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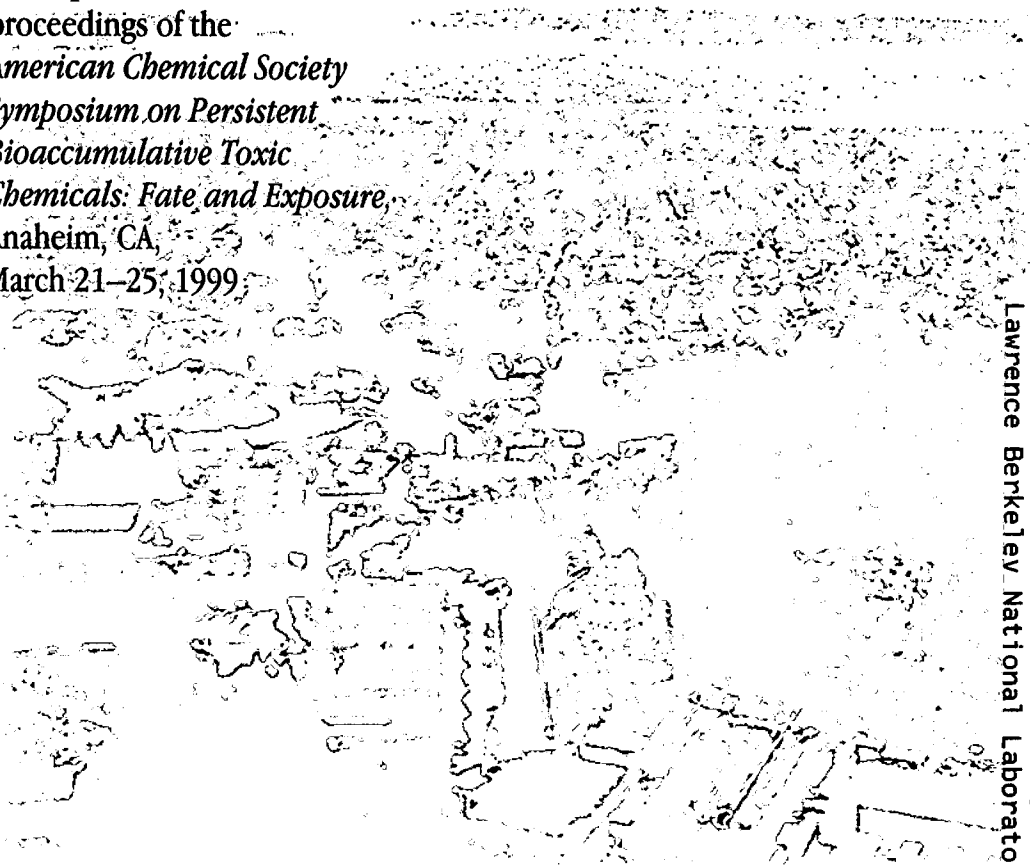
## Relationship Between Persistence and Spatial Range of Environmental Chemicals

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# Relationship between Persistence and Spatial Range of Environmental Chemicals

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Several approaches to calculate the spatial range or travel distance of environmental chemicals have been proposed in the literature. Here we evaluate the relationship between different definitions of spatial range and travel distance and between these quantities and the chemical's atmospheric residence time. We show that the results from a simple global multimedia fate and transport model can account for the analytical relationship. In contrast, the relationship between a chemical's overall persistence and spatial range cannot be described by an analytical expression. A plot of the spatial range versus the overall persistence does not show a well defined relationship between these two measures. The deviations from the analytical relation between atmospheric residence time and spatial range are caused by differences in the phase partitioning of the chemicals. In addition, deviations are strongly influenced by the release media. These effects are demonstrated by correlating the deviations from the analytical relation with the octanol-air partitioning coefficient for each chemical.

## Introduction

The spatial range or characteristic travel distance of an environmental chemical has been introduced as a measure of the chemical's mobility and potential for long-range transport (LRT) (1-7). In analogy to persistence, which quantifies the duration of the environmental exposure, the spatial range is used as a measure of the spatial extent or "effective length" of the spatial distribution of a chemical in the environment. Indicating the extent of an exposure pattern, the spatial range helps to distinguish among local, regional, and global pollution problems. Local, regional, and global scale pollutants require different distribution models, exposure models, measurement programs, and regulatory approaches.

Spatial range and persistence are attributes that can be used to compare and classify chemicals. These two quantities provide exposure screening indicators which can be seen in analogy to hazard indicators such as toxicity or mutagenicity on the effect level. Spatial range and persistence are of particular importance for the characterization and identification of Persistent Organic Pollutants (POPs) (8) but they can also be used in a general framework for the assessment of chemicals (9, 10).

Since a chemical cannot be transported in the environment if it is not persistent for some time, it seems to be obvious that persistence and spatial range are correlated. However, this is not an ideal correlation for several reasons. First, there are different approaches to calculate a chemical's spatial range and persistence, leading to a variety of persistence-spatial range relations. Second, persistence and spatial range are influenced in a complex way by the chemical's partitioning between the environmental media soil, water and air. These media differ in their mobility and in the chemical's degradation rate constants, which can lead to different spatial ranges for a given persistence. Additionally, if the chemical is released to a different environmental medium, the distribution of the chemical between the environmental media will change, affecting the overall persistence.

In this paper, we first investigate the relationship between three definitions of spatial range (denoted by  $R$ ,  $\rho$ , and  $L$ ) and between spatial range and the chemical's residence time in the mobile medium (usually air), denoted by  $\tau_a$ . Based on advective and macro-diffusive transport processes, we develop analytical relationships between  $R$ ,  $\rho$ ,  $L$ , and  $\tau_a$ . We next compare the analytical relationships between atmospheric residence time and spatial range obtained for macro-diffusive flow with numerical results from a simple model of the global circulation of chemicals. Then the relation between spatial range and overall persistence, which is not accessible in an analytical form, is investigated with the model. Finally, the significant influence of the medium the chemical is released into is demonstrated by comparing release to soil and release to air.

## Approaches to Calculating Spatial Range

Several definitions of the spatial range or travel distance have been proposed and are currently used:

- Müller-Herold and Nickel (5) calculate the Shannon entropy  $S$  of the spatial concentration or exposure distribution and subsequently the entropy rank  $\rho = \exp\{-S\}$ .  $\rho$  is a measure of the spread of a distribution.
- Bennett et al. (6) and van Pul et al. (7) define the travel distance  $L$  of a chemical by the point where a monotonously decreasing function  $c(x)$  has dropped to  $c_0/e \approx 0.368 \cdot c_0$ .
- Scheringer (3) introduced the spatial range  $R$  as the 95% interquantile distance of the spatial concentration distribution. This quantity can be determined for any kind of spatial distribution, e.g. for nearly uniform distributions that are obtained for CFCs in the troposphere and for distributions with more than one maximum, such as the accumulation of POPs in polar regions.

All of these definitions were introduced in the context of multimedia models that are used to calculate the environmental concentrations as functions of location. However, spatial range and persistence are not part of a specific model but can be determined from a variety of models or measured concentration data.

## Calculating Spatial Range for Advective and Diffusive Air Flow

The results for spatial range or travel distance presented in the literature differ with respect to the underlying multimedia models and the assumed transport mechanisms. There are several regional models that have advective flow in the atmosphere as the basic transport mechanism (6, 7). There are also global models that include macro-diffusive transport processes in water and air (4, 11, 12, 13). The use of both types of models in calculating spatial range and travel distance is described in the following subsections.

### Transport through Advective Flow

The regional models consist of a multimedia environment with advective inflow and outflow. Air (or water) moves through the system with a constant wind speed of 4 m/s (6) or 5 m/s (7). The transport process is driven by this advective flow, and a certain parcel of air travels without mixing with the surrounding air (plug flow). The direction of the transport is defined by the direction of the air flow.

The assumption of a steady-state mass distribution and first-order removal processes (atmospheric degradation and transfer to, and subsequent degradation in, soil and water) with a constant advective flow results in the following spatial concentration profile (6)

$$c(x) = c(x_0) \cdot \exp \left\{ -\frac{k}{u} \cdot x \right\}. \quad (1)$$

$k$  (in  $s^{-1}$ ) is the effective atmospheric removal rate constant which is given by the net flow through the air compartment (in kg/s) divided by the mass in air (in kg) (6).  $\tau_a = 1/k$  is then the atmospheric residence time.  $u$  is the wind speed in m/s, and  $x$  is the distance from the point of inflow into the system,  $x_0$ . The quantity  $L = u/k$  denotes the point where the concentration has dropped to  $c_0/e$ , which is defined as the characteristic travel distance (6). Accordingly, a linear relation

$$L = u \cdot \tau_a \quad (2)$$

between travel distance and residence time is obtained for this model.

The spatial range  $R$  is given by the point  $q_{0.95}$  with

$$\int_0^{q_{0.95}} c(x) dx / \int_0^{\infty} c(x) dx = 0.95, \quad (3)$$

see ref (3). Inserting the exponential function from eq 1 for  $c(x)$  in eq 3, we obtain

$$R = q_{0.95} \approx 3.00 \cdot u/k = 3.00 \cdot u \cdot \tau_a = 3.00 \cdot L. \quad (4)$$

For atmospheric residence times of 100 days or greater, the assumption of a single advective flow leads to travel distances larger than the circumference of the earth. Accordingly, models with advective flow are appropriate for local and regional transport processes, but are not predictive on the global scale, only indicating if a chemical is likely to be dispersed globally.

### Transport through Macroscopic Diffusion

Macroscopic diffusion in water and air is the relevant transport mechanism in global models (4, 11, 12, 13). The transport is driven by the concentration gradient between adjacent air or water compartments and finally leads to uniform concentration distributions. The direction of the transport is determined by the concentration gradient, which means that the chemical can travel in two or more directions at the same time (depending on the model geometry). Combining the second law of diffusion with a first-order removal term yields the following relationship:

$$\dot{c}(x, t) = D_{\text{eddy}} \frac{\partial^2 c(x, t)}{\partial x^2} - k \cdot c(x, t). \quad (5)$$

$D_{\text{eddy}}$  is the macroscopic diffusion coefficient (in  $\text{m}^2/\text{s}$ ) and  $k$  is the atmospheric removal rate constant in  $\text{s}^{-1}$  (the same  $k$  as used in the advective model). Typical values for  $D_{\text{eddy}}$  in air are in the range of  $5 \cdot 10^5 \text{m}^2/\text{s}$  to  $4 \cdot 10^6 \text{m}^2/\text{s}$  (3, 11, 14).

The steady state ( $\dot{c}(x, t) = 0$ ) relationship obtained from eq 5 is:

$$D_{\text{eddy}} \frac{d^2 c(x)}{dx^2} = k \cdot c(x)$$

and the steady state solution follows as

$$c(x) = c(x_0) \cdot \exp \left\{ -\sqrt{\frac{k}{D_{\text{eddy}}}} \cdot x \right\} \quad (6)$$

(with the boundary conditions  $c(0) = c_0$  and  $c(x \rightarrow \infty) = 0$ ).

In this case, the travel distance  $L$  is given by

$$L = \sqrt{D_{\text{eddy}}/k} = \sqrt{D_{\text{eddy}} \cdot \tau_a}. \quad (7)$$

Corresponding to the case of advective transport, the spatial range follows as

$$R \approx 3.00 \cdot L = 3.00 \sqrt{D_{\text{eddy}} \cdot \tau_a}. \quad (8)$$

As shown in ref (5), the result for the entropy rank is

$$\rho = e \cdot \sqrt{D_{\text{eddy}}/k} \approx 2.72 \sqrt{D_{\text{eddy}} \cdot \tau_a}. \quad (9)$$

For two-sided distributions, a factor of 2 applies to all of these quantities.



## Spatial Range–Persistence Diagrams

### Analytical Expressions and Results from a Model for Diffusive Flow

As described in the previous section, the analytical relationships between spatial range  $R$  or travel distance  $L$  and atmospheric residence time  $\tau_a$  are  $L = u \cdot \tau_a$  for advective transport in one direction and  $R = 6.00 \sqrt{D_{\text{eddy}} \cdot \tau_a}$  for diffusive transport in two directions. These relationships are plotted in Figure 1 with  $u = 5 \text{ m/s}$  and  $D_{\text{eddy}} = 2 \cdot 10^6 \text{ m}^2/\text{s}$ . This plot illustrates how the travel distance  $L$  and the spatial range  $R$  can be calculated from the atmospheric residence time and how they compare for two different transport mechanisms.

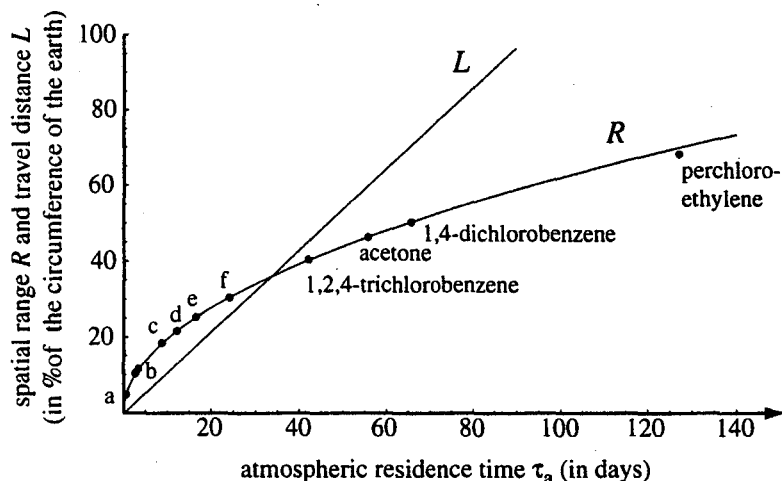


Figure 1. Relationships between atmospheric residence time  $\tau_a$  and atmospheric spatial range  $R$  and travel distance  $L$ . The lines show the analytical expressions for advective and macro-diffusive transport. The dots indicate the model results obtained for selected chemicals with a global model for diffusive transport described in ref (3); the chemicals are released to air. The letters indicate: a) *p*-cresol; b) dioxane, cyclohexane, toluene, octane (similar results); c) methyl *t*-butyl ether; d) chlorotoluene; e) benzene; f) chlorobenzene.

Additionally, the results for the atmospheric residence time and the spatial range calculated with a global fate model are shown for selected chemicals (dots). This model, which is described in ref (3), is based on the analytical diffusive transport model, and is a steady-state multimedia model including diffusive transport in air and water. In Figure 1, the comparison of the model results with the analytical expression  $R = 6.00 \sqrt{D_{\text{eddy}} \cdot \tau_a}$  is based on release to air. In the next subsection, this model is used with release to soil and the results are plotted in Figure 4 to investigate the correlation between spatial range and overall persistence.

The model consists of a closed loop of 80 cells, each identical to a single level III multimedia model with soil, water and air subcompartments. In this loop with circumference  $G = 40\,000$  km, the one-dimensional global circulation of chemicals is modelled. Based on macro-diffusive transport in air with  $D_{\text{eddy}} = 2 \cdot 10^6 \text{ m}^2/\text{s}$  (and first order degradation and phase partitioning), the model yields the steady-state concentrations for each subcompartment of the 80 cells. The atmospheric concentration distribution of perchloroethylene is shown as an example in Figure 2. For details of the model, see ref (3).

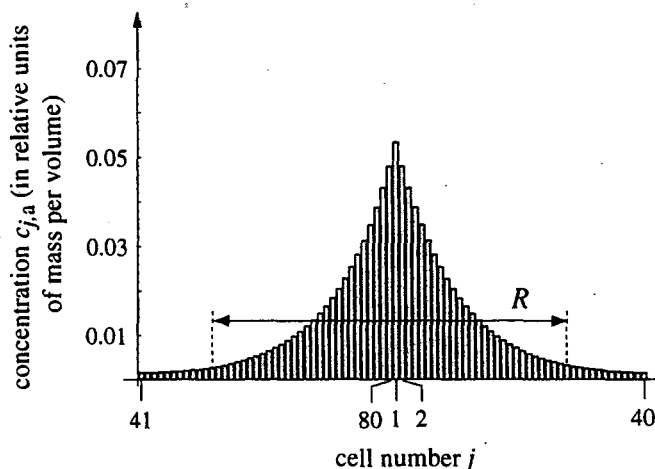


Figure 2. Atmospheric steady-state concentrations  $c_{j,a}$  of perchloroethylene vs. cell number  $j$  in the circular global model. The distribution  $\{c_{j,a}\}_{j=1,\dots,80}$  is normalized to 1. The chemical is released to air at  $j = 1$ . In this graphic representation of the circular system, the adjacent cells 40 and 41 appear separated. The spatial range is  $R = 68.5\%$ , see dot "perchloroethylene" in Figure 1.

The atmospheric residence time after emission to air at cell  $j = 1$  was calculated according to

$$\tau_a = \frac{1}{Q} \sum_{j=1}^{80} c_{j,a} \cdot v_j = \frac{M_{\text{air}}^{\text{stst}}}{Q} \quad (10)$$

with the continuous source term  $Q$  (in kg/s), the atmospheric steady state concentrations  $c_{j,a}$  in the cells  $j$  with volume  $v_j$ , and the steady-state mass in air  $M_{\text{air}}^{\text{stst}}$  (in kg). The spatial range was derived as the 95% interquartile range from the spatial concentration distributions, see Figure 2 and eq 3.

For chemicals with  $\tau_a < 100$  d, the model results are described by the analytical expression  $R = 6.00 \sqrt{D_{\text{eddy}} \cdot \sqrt{\tau_a}}$ . Perchloroethylene with  $\tau_a = 127$  d shows a slightly lower spatial range than predicted by this analytical expression. This is due to the fact that the model assumes a closed circular world with an upper limit for the spatial range of  $G = 40\,000$  km while the analytical expression is valid for an "open" world and

predicts unlimited spatial ranges for increasing  $\tau_a$ . Chemicals with even higher atmospheric residence time such as tetrachloromethane and CFCs do not follow the analytical expression but show a constant spatial range of 95% of the global circumference. In Figure 3, the model results for an expanded set of chemicals, including very persistent ones, are shown on a logarithmic scale for the atmospheric residence time.

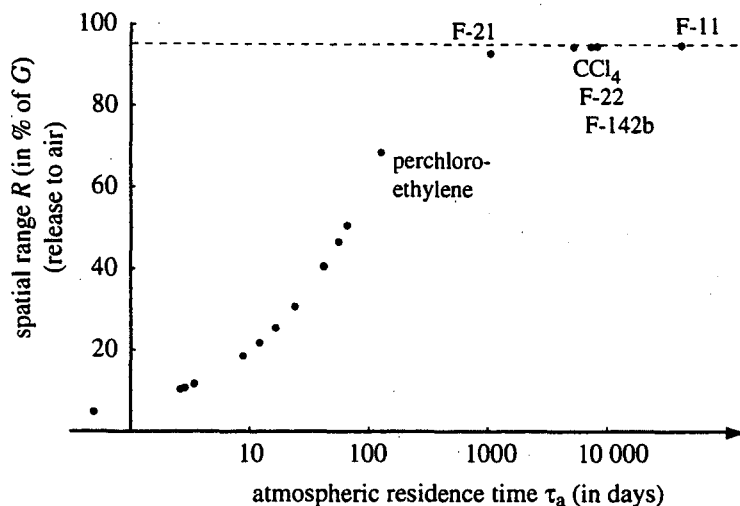


Figure 3. Model results for atmospheric spatial range  $R$  and atmospheric residence time  $\tau_a$  for an expanded set of chemicals. The chemicals are released to air.  $\tau_a$  is given on a logarithmic scale. The chemicals at the lower end of the scale are the same as in Figure 1. The dashed horizontal line indicates the upper limit of  $R = 95\%$  of  $G$ .

#### Relationship between Spatial Range and Overall Persistence

The analytical relationships plotted in Figure 1 demonstrate that  $R$  and  $L$  can be calculated directly from the atmospheric residence time  $\tau_a$ . On the one hand, this is useful but on the other hand,  $\tau_a$  is a compartment specific residence time which does not provide the most comprehensive information on a chemical's environmental lifetime because it is determined by both degradation *and* transfer to other compartments (15). Efficient removal through deposition processes can lead to a low atmospheric residence time for a chemical that may be persistent in water or soil. Therefore, it is more informative to combine the spatial range with the *overall* persistence of the chemicals in one diagram so that information on the chemicals' actual lifetime and their phase partitioning is included. However, the relation between overall persistence (denoted by  $\tau$ ) and spatial range cannot be described by an analytical expression. Figure 4 shows the plot of  $R$  versus  $\log \tau$  for the same set of chemicals plotted in Figure 3 (dots) and, in addition, for the 12 POPs and lindane (lines) (4). As can be seen in the figure, there is not a

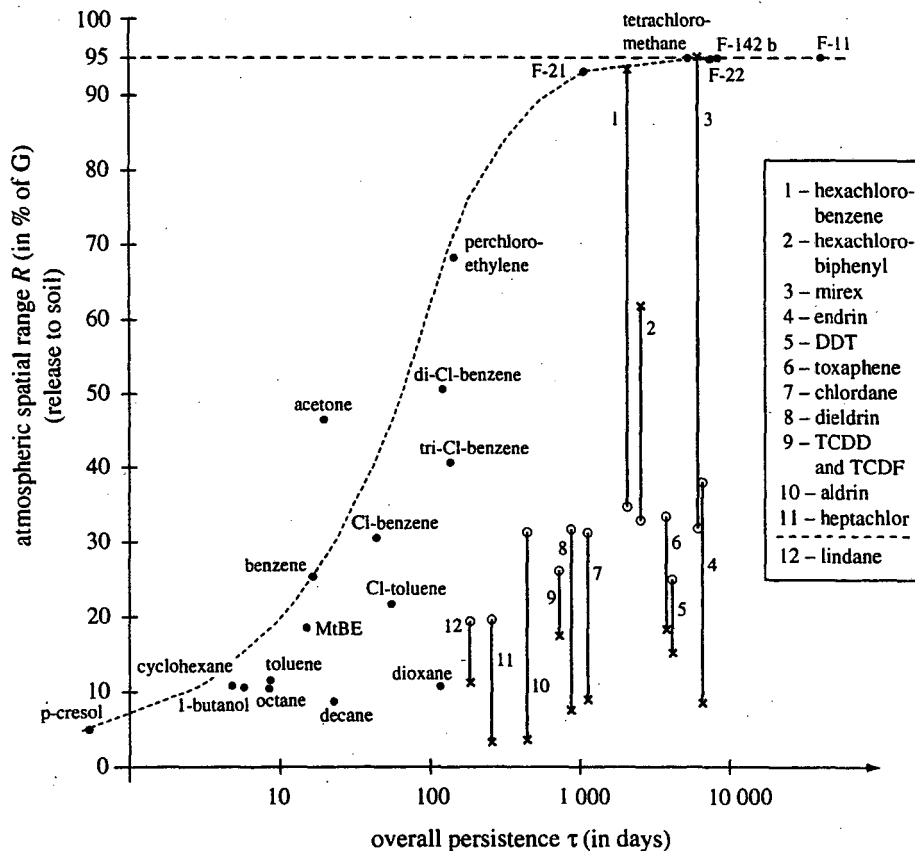


Figure 4. Model results for atmospheric spatial range  $R$  and overall persistence  $\tau$  for the chemicals from Figure 3 and for the 12 POPs and lindane. All chemicals are released to the soil. The persistence values are given on a logarithmic scale. The dashed curve is the interpolated  $R(\tau_a)$  relation of Figure 3. The dashed horizontal line indicates the upper limit of  $R = 95\%$ . The vertical lines represent spatial range intervals which are obtained if the adsorption of the POPs to aerosol particles is varied between 0% (x) and 100% (o).

well defined relationship between these two measures. All chemicals were released to the soil, i. e. the immobile compartment, so that they have to volatilize before they are transported with the macro-diffusive air flow. However, the dynamics of the transport in air is independent of the size of the airborne fraction of the chemical. This means that the numerical values of the atmospheric spatial range  $R$  for release to soil (Figure 4) are almost the same as for release to air (Figure 3).

The overall persistence  $\tau$  was calculated according to

$$\tau = \frac{1}{Q} \sum_{i=s,w,a} \sum_{j=1}^{80} c_{i,j} \cdot v_{i,j} = \frac{M_{\text{tot}}^{\text{sst}}}{Q}, \quad (11)$$

compare eq 10.  $M_{\text{tot}}^{\text{sst}}$  is the amount of chemical that is contained in the entire model system in the steady state.

The dashed curve in Figure 4 is the interpolated  $R(\tau_a)$  relation of Figure 3. Most of the chemicals lie on the right of this line. This is due to the fact that their degradation rate constants in soil are lower than the degradation rate constants in air so that the fraction in soil is degraded more slowly than the fraction in air. Under this conditions, the overall persistence  $\tau$  is higher than the atmospheric residence time  $\tau_a$  while the spatial range is nearly the same as for release to the air. This effect is very pronounced for dioxane and the the semivolatile organochlorines at the lower ends of the lines.

There are some chemicals whose overall persistence  $\tau$  is very close to the atmospheric residence time  $\tau_a$  (benzene, perchloroethylene, the CFCs). This is observed if the degradation rate constants in soil, water and air are (almost) the same or if the chemical is so volatile that the overall persistence is essentially independent of the degradation rate constants in water and soil.

Finally, acetone has an atmospheric degradation rate constant which is *lower* than that in the soil. In this case, release to the soil leads to an overall persistence  $\tau$  which is lower than the atmospheric residence time  $\tau_a$ . For this reason, acetone is on the left of the  $R(\tau_a)$  line in Figure 4.

The spatial ranges of the semivolatile organochlorines are subject to considerable uncertainty because the atmospheric degradation and transport of these chemicals is strongly influenced by adsorption to aerosol particles (16, 17, 18). The vertical lines shown in Figure 4 represent the entire range from 0% adsorption (indicated by  $\times$ ) to 100% adsorption (indicated by  $\circ$ ); for details, see (4). Although these extremes do not reflect realistic conditions for all of the chemicals (rather volatile compounds such as hexachlorobenzene are not completely adsorbed to particles under most environmental conditions), they are shown here to illustrate the possible influence of the aerosol particles and the sensitivity of the spatial range to this model parameter.

### Influence of Phase Partitioning and Path of Release

As apparent from Figure 4, many chemicals that have a large overall persistence do not necessarily have a large spatial range. It is desirable to try to understand the relationship between the spatial range and the overall persistence in the environment. To this end, we calculated the ratio of the atmospheric spatial range after release to the soil (the  $R$  values of the dots in Figure 4) and the atmospheric spatial range given by the  $R(\tau_a)$  line for the given  $\tau$  value. Thus, this ratio, which is denoted by  $r$ , quantifies the vertical deviation of the dots in Figure 4 from the dashed  $R(\tau_a)$  line in Figure 4. The ratio  $r$  is lower for chemicals that tend to partition out of the atmosphere, such that there is a positive correlation to vapor pressure and Henry's law constant ( $H$ ) and a negative correlation

to the octanol-water and octanol-air ( $K_{oa}$ ) partitioning coefficients. The comparisons revealed that  $\log K_{oa}$  is actually the best descriptor for this trend. In Figure 5, we plot  $r$  versus  $\log K_{oa}$  for the chemicals from Figure 4. The plot shows a continuous trend to lower  $r$  values if  $\log K_{oa}$  increases. The chemicals with  $r \approx 1$  are the CFCs, perchloroethylene, benzene, and p-cresol; they lie on the  $R(\tau_a)$  line in Figure 4. Acetone is the only chemical with  $r > 1$ ; dioxane has  $r = 0.15$  and  $\log K_{oa} = 0.036$ . For the POPs, the arithmetic means of the  $R$  intervals of Figure 4 were used in this analysis.

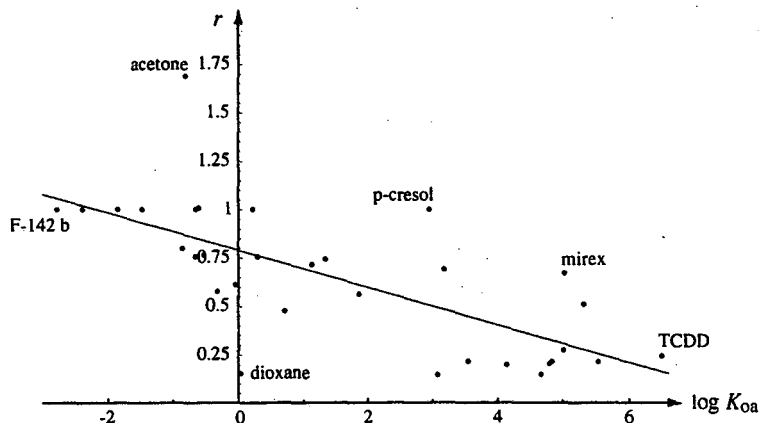


Figure 5. Correlation of  $\log K_{oa}$  with the ratio  $r$  of the calculated spatial range indicated by the dots in Figure 4 and the spatial range determined by the curve  $R(\tau_a)$  in Figure 4. The chemicals are released to soil.  $K_{oa}$  equals  $K_{ow}/H$  with  $H$  in  $\text{Pa m}^3/\text{mol}$ . The line is obtained by linear regression.

It is important to note that there is not a perfect correlation between  $r$  and  $\log K_{oa}$  in Figure 5 because a chemical's partitioning between the environmental media in a steady-state condition is not influenced by the partitioning coefficients alone, but also by advective exchange processes such as wet deposition and by the degradation rates in the environmental media, which can be very different for the same  $\log K_{oa}$  value.

Another factor influencing the spatial range relative to the overall persistence is whether a chemical is released to the air or to the soil. Many chemicals are degraded more rapidly in the air than in the soil. Thus, if a chemical is released to the air, the overall persistence is likely to be lower than if the chemical is released to the soil. Figure 6 shows the  $r$ - $\log K_{oa}$  correlation for this situation. It can be seen that all non-adsorbing chemicals (dots in Figure 4) except dioxane have  $r$  values close to 1. There is a sharp decrease in  $r$  at  $\log K_{oa} \approx 3$ , leading to  $r$  values below 0.3 for most of the POPs. These results indicate that the overall persistence of the volatile chemicals is dominated by the atmospheric degradation rate constant while the degradation rate constants in water and soil and the partitioning coefficients do not have a significant influence on  $\tau$ . Thus, the overall persistence  $\tau$  is close to the atmospheric residence time  $\tau_a$  and much lower than for the "release to soil" scenario. The POPs, on the other hand, are transferred to the soil by diffusion and deposition, where they have low degradation rate constants. Thus

their overall persistence is not as strongly influenced by the degradation rate constant in air and their overall persistences are higher than their atmospheric residence times.

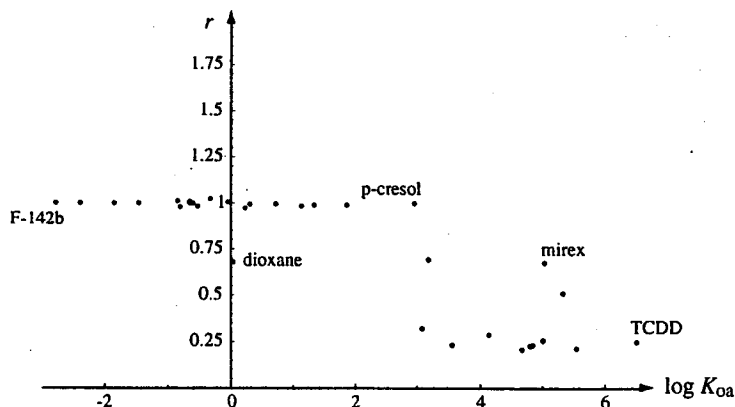


Figure 6. Correlation of  $\log K_{0a}$  with the ratio  $r$  of the calculated spatial range and the spatial range determined by the curve  $R(\tau_a)$ . In this case, the chemicals are released to air. A plot such as in Figure 4 is not shown for this case because most of the  $(\tau, R)$  points would be very close to the  $R(\tau_a)$  curve.

These results illustrate that modeling a release to air is suitable only if we want to calculate the atmospheric residence time or if the chemical is actually released to the air. In general, this scenario is less interesting than release to the soil because there is often less multimedia partitioning for a release to air than to soil, and thus the different degradation rate constants are not as influential if the release is to air. If one is not sure what medium the chemical will be released to, model calculations with release to the air should be complemented by calculations with release to the soil which provide more insight into the chemicals' phase partitioning and overall degradability.

## Conclusions

In conclusion,  $R, \tau$ -diagrams such as in Figure 4 are useful for the screening of the exposure behavior of larger sets of chemicals. High overall persistence and high spatial range are unwanted properties which indicate a chemical's potential to cause problematic environmental exposure.

In addition to the screening of a variety of chemicals,  $R, \tau$ -diagrams can be used to visualize details of the complex environmental fate of specific chemicals such as the POPs. In Figure 4, the sensitivity of the atmospheric spatial range of the POPs to the extent of adsorption to particles is shown. The modeling results of such a particular focus can be aggregated and communicated by means of a  $R, \tau$ -diagram.

Both aspects, exposure screening of a larger set of chemicals and analyzing details of the transport and degradation behavior of selected chemicals, are relevant for the future debate on chemicals regulation and for the assessment of possible POPs candidates.

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