1479	711	2.1	983	1016	1001	208	21	7	4	3	5.0	5.0	5.1
PCP	147	71	2.1	98	102	100	21	21	18	16	2	17.0	17.0	17.0
DEP	372	22	17	40	33	66	108	164	23	15	8	21.1	22.0	21.2
DBP	48	23	2.1	32	33	32	6.8	21	22	20	2	21.0	21.0	21.0
CCl ₄	1438	437	3.3	712	690	761	309	41	14	3	11	10.9	13.0	11.7
aldrin	989	1.8	553	83	99	262	327	125	22	13	9	17.7	20.0	18.1
chlordane	1481	713	2.1	1002	1022	1017	193	19	8	2	6	2.7	2.0	3.2
γ-HCH	1447	695	2.1	950	1008	970	214	22	13	8	5	11.0	11.5	11.1
heptachlor	144	46	3.2	90	100	93	27	28	20	18	2	19.0	19.0	19.0
methoxychlor	147	71	2.1	98	102	100	21	21	19	17	2	17.8	18.0	17.8
atrazine	1392	106	13	173	122	272	399	147	16	2	14	12.5	15.0	14.0
dalapon	147	71	2.1	93	90	96	23	24	20	15	5	17.7	17.5	17.8
α-HCH	1345	446	3.0	878	1006	915	255	28	14	5	9	11.2	12.0	11.6

Table 17 Overall persistence in hours as calculated by various models for 26 chemicals assuming emission to air, water, and soil.

Model	TAPL	WAN1	WAN2	PEN1	PEN2	VDM1	VDM2	VDM3	VDM4
benzene	5.1	5.3	5.3	2.7	5.5	6.6	7.1	7.0	4.2
HCB	3925	2959	3299	1774	2407	3008	3023	3187	2405
2,3,7,8-TCDD	1849	612	625	859	2005	927	988	575	1347
1,3-butadiene	3.0	3.4	3.5	1.7	4.1	1.1	0.9	3.6	0.6
styrene	11	4.6	4.6	5.7	8.6	11	11	13	9.9
toluene	8.8	11	11	5.0	6.6	16	19	19	10
acenaphthylene	168	164	165	82	84	119	124	125	116
pyrene	1109	731	750	492	730	606	671	413	774
fluoranthene	1144	731	751	506	766	639	683	414	776
chrysene	1968	743	764	911	2379	997	1019	511	1370
B[a]A	1906	738	758	863	2356	929	969	486	1254
B[a]P	2082	745	766	974	3005	1031	1069	558	1403
perylene	2176	748	769	1026	3861	1050	1108	617	1426
B[k]F	2065	747	768	967	2874	1032	1065	557	1405
PCP	142	76	76	63	178	83	112	59	152
DEP	33	20	20	16	237	21	21	19	23
DBP	32	21	21	14	39	32	29	17	30
CCl ₄	1397	107	110	668	714	523	455	361	1007
aldrin	51	20	20	28	28	718	243	202	117
chlordane	1900	854	885	1020	16664	945	1025	1097	889
γ-HCH	1219	893	935	546	573	921	911	929	648
heptachlor	75	65	65	36	142	71	62	47	44
methoxychlor	77	50	50	34	66	86	77	39	75
atrazine	677	115	117	313	1146	499	534	585	289
dalapon	147	100	102	71	97	89	89	92	86
α-HCH	795	885	925	368	381	819	820	904	425
average	960	467	491	448	1568	584	582	455	619
geomean	264	140	143	126	285	200	196	158	183
maximum	3925	2959	3299	1774	16664	3008	3023	3187	2405
95 percentile	2152	891	933	1024	3647	1046	1098	1055	1421
75 percentile	1887	745	766	862	2268	929	983	571	1192
median	736	139	141	341	477	564	494	387	357
25 percentile	57	28	28	30	70	74	65	41	52
5 percentile	6.0	4.8	4.8	3.3	5.8	7.6	8.1	8.4	5.6
minimum	3.0	3.4	3.5	1.7	4.1	1.1	0.9	3.6	0.6

Table 18 Correlation between the calculated overall persistence values listed in Table 17.

	TAPL	WAN1	WAN2	PEN1	PEN2	VMD1	VDM2	VDM3	VDM4
TAPL	1	0.88	0.87	1	0.47	0.93	0.95	0.82	0.99
WAN1	0.88	1	1	0.86	0.32	0.95	0.97	0.96	0.84
WAN2	0.87	1	1	0.85	0.31	0.95	0.97	0.96	0.83
PEN1	1	0.86	0.85	1	0.53	0.92	0.94	0.81	0.98
PEN2	0.47	0.32	0.31	0.53	1	0.35	0.38	0.36	0.39
VMD1	0.93	0.95	0.95	0.92	0.35	1	0.99	0.94	0.90
VDM2	0.95	0.97	0.97	0.94	0.38	0.99	1	0.94	0.92
VDM3	0.82	0.96	0.96	0.81	0.36	0.94	0.94	1	0.76
VDM4	0.99	0.84	0.83	0.98	0.39	0.90	0.92	0.76	1
average	0.88	0.86	0.86	0.88	0.46	0.88	0.90	0.84	0.84

Table 19 Overall persistence rank among the 26 chemical as calculated by various models assuming emission to air, water, and soil.

Model	TAPL	WAN1	WAN2	PEN1	PEN2	VDM1	VDM2	VDM3	VDM4
benzene	25	24	24	25	25	25	25	25	25
HCB	1	1	1	1	5	1	1	1	1
2,3,7,8-TCDD	8	12	12	8	8	8	7	7	6
1,3-butadiene	26	26	26	26	26	26	26	26	26
styrene	23	25	25	23	23	24	24	24	24
toluene	24	23	23	24	24	23	23	21	23
acenaphthylene	15	13	13	15	19	16	16	16	17
pyrene	12	11	11	12	11	13	12	13	11
fluoranthene	11	10	10	11	10	12	11	12	10
chrysene	5	8	8	6	6	5	6	10	5
B[a]A	6	9	9	7	7	7	8	11	7
B[a]P	3	7	7	4	3	4	3	8	4
perylene	2	5	5	2	2	2	2	5	2
B[k]F	4	6	6	5	4	3	4	9	3
PCP	17	17	17	17	16	19	17	18	15
DEP	21	22	22	21	15	22	22	22	22
DBP	22	20	20	22	21	21	21	23	21
CCl ₄	9	15	15	9	12	14	14	14	8
aldrin	20	21	21	20	22	11	15	15	16
chlordane	7	4	4	3	1	6	5	2	9
γ-HCH	10	2	2	10	13	9	9	3	12
heptachlor	19	18	18	18	17	20	20	19	20
methoxychlor	18	19	19	19	20	18	19	20	19
atrazine	14	14	14	14	9	15	13	6	14
dalapon	16	16	16	16	18	17	18	17	18
α-HCH	13	3	3	13	14	10	10	4	13

Table 20 Correlation between the calculated overall persistence rankings listed in Table 19.

	TAPL	WAN1	WAN2	PEN1	PEN2	VMD1	VDM2	VDM3	VDM4
TAPL	1	0.90	0.90	0.99	0.94	0.95	0.97	0.86	0.98
WAN1	0.90	1	1	0.91	0.84	0.90	0.93	0.94	0.86
WAN2	0.90	1	1	0.91	0.84	0.90	0.93	0.94	0.86
PEN1	0.99	0.91	0.91	1	0.95	0.95	0.97	0.88	0.97
PEN2	0.94	0.84	0.84	0.95	1	0.89	0.93	0.84	0.92
VMD1	0.95	0.90	0.90	0.95	0.89	1	0.99	0.90	0.96
VDM2	0.97	0.93	0.93	0.97	0.93	0.99	1	0.92	0.97
VDM3	0.86	0.94	0.94	0.88	0.84	0.90	0.92	1	0.85
VDM4	0.98	0.86	0.86	0.97	0.92	0.96	0.97	0.85	1
average	0.95	0.92	0.92	0.95	0.91	0.94	0.96	0.90	0.93

Table 21 Summary statistics on the overall persistence comparison assuming emission to air, water, and soil.

ID	absolute value								rank					
	max	min	max/min	geomean	median	average	stdev	%stdev	max	min	range	geomean	median	average
benzene	7.1	2.7	2.6	5.2	5.3	5.4	1.4	26	25	24	1	24.8	25.0	24.8
HCB	3925	1774	2.2	2823	3008	2887	620	21	5	1	4	1.2	1.0	1.4
2,3,7,8-TCDD	2005	575	3.5	984	927	1087	534	49	12	6	6	8.2	8.0	8.4
1,3-butadiene	4.1	0.6	6.9	2.0	3.0	2.4	1.4	56	26	26	0	26.0	26.0	26.0
styrene	13	4.6	2.8	8.3	9.9	8.9	3.1	35	25	23	2	23.9	24.0	23.9
toluene	19	5.0	3.9	11	11	12	5.2	43	24	21	3	23.1	23.0	23.1
acenaphthylene	168	82	2.1	123	124	127	33	26	19	13	6	15.5	16.0	15.6
pyrene	1109	413	2.7	673	730	697	198	28	13	11	2	11.8	12.0	11.8
fluoranthene	1144	414	2.8	687	731	712	204	29	12	10	2	10.7	11.0	10.8
chrysene	2379	511	4.7	1062	997	1185	616	52	10	5	5	6.4	6.0	6.6
B[a]A	2356	486	4.8	1020	929	1140	609	53	11	6	5	7.8	7.0	7.9
B[a]P	3005	558	5.4	1130	1031	1293	783	61	8	3	5	4.4	4.0	4.8
perylene	3861	617	6.3	1198	1050	1420	1027	72	5	2	3	2.7	2.0	3.0
B[k]F	2874	557	5.2	1123	1032	1276	746	58	9	3	6	4.6	4.0	4.9
PCP	178	59	3.0	97	83	105	43	41	19	15	4	17.0	17.0	17.0
DEP	237	16	14.9	28	21	46	72	158	22	15	7	20.9	22.0	21.0
DBP	39	14	2.8	25	29	26	8	31	23	20	3	21.2	21.0	21.2
CCl ₄	1397	107	13.0	445	523	594	416	70	15	8	7	11.9	14.0	12.2
aldrin	718	20	35.8	74	51	158	226	142	22	11	11	17.5	20.0	17.9
chlordane	16664	854	19.5	1417	1020	2809	5205	185	9	1	8	3.8	4.0	4.6
γ-HCH	1219	546	2.2	816	911	842	215	26	13	2	11	6.3	9.0	7.8
heptachlor	142	36	3.9	63	65	67	31	46	20	17	3	18.7	19.0	18.8
methoxychlor	86	34	2.5	59	66	62	19	30	20	18	2	19.0	19.0	19.0
atrazine	1146	115	10.0	375	499	475	321	68	15	6	9	12.1	14.0	12.6
dalapon	147	71	2.1	95	92	97	21	22	18	16	2	16.9	17.0	16.9
α-HCH	925	368	2.5	659	819	702	237	34	14	3	11	7.8	10.0	9.2

Discussion of the Comparison of Overall Persistence Values

Absolute values: There are large differences in the absolute persistence values calculated by the various models (Table 2, 7, 12, and 17). The difference between highest and lowest value calculated for one chemical is regularly bigger than one order of magnitude (Tables 6, 11, 16, 21). However, these differences are dependent on both physical-chemical properties and mode of entry. In particular, differences between models are small (max/min ratios of 2 or 3) if the dominant medium of partitioning is obvious, namely for:

- volatile substances (e.g. benzene, styrene, toluene) being emitted to air,
- highly sorptive compounds (PAHs, HCHs) emitted to soil, and
- water soluble compounds (atrazine, dalapon) emitted to water

The overall persistence of such chemicals is essentially controlled by the degradation half-life in the medium of emission, which is also the primary medium of partitioning. Rates of intermedia transfer process have little impact on the calculated overall persistence values under such circumstances. In other words, under certain emission conditions, selected chemicals are not multimedia pollutants and an assessment of their persistence can be based on the persistence in a single environmental medium.

On the other hand, differences between models tend to be higher if the medium of emission is different from the medium of primary residence and thus degradation, examples being volatile substances emitted to soil, highly sorptive substances emitted to air, and volatile or highly sorptive chemicals emitted to water. In such cases the rates of evaporation from soil, atmospheric deposition, and volatilisation from water or transfer to sediments, respectively become decisive.

Partly, these differences can be attributed to differences in the numbers and relative dimensions of the model compartments. For example, with emission to air the three-compartment models, i.e. those without a sediment compartment (SCHE, HELD, BENN, WAN1, WAN2), tend to estimate lower overall persistences (median for the 26 chemicals 21 to 53 hours) than the four compartment models (median between 104 and 322 hours). With emissions to water BEN and WANX estimate significantly lower persistences for PAHs (around 100 hours) than the other models (>1000 hours). Degradation half-lives in sediments tend to be longer than in water (Table 1) and the elimination of a sediment compartment thus typically results in shortened overall persistences. BENN and WANX do not have a sediment compartment, and thus no pathway from water to soil/sediment. In these models PAHs partition into water and are degraded rapidly, whereas in the other models they partition into sediments and are degraded slowly.

High discrepancies between models are also notable for chemicals, for which half-lives differ very strongly between compartments. The persistence values calculated for aldrin always have high variability because it is very rapidly degraded in air, but not in the other media. Small differences in the calculated extent of partitioning into air results in large differences. On the other hand, the persistence of a chemical such as HCB, which is more or less equally persistent in all media, has a very low variability.

Correlation between absolute persistence values: Despite the large differences in absolute values, the correlation between the overall persistence values obtained by various models was high, with correlation coefficients averaging higher than 0.8 for emission to air (Table 3), soil (Table 13) and all three media (Table 18). The correlation is relatively poor when emission is assumed to occur into water only (Table 8). However, this can be attributed to the issue of a

sediment compartment discussed above. The three compartment model results for emission to water are highly correlated, as are the four compartment model results.

As expected, the SCHE and HELD models gave virtually identical results, the results of the two WAN models were perfectly correlated, as were the results from TAPL and the PEN1 model which are both based on EQC or its predecessor, the "generic" model. The only model results that were less well correlated with the others with all emission scenarios were those from PEN2. The simplifications and reductions in data input requirements of the "heuristic" model approach obviously cause significant deviations from the other models. A more thorough comparison between PEN1 and PEN 2 would reveal whether these deviations are potentially of concern, i.e. leading to false negatives decisions, or not. It may also be worthwhile to comparatively evaluate the various approaches with reduced input parameter requirements, such as PEN2 and the CART approach.

Rankings: Persistence rankings were more similar between the models than the absolute persistence values. But large discrepancies in rank did occur, and the range of rankings for the same chemical and the same mode of entry regularly exceeded 10, especially if emission takes place into water. The same reasons that caused differences in absolute persistence values are responsible for the differences in rankings, namely the inclusion/exclusion of a sediment compartment, and large differences in half-lives among media.

The persistence rankings calculated by the various models were highly correlated (Table 5, 10, 15, and 20, with correlation coefficients consistently higher than those between the absolute persistence values. Especially with emission to soil correlation coefficients were very high (Table 15), but it is also true in the case of emission to water (Table 10); The correlation of the rankings is almost as high as the correlation of rankings for the other emission scenarios, whereas the correlation for the absolute values was substantially lower (Table 8). The rankings of the SCHE and the HELD models were identical, as generally were those from the two WANX models. Also the rankings of the PEN2 model were better correlated with the other models than the absolute values.

Comparison of Atmospheric Travel Distance Values

Long range transport is generally perceived to occur mostly in the atmosphere. Accordingly, so far virtually all modelling approaches making estimates of LRT potential are estimating some sort of characteristic travel distance within the atmosphere. Beyer et al. (2000) however indicated that in principle a characteristic distance can also be calculated for other mobile environmental phases, such as water.

Models Included in the Comparison of Atmospheric Travel Distances

Eight models were included in the comparison of estimated atmospheric travel distance. These are:

1. **SCHE:** The circular model as developed and described by Scheringer (1996; 1997).
2. **HELD_2D:** A recoded version of the SCHE model developed by Held using a different numerical technique.
3. **HELD_3D:** A version of the SCHE-model in which the ring of the SCHE-model is replaced by a sphere.
4. **BENN:** The 3-compartment (air, water, soil) multimedia model described in Bennett et al. (1998).

5. **WANIA**: The persistence criterion model by Wania (1998), which is a level III fugacity model with three compartments (air, water, soil). For the sake of this comparison, advective transport of air and water has been added to the model.
6. **TAPL**: The TAPL3 model by Mackay and co-workers (Beyer et al., 2000), which in turn is based on the “generic” model (Mackay et al., 1992).
7. **VDM1**: van de Meent et al. (1999) used again a modification of the SIMPLEBOX model (Brandes et al., 1996; van de Meent, 1993) Specifically, they used the nested two-scale model, SimpleBox 2.1, with the regional, arctic and tropic scales set to negligible small dimensions. The continental scale was set to regional dimensions (200 km^2), and the global scale set to N-hemispheric dimensions ($255 \cdot 10^6 \text{ km}^2$). Advection occurs between inner and outer scale and emissions take place to the inner scale only.
8. **PENN**: The long range transport model described in Rodan et al. (1999)

Again the model approaches are similar in that they are all based on level III multimedia calculations. There is however a difference in principle in how LRT potential is assessed in the SCHE, HELD_2D and HELD_3D models vis-à-vis in the remaining models. Scheringer (1996) introduced the concept of spatial range, defined as the 95%-interquantile range of the spatial exposure distribution calculated by his ring model. Exposure in this context is the time integral over the concentration. This spatial range can be calculated and is different for each of the three phases. The atmospheric exposure distribution was employed in the assessment of the atmospheric LRT potential.

The five remaining models assess LRT potential by estimating a characteristic travel distance. The approach taken in the PENN model is more complex, in that the multimedia model serves the triple purpose of calculating the media distribution (and thus the air concentration) within an initial mixing zone, estimating the effective atmospheric loss rate constant k_{Eff} , and relating the concentration in the advected air with an “average environmental concentration” (Rodan et al., 1999). Whereas BENN, TAPL, and WANIA define the travel distance as the point where the initial air concentration has dropped to a certain fraction such as $1/e$ (37 %) or $1/2$, the PENN approach defines this distance as the point where an arbitrary emission rate of 3000 kg/h leads to a remote “average environmental concentration” of 10^{-11} g/m^3 . This allows to account for the influence of the mode-of-entry on the LRT potential. A chemical which is not emitted into the atmosphere may have a much smaller potential for atmospheric transport than is suggested by its characteristic travel distance. Beyer et al. (2000) also noted the effect of mode-of-emission on travel distance, and introduced the concept of an effective travel distance. Scheringer’s spatial range can be calculated for any mode-of-entry. In this comparison, only one mode-of-entry of the chemical into the environment was considered; emission was assumed to occur into air only.

Results of the Comparison of Atmospheric Travel Distances

The results of the model calculations are again shown in a series of tables. Table 22 shows the calculated **atmospheric travel distance** calculated by the various models for the 26 chemicals. This table also contains the arithmetic and geometric mean, the median, the minimum, the maximum and various percentiles of the travel distance calculated by one model for the 26 chemicals. Table 23 shows the **correlation coefficients between the results for atmospheric travel distance** of the various models. The travel distances calculated for the 26 chemicals by each model have been ranked and each chemical assigned a rank between 1 and 26 (1: chemical transported the furthest, 26: least mobile chemical). Table 24 shows these

travel distance rankings for all models. The **correlation among the rankings** calculated by various models is shown in Table 25.

A number of **statistical parameters**, namely the maximum, the minimum, the ratio between maximum and minimum, the geometric mean, the median, and the average (i.e. arithmetic mean) and standard deviation (absolute and as percent of average) of the atmospheric travel distance values calculated for one chemical were determined and are listed in Table 26. Similarly, the maximum, minimum, range, geometric mean, median and arithmetic mean of the rankings calculated for each of the chemical are included in this table.

Discussion of the Comparison of Atmospheric Travel Distances

Absolute values: As is the case with the overall persistence values, the differences in the absolute atmospheric travel distances calculated by the various models are large (Table 22). The difference between highest and lowest value calculated for one chemical is regularly one order of magnitude or higher (Tables 26). There are two primary reasons for these differences, which can be illustrated with two graphs comparing the results of two of the models each (Fig. 1).

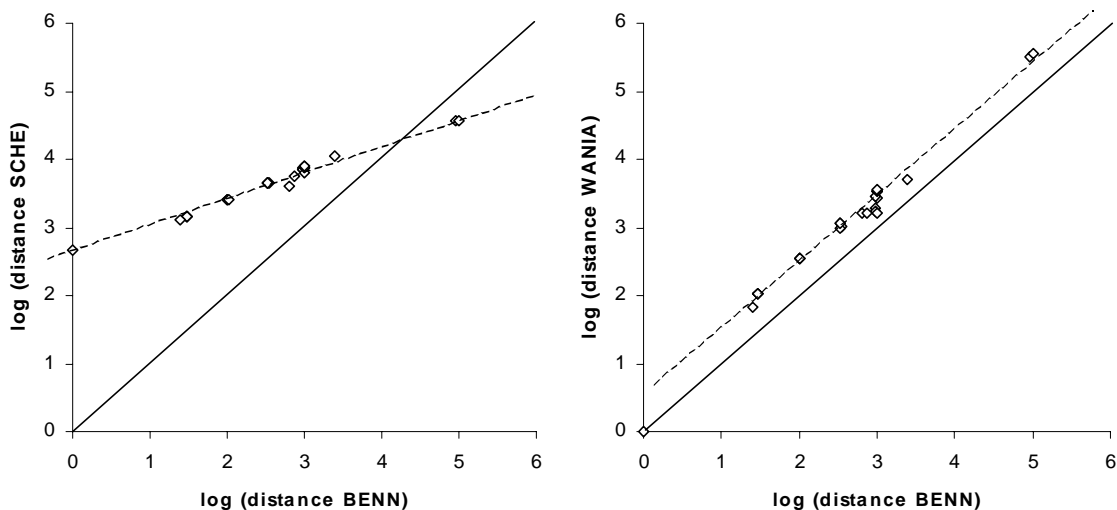


Figure 1

The graph of the right shows that certain models (e.g. WANIA) predict consistently higher distances than others (e.g. BENN) across the entire range of transport distances. Such differences can simply be explained by different environmental input parameters of the models, specifically the assumptions made concerning atmospheric advection rates.

Other discrepancies are more complex, but can be explained by the different way the SCHE model and its derivatives calculate transport distance. These models tend to estimate higher transport distances than the other models, except for the most mobile substances (CCl_4 and HCB). For these substances, the other models, in particular TAPL3 and WANIA, predict extremely large distances in excess of 200,000 km. This amounts to more than five times the circumference of the Earth and essentially suggests complete mixing of such compounds in the Earth's atmosphere. On the other hand, the SCHE model, and the HELD models derived from it, have an upper limit for the atmospheric travel distance given by the circumference of the world (approx. 37,000 km), and CCl_4 and HCB indeed approach this maximum value. The VDM1 model also seems to be limited by a fairly low upper threshold of about 12,500 km.

Table 22 Atmospheric travel distance as calculated by various models for 26 chemicals assuming emission to air.

Model	BENN	SCHE	HELD_2D	HELD_3D	WANIA	TAPL3	VDM1	PENN
benzene	102	2532	2517	3351	353	508	297	6257
HCB	92606	37146	37146	33580	319709	200914	12331	3680403
2,3,7,8-TCDD	977	7766	7729	10155	2672	711	683	21186
1,3-butadiene	30	1451	1365	1844	104	150	88	1732
styrene	30	1451	1365	1844	104	150	88	1734
toluene	102	2532	2517	3351	353	508	298	6260
acenaphthylene	330	4500	4500	5982	1139	1603	826	21255
pyrene	997	7716	7683	10099	3356	3816	1422	67873
fluoranthene	995	7729	7694	10110	3363	3716	1386	67428
chrysene	962	7225	7173	9436	1901	642	701	18789
B[a]A	975	7666	7639	10009	2807	1476	997	39869
B[a]P	950	7062	6997	9220	1745	493	615	13881
perylene	624	3947	3828	5089	1579	451	596	11857
B[k]F	997	6196	6119	8092	1629	459	592	12644
PCP	2447	11131	11059	14276	5131	2554	3007	62103
DEP	731	5595	5534	7311	1665	413	198	10838
DBP	351	4439	4414	5864	1008	812	571	15421
CCl ₄	101877	37152	37152	33585	352046	498958	11753	6404215
Aldrin	30	1451	1365	1844	104	150	92	1788
chlordane	331	4517	4511	5994	997	1357	870	24888
γ-HCH	1000	7645	7615	10002	3363	3021	1765	58396
heptachlor	330	4537	4527	6020	1142	1636	899	20914
methoxychlor	103	2514	2506	3336	351	401	235	6854
atrazine	25	1257	966	1284	67	16	82	449
dalapon	0	475	4	6	1	0	81	0
α-HCH	1014	7934	7887	10353	3495	4473	2123	72441
Average	8035	7445	7377	8540	27315	28053	1638	409595
Geomean	330	4687	3823	4922	1139	703	608	12842
Maximum	101877	37152	37152	33585	352046	498958	12331	6404215
95 percentile	70066	30642	30624	28754	241065	151804	9566	2778413
75 percentile	996	7704	7672	10077	3219	2325	1289	53765
Median	677	5066	5031	6665	1604	676	649	17105
25 percentile	102	2532	2517	3351	353	422	251	6409
5 percentile	26.0	1305.6	1065.6	1424.2	76.2	49.7	83.5	769.7
Minimum	0.0	475.0	4.2	5.7	0.8	0.0	81.1	0.1

Table 23 Correlation between the calculated atmospheric transport distances listed in Table 23

	BENN	SCHE	HELD_2D	HELD_3D	WANIA	TAPL3	VDM1	PENN
BENN	1	0.96	0.96	0.91	1	0.93	0.98	0.97
SCHE	0.96	1	1	0.99	0.96	0.87	0.99	0.92
HELD_2D	0.96	1	1	0.99	0.96	0.87	0.98	0.92
HELD_3D	0.91	0.99	0.99	1	0.90	0.82	0.96	0.87
WANIA	1	0.96	0.96	0.90	1	0.93	0.97	0.97
TAPL3	0.93	0.87	0.87	0.82	0.93	1	0.88	0.99
VDM1	0.98	0.99	0.98	0.96	0.97	0.88	1	0.93
PENN	0.97	0.92	0.92	0.87	0.97	0.99	0.93	1
average	0.96	0.97	0.97	0.94	0.96	0.90	0.97	0.95

Table 24 Atmospheric travel distance rankings among the 26 chemical as calculated by various models assuming emission to air.

Model	BENN	SCHE	HELD_2D	HELD_3D	WANIA	TAPL3	VDM1	PENN
benzene	21	20	20	20	20	16	19	21
HCB	2	2	2	2	2	2	1	2
2,3,7,8-TCDD	9	5	5	5	9	13	13	11
1,3-butadiene	23	23	23	23	22	22	23	24
styrene	24	24	24	24	24	24	24	23
toluene	20	19	19	19	19	15	18	20
acenaphthylene	18	16	16	16	16	9	11	10
pyrene	7	7	7	7	7	4	6	4
fluoranthene	8	6	6	6	5	5	7	5
chrysene	11	10	10	10	10	14	12	13
B[a]A	10	8	8	8	8	10	8	8
B[a]P	12	11	11	11	11	17	14	15
perylene	14	18	18	18	14	19	15	17
B[k]F	6	12	12	12	13	18	16	16
PCP	3	3	3	3	3	7	3	6
DEP	13	13	13	13	12	20	21	18
DBP	15	17	17	17	17	12	17	14
CCl ₄	1	1	1	1	1	1	2	1
aldrin	22	22	22	22	23	23	22	22
chlordane	16	15	15	15	18	11	10	9
γ-HCH	5	9	9	9	6	6	5	7
heptachlor	17	14	14	14	15	8	9	12
methoxychlor	19	21	21	21	21	21	20	19
atrazine	25	25	25	25	25	25	25	25
dalapon	26	26	26	26	26	26	26	26
α-HCH	4	4	4	4	4	3	4	3

Table 25 Correlation between the calculated atmospheric travel distance rankings listed in Table 24.

	BENN	SCHE	HELD_2D	HELD_3D	WANIA	TAPL3	VDM1	PENN
BENN	1	0.96	0.96	0.96	0.97	0.81	0.88	0.89
SCHE	0.96	1	1	1	0.98	0.86	0.91	0.92
HELD_2D	0.96	1	1	1	0.98	0.86	0.91	0.92
HELD_3D	0.96	1	1	1	0.98	0.86	0.91	0.92
WANIA	0.97	0.98	0.98	0.98	1	0.86	0.91	0.91
TAPL3	0.81	0.86	0.86	0.86	0.86	1	0.96	0.96
VDM1	0.88	0.91	0.91	0.91	0.91	0.96	1	0.97
PENN	0.89	0.92	0.92	0.92	0.91	0.96	0.97	1
average	0.93	0.95	0.95	0.95	0.95	0.90	0.93	0.94

Table 26 Summary statistics on the atmospheric travel distance comparison assuming emission to air

ID	absolute value								rank					
	max	min	max/min	geomean	median	average	stdev	%stdev	max	min	range	geomean	median	average
benzene	6257	102	61	961	1513	1990	2136	107	21	16	5	19.6	20.0	19.6
HCB	3680403	12331	298	102838	64876	551729	1268594	230	2	1	1	1.8	2.0	1.9
2,3,7,8-TCDD	21186	683	31	3363	5201	6485	7017	108	13	5	8	8.1	9.0	8.8
1,3-butadiene	1844	30	61	356	757	845	819	97	24	22	2	22.9	23.0	22.9
styrene	1844	30	61	356	757	846	819	97	24	23	1	23.9	24.0	23.9
toluene	6260	102	61	961	1513	1990	2137	107	20	15	5	18.6	19.0	18.6
acenaphthylene	21255	330	64	2446	3051	5017	6880	137	18	9	9	13.6	16.0	14.0
pyrene	67873	997	68	5413	5749	12870	22460	175	7	4	3	6.0	7.0	6.1
fluoranthene	67428	995	68	5377	5705	12803	22311	174	8	5	3	5.9	6.0	6.0
chrysene	18789	642	29	3053	4537	5854	6291	107	14	10	4	11.2	10.5	11.3
B[a]A	39869	975	41	4185	5223	8930	12989	145	10	8	2	8.5	8.0	8.5
B[a]P	13881	493	28	2740	4371	5120	4948	97	17	11	6	12.6	11.5	12.8
perylene	11857	451	26	1986	2703	3496	3824	109	19	14	5	16.5	17.5	16.6
B[k]F	12644	459	28	2537	3874	4591	4420	96	18	6	12	12.6	12.5	13.1
PCP	62103	2447	25	7547	8095	13963	19982	143	7	3	4	3.6	3.0	3.9
DEP	10838	198	55	1987	3600	4036	3893	96	21	12	9	15.0	13.0	15.4
DBP	15421	351	44	2032	2711	4110	5048	123	17	12	5	15.6	17.0	15.8
CCl ₄	6404215	11753	545	125728	69515	934592	2217256	237	2	1	1	1.1	1.0	1.1
aldrin	1844	30	61	360	757	853	827	97	23	22	1	22.2	22.0	22.3
chlordane	24888	331	75	2422	2934	5433	8139	150	18	9	9	13.3	15.0	13.6
γ-HCH	58396	1000	58	5286	5489	11601	19178	165	9	5	4	6.8	6.5	7.0
heptachlor	20914	330	63	2481	3082	5001	6757	135	17	8	9	12.5	14.0	12.9
methoxychlor	6854	103	67	915	1454	2038	2325	114	21	19	2	20.4	21.0	20.4
atrazine	1284	16	78	188	265	518	564	109	25	25	0	25.0	25.0	25.0
dalapon	475	0	125008	1	3	71	166	234	26	26	0	26.0	26.0	26.0
α-HCH	72441	1014	71	5954	6180	13715	23943	175	4	3	1	3.7	4.0	3.8

This difference is reflected in Table 22, where the arithmetic means of the travel distances calculated by the SCHE-type models is lower than those calculated by BENN, WANIA and TAPL3. For the geometric means and medians the situation is reversed, because these parameters are less skewed by a few very high values.

Both graphs in Figure 1, however also show that despite the large differences in the absolute values calculated by the models, there are very strong linear relationships between the logarithms of the transport distances (see also correlation coefficients discussed below).

The approach by Scheringer seems to have less ability to discriminate between chemicals. For example, for the five PAHs pyrene, fluoranthene, chrysene, B[a]A, and B[a]P, SCHE calculates travel distances which are virtually identical, whereas in TAPL3 pyrene travels almost eight times as far as B[a]P. However, our knowledge of the real transport potential of these PAHs is insufficient to judge which of these assessment is more realistic.

The absolute values for spatial range calculated by SCHE and HELD_2D tend to be identical for highly mobile chemicals, yet to differ significantly for very immobile substances such as dalapon and atrazine. This indicates that the numerical technique used in SCHE has limited resolution at the lower end of the spatial range scale. The spatial range calculated by Held_2D is typically three quarters of that calculated by Held_3D. Exceptions are the highly mobile chemicals CCl₄ and HCB which have higher transport distances in HELD_2D than in HELD_3D.

Correlation between absolute transport distance values: That the model predictions for atmospheric mobility are fairly consistent among the seven models can also be seen from the correlation coefficients (Table 23), which are always higher than 0.90. The exception is the TAPL3 model, which is less well correlated with all others. As expected, TAPL3 results correlate better with the results from BENN and WANIA than with those calculated by models derived from Scheringer's circular model.

Rankings: The calculated rankings were very similar among the models (Table 24). In particular, virtually all models agreed which are the four most (CCl₄, HCB, PCP, and α -HCH) and five least mobile chemicals (dalapon, atrazine, styrene, 1,3-butadiene, and aldrin). There were larger differences in the intermediate rankings, but this is not surprising because there were several chemicals with similar properties, and the relative differences between travel distances were minor. The rankings calculated by the various models were highly correlated (Table 25), but again slightly lower with the TAPL3 model. The rankings of the SCHE and the HELD models were identical.

Summary and Conclusions

The absolute values for overall persistence and atmospheric travel distance calculated by different models differ substantially. It is thus not reasonable to define an absolute threshold value for overall persistence (e.g 2 month) or travel distance (e.g 10,000 km) which would apply to all models. These criteria are presently and probably will remain model-specific.

The relative ranking of the chemicals according to persistence calculated by different models is similar, but there are significant numbers of chemicals which are ranked quite differently in some of the models. The most notable reasons for this are:

- the underestimation of persistence in models that have no sediment compartment for chemicals that have a higher persistence in sediments than in water (or an overestimation for chemicals which are less persistent in sediments than in water). Note that it may be possible to avoid the introduction of a full sediment compartment into three compartment

models by considering the “soil” compartment as a composite of soil and sediment and defining a transport process that can deliver chemical from water to this “soil”.

- chemicals which have highly variable degradation rates in various media and for which minor shifts in the calculated media distribution can result in large shifts in the estimated overall persistence.

If the number and type of compartments and the relative size of the aquatic and terrestrial environments is specified, various level III models are likely to give very similar rankings according to overall persistence, and it may be feasible to define benchmark chemicals, which separate persistent from non-persistent substances irrespective of which model is used. Such a benchmark obviously should not have highly variable persistences in various media.

The relative ranking of the chemicals according to travel distance calculated by different models is very similar. Of particular significance is that all models identify the same chemicals as being subject to long range transport, and these chemicals are indeed believed to be subject to atmospheric transport into remote regions. It should thus also be feasible to define benchmark chemicals, which separate substances that can undergo long range transport from those that do not irrespective of which model is used.

Criteria for persistence and LRT potential could thus take the following form:

“A chemical shall be considered persistent if its calculated overall persistence in a typical regional level III multimedia model with four compartments (air, soil, water, sediment) exceeds that of chemical X calculated under the same conditions.”

“A chemical shall be considered as having the potential for atmospheric long range transport if its calculated transport distance/spatial range in a typical regional level III multimedia model exceeds that of chemical X calculated under the same conditions.”

Approaches using benchmark chemicals have the advantage that they are adaptable to a specific regulatory context. What is required is a judgement of which well-characterised contaminants are and are not considered persistent or as having LRT potential within the context of interest. This is probably as much a policy decision as it is a scientific question. It is quite likely that a regional and a global assessment may thus derive different sets of benchmark chemicals, as a particular contaminant (e.g. TCDD) may be considered as having LRT potential on a regional but not on a global scale.

Recommendations and Discussion of Paths Forward

An aspect of this issue which has not been fully addressed in this report is the desirability of developing a tiered system of evaluating persistence and long range transport. The data requirements of these models are considerable and it is unlikely that resources will be available to obtain the required data for the some 60,000 chemicals of commerce. A current study at the Canadian Environmental Modelling Centre (which has developed in part from this report) suggests a tiered “factor of 8” system in which the chemicals are screened as shown in Fig. 2.

- Tier 1 is envisaged as being a simple comparison of chemical properties against criteria values. For persistence it could be half-lives in various media that are compared with certain threshold values. For long range transport, it could be a half-life in the atmosphere.
- Tier 2 is envisaged as an equilibrium or Level II evaluation. Examples would be the approach of Gouin et al. (2000) for persistence, and a modification of the Beyer et al. (2000) approach (with a criterion of velocity x half-life in air x fraction in air at equilibrium) for long range transport.

- Tier 3 is envisaged as a non-equilibrium or Level III evaluation of the type compared in this report. Examples are the approach by Webster et al. (1998) for persistence and Beyer et al. (2000) for long range transport.
- Tier 4 is a full site-specific assessment of fate and ultimately risk.

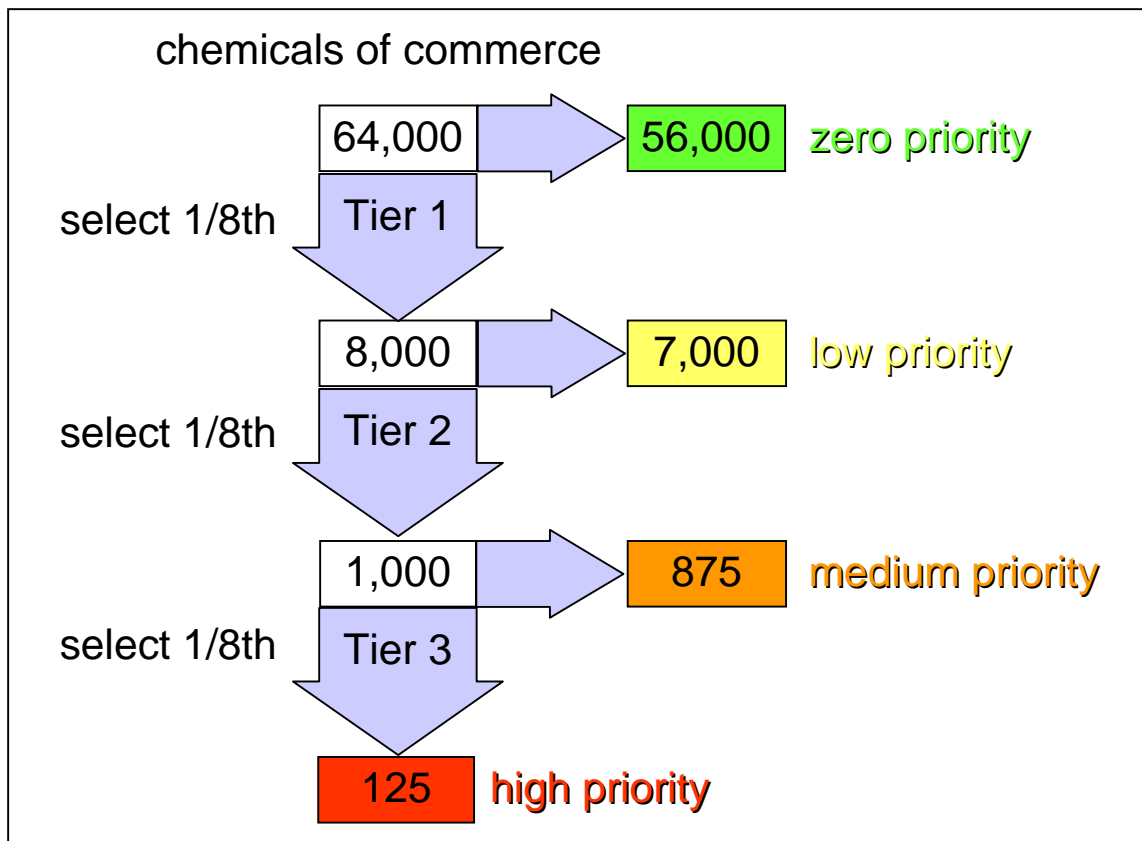


Figure 2

Such a system would be economical, simple, transparent and by applying a progressively more detailed evaluation would focus attention and resources where they are most needed. A report on this approach is presently in preparation.

In summary, considerable efforts have been, and are being, devoted to developing systems for evaluating the persistence and long range transport characteristics of chemicals. These efforts are in large part derived from the 1998 SETAC workshop on this topic. A healthy diversity of models has been developed and it is encouraging that they are in general agreement with each other, and that they appear to give results consistent with environmental observations. It is likely that a tiered system of models will emerge in the near future which will enable decisions to be made on priority, based on benchmark chemicals and/or specific criteria.

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