Supplementary Information


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1 Chemical Property Data for the 14 Reference Chemicals

Table S1: Physical-chemical properties and degradation rate constants of the 14 chemicals selected for the $P_{sv}$ and LRTP rankings.

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Vapor pressure $P_{sv}$ (25ºC)</th>
<th>Solubility $K_{sv}$</th>
<th>$K_{aw}$</th>
<th>$K_{ow}$</th>
<th>$k_{air}$</th>
<th>$k_{soil}$</th>
<th>$k_{water}$</th>
<th>$k_{sed}$</th>
<th>$k_{veg}$</th>
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<tbody>
<tr>
<td>aldrin</td>
<td>6.37E-2</td>
<td>2.63E-3</td>
<td>9.77E-3</td>
<td>1.78E+6</td>
<td>6.64E-5</td>
<td>5.03E-8</td>
<td>7.20E-8</td>
<td>7.20E-9</td>
<td>6.64E-5</td>
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<tr>
<td>atrazine</td>
<td>3.87E-5</td>
<td>1.42E-1</td>
<td>1.10E-7</td>
<td>5.62E+2</td>
<td>3.11E-5</td>
<td>2.36E-7</td>
<td>2.33E-7</td>
<td>1.91E-8</td>
<td>3.11E-5</td>
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<tr>
<td>BDE-47</td>
<td>2.15E-4</td>
<td>1.94E-4</td>
<td>4.46E-4</td>
<td>2.43E+6</td>
<td>7.52E-7</td>
<td>9.63E-9</td>
<td>9.63E-9</td>
<td>7.52E-7</td>
<td>7.52E-7</td>
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<td>biphenyl</td>
<td>4.21E</td>
<td>1.66E-1</td>
<td>1.05E-2</td>
<td>1.10E+4</td>
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<td>3.50E-7</td>
<td>1.13E-6</td>
<td>1.13E-7</td>
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<td>CCl4</td>
<td>1.65E+4</td>
<td>4.64E</td>
<td>1.44E</td>
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<td>2.90E-10</td>
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<td>3.09E-2</td>
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<td>5.64E-9</td>
<td>5.64E-9</td>
<td>5.64E-10</td>
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<td>2.42E+4</td>
<td>1.62E-8</td>
<td>4.58E-8</td>
<td>8.02E-8</td>
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<td>1.62E-8</td>
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<td>3.02E-5</td>
<td>7.41E-3</td>
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<td>3.50E-10</td>
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<td>1.16E-7</td>
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<td>1.32E-4</td>
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<td>3.09E-3</td>
<td>1.41E+7</td>
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<td>1.13E-8</td>
<td>7.55E-7</td>
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<tr>
<td>p-cresol</td>
<td>1.51E+1</td>
<td>1.10E+2</td>
<td>5.51E-5</td>
<td>9.33E+1</td>
<td>3.21E-5</td>
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<td>α-HCH</td>
<td>2.26E-1</td>
<td>3.55E-1</td>
<td>2.57E-4</td>
<td>7.59E+3</td>
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<td>5.94E-8</td>
<td>5.94E-8</td>
<td>3.50E-9</td>
<td>1.02E-7</td>
</tr>
</tbody>
</table>

2 Description of the Seven Models

**EVn-BETR**

The European Variant Berkeley–Trent model (EVn-BETR) is a fugacity-based model (Mackay, 2001) that comprises 50 regions, with 4 regions in the periphery to describe the world outside Europe. Each region represents an area of approximately 500 km x 500 km (5°x5°), with the whole model domain covering an area from 38.7 °N to 61.1 °N latitude and 10.1°W to 39.4 °E longitude (Prevedouros et al., 2004). Each region consists of seven environmental compartments: lower (0–1000 m) and upper air (1000–2000 m), soil, vegetation, ocean water, fresh water and sediment. Detailed information on the model construction can be found in MacLeod et al. (2001) and Woodfine et al. (2001). In Evn-BETR, the long-range transport potential of chemicals is calculated as the average distance from a point source at which the chemical’s concentration has dropped to 38% (1/e) of its initial concentration. The average distance is calculated using the predicted air concentrations in the eight boxes surrounding the source box.

The atmospheric transport between EVn BETR grid cells has been derived from historical data derived from the European Centre for Medium-Range Weather Forecasts (ECMWF) global circulation model. Forward trajectory data were calculated using 6-hourly operational analyses of the three components of the wind and surface pressure, which were then interpolated on to a 1.5° by 1.5° grid. The output data from the trajectories consisted of latitude, longitude and pressure of the trajectory every 30 min. Air was allowed to move freely to all other regions within the two atmospheric heights of 500 and 2000 m above sea level. The trajectory data were then used to produce an average wind rose for all the model segments for the period of study (1997–2001). The wind roses were then converted into a connectivity flux matrix for each atmospheric height, using a matrix technique described by Woodfine et al. (2001).

**MSCE-POP**

MSCE-POP is a multi-compartment atmospheric transport model, describing processes in and exchange between four environmental compartments (atmosphere, soil, sea water, and vegetation). Except the vegetation compartment, all compartments are vertically segmented into a number of layers. There are regional and
hemispherical versions of the model. The spatial resolution of the latter version, which was used in the EMEP POP model inter-comparison study, is 2.5 x2.5° and the model domain covers the total Northern Hemisphere. Lateral transport of compounds by air and by seawater is taken into account in the model. (Malanichev et al., 2004, Gusev et al., 2005).

ClimoChem

ClimoChem is a multi-compartment mass balance box model that covers the entire global system. Compartments included are soil, oceanic surface water, troposphere air, vegetation and vegetation soil. ClimoChem consists of a flexible number (typically 10 to 30) of latitudinal zones with different temperatures and compartment volumes. ClimoChem does not have a spatial resolution in the East-West direction; in North-South direction, the spatial resolution is given by the number of zones, $n$, and the width of a zone is equal to $180/n$ degrees latitude (Scheringer et al., 2000). The transport mechanism implemented in the model is large-scale eddy diffusion in atmosphere and oceans. Eddy diffusion coefficients have been derived from tracer measurements in atmosphere and ocean water (Keeling and Heimann, 1986; Okubo, 1971). For the atmosphere, these eddy diffusion coefficients represent the long-term average of the intra- and interhemispheric mixing. For the ocean, they represent the growth of a “patch” of contaminant that is caused by turbulent mixing caused by large-scale eddies. In the ClimoChem model, they describe the exchange of air and water between adjacent latitudinal zones.

SimpleBox

SimpleBox is a nested level III and level IV ‘Mackay type’ multimedia fate model consisting of ten environmental compartments on local, regional, continental and global scales (Brandes et al., 1996; Den Hollander et al., 2004). The regional and continental scales distinguish an air compartment (atmospheric mixing layer), a sea water compartment with a sediment compartment, a fresh water compartment with a sediment compartment, and three types of soil compartments (natural, agricultural, other soil) with corresponding vegetation compartments. SimpleBox is a generic model, in which the default settings are set to match the European Union procedures for the evaluation of substances (Brandes et al., 1996). Advective transport (e.g. wet and dry deposition, wind flow, water transport, sedimentation), as well as diffusive
transport (e.g. gaseous deposition, volatilization) between the different environmental compartments and spatial scales is accounted for in the model. Since SimpleBox is a non-spatial model, transport distances of chemicals are not calculated directly. The relative long-range transport potential of a compound can be estimated based on the fraction of the amount released that is exported across the boundaries of the model: for chemicals with high LRT, this fraction is close to one, for chemicals with low LRT, this fraction is close to zero.

ADEPT

ADEPT (Atmospheric DEPosition and Transport model for risk assessment) is a diagnostic model that calculates concentrations in air and deposition fluxes to the underlying surface; Roemer et al., 2004). The model is derived from the LOTOS-EUROS model (Schaap et al., 2005). It covers the European continent (30°N-70°N; and 10°W to 60°E), but it can be adjusted to sub-domains. There is no exchange with water, soil and vegetation, only a flux (loss term) to the underlying surface. Transport characteristics are taken from the LOTOS-EUROS model by means of source receptor matrices for inert species. Loss by chemistry, wet and dry deposition is modeled on the basis of the average transport time from source to receptor, and by means of average values for OH, O3, photolysis, atmospheric and surface resistances, precipitation and Henry coefficients.

G-CIEMS

G-CIEMS is a GIS-based geo-referenced multimedia fate model consisting of environmental compartments of gridded air cells, polygon and line-based surface catchments and river structures, and polygon-based sea segments (Suzuki et al., 2005). The model is now mainly applied to the Japan-regional environment with detailed (ca. 5 km) resolutions. As the model is flexible to any geographical conditions within the computational limitations, a generic simple framework consisting of only several boxes including the specified European modeling domain and surrounding areas was used in this study, so that essential comparison of the multimedia fate processes would be possible.
# Statistics of $P_{ov}$ and LRTP Rankings of the 14 Reference Chemicals

Table S2: average deviations of $P_{ov}$ rankings from average ranking of the 14 chemicals: average over all 14 chemicals in each of the 6 models (left) and average over the 6 models for each chemical (right).

<table>
<thead>
<tr>
<th>model</th>
<th>average deviation of all 14 chemicals</th>
<th>chemical</th>
<th>average deviation of all 6 models</th>
</tr>
</thead>
<tbody>
<tr>
<td>CliMoChem</td>
<td>0.428</td>
<td>p-cresol</td>
<td>0.333</td>
</tr>
<tr>
<td>MSCE-POP</td>
<td>0.428</td>
<td>CCl4</td>
<td>0.333</td>
</tr>
<tr>
<td>G-CIEMS</td>
<td>0.428</td>
<td>a-HCH</td>
<td>0.50</td>
</tr>
<tr>
<td>OECD Tool</td>
<td>0.571</td>
<td>BDE-47</td>
<td>0.50</td>
</tr>
<tr>
<td>SimpleBox</td>
<td>1.0</td>
<td>aldrin</td>
<td>0.667</td>
</tr>
<tr>
<td>EVN-BETR</td>
<td>1.29</td>
<td>biphenyl</td>
<td>0.667</td>
</tr>
<tr>
<td></td>
<td></td>
<td>BDE-99</td>
<td>0.667</td>
</tr>
<tr>
<td></td>
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<td>HCB</td>
<td>0.667</td>
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<td></td>
<td>PCB-180</td>
<td>0.667</td>
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<td></td>
<td></td>
<td>atrazine</td>
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<td></td>
<td></td>
<td>BaP</td>
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<td></td>
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<td>PCB-28</td>
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<td>PCB-153</td>
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<tr>
<td></td>
<td></td>
<td>HCBD</td>
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<tr>
<td></td>
<td>average of all 14 chemicals</td>
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<td>0.69</td>
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</table>

average of all 14 chemicals
Table S3: average deviations of LRTP rankings from average ranking of the 14 chemicals: average over all 14 chemicals in each of the 8 models (left) and average over the 8 models for each chemical (right).

<table>
<thead>
<tr>
<th>model</th>
<th>average deviation of all 14 chemicals</th>
<th>chemical</th>
<th>average deviation of all 8 models</th>
</tr>
</thead>
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<td>OECD Tool (CTD)</td>
<td>0.714</td>
<td>p-cresol</td>
<td>0.375</td>
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<td>OECD Tool (TE)</td>
<td>1.0</td>
<td>aldrin</td>
<td>0.5</td>
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<td>1.29</td>
<td>BaP</td>
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<td>MSCE-POP</td>
<td>1.29</td>
<td>BDE-47</td>
<td>1.125</td>
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<td>1.29</td>
<td>HCB</td>
<td>1.375</td>
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<tr>
<td>EVN-BETR</td>
<td>1.43</td>
<td>CCl4</td>
<td>1.375</td>
</tr>
<tr>
<td>ADEPT</td>
<td>2.0</td>
<td>PCB-153</td>
<td>1.375</td>
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<tr>
<td>CliMoChem</td>
<td>2.43</td>
<td>HCBD</td>
<td>1.5</td>
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<tr>
<td></td>
<td></td>
<td>biphenyl</td>
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<td>atrazine</td>
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<td>PCB-180</td>
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<td>BDE-99</td>
<td>2.25</td>
</tr>
<tr>
<td></td>
<td></td>
<td>average of all 14 chemicals</td>
<td>1.43</td>
</tr>
</tbody>
</table>
### Mass Balance Estimates for PCB-153 in the Year 2000

#### Volumes

**MSGE-COP** | **CMBChrom** | **SimpleBox** | **I-Va-HRET** | **G-CHEM**
---|---|---|---|---
air (m³) | 1.28E+17 | 6.18E+16 | 9.80E+15 | 1.06E+16 | 1.20E+17
water (m³) | 9.69E+14 | 8.41E+14 | 1.05E+14 | 4.29E+14 | 3.94E+14
sediment (m³) | 3.12E+12 | 5.02E+11 | 1.18E+11 | 1.56E+10 | 3.55E+11
vegetation (m³) | nr | 5.01E+09 | 8.34E+09 | 3.26E+09 | 6.28E+08

#### Concentration 2000

**C**

- **air (pg/m³):**
  - Interface with ocean: 3.7
  - Interface with soil: 7.4
  - Interface with vegetation: 7.4

- **water (pg/L):**
  - Interface with atmosphere: 0.18

- **sediment (pg/g):**
  - Interface with atmosphere: 6.2

#### Mass 2000

**kg**

- **air:**
  - Total: 107

- **water:**
  - Total: 1258

- **sediment:**
  - Total: 604

- **soil:**
  - Total: 11187

- **vegetation:**
  - Total: 101

#### Changes in inventory from 1999 to 2000

**kg/yr**

- **air:**
  - Total: 107

- **water:**
  - Total: 1258

- **sediment:**
  - Total: 604

- **soil:**
  - Total: 11187

- **vegetation:**
  - Total: 101

#### Mass balances for individual media

**kg/yr**

- **air:**
  - Total: 107

- **water:**
  - Total: 1258

- **sediment:**
  - Total: 604

- **soil:**
  - Total: 11187

- **vegetation:**
  - Total: 101

#### Mass budget

- **emission to model domain:**
  - Total: 586

- **net export from domain:**
  - Total: 584

- **reaction in air:**
  - Total: 45

- **reaction in water:**
  - Total: 33

- **reaction in sediment:**
  - Total: 2276

- **reaction in soil:**
  - Total: 4343

- **reaction in vegetation:**
  - Total: 0

- **burial in sediment:**
  - Total: 75

- **leaching from soil:**
  - Total: 0.44

- **deposition of dry fall:**
  - Total: 1213

- **deposition of wet fall:**
  - Total: 9660

#### Intermedia flow

- **dry deposition to water:**
  - Total: 35

- **wet deposition to water:**
  - Total: 40

- **gas absorption to water:**
  - Total: 420

- **dry deposition to soil:**
  - Total: 1140

- **wet deposition to soil:**
  - Total: 235

- **gas absorption to soil:**
  - Total: 4200

- **dry deposition to vegetation:**
  - Total: 246

- **wet deposition to vegetation:**
  - Total: 26

- **gas absorption to vegetation:**
  - Total: 1410

- **total deposition to vegetation:**
  - Total: 1247

- **total atmospheric deposition:**
  - Total: 2057

- **sedimentation:**
  - Total: 590

- **run off to surface water:**
  - Total: 35

- **litter fall to soil:**
  - Total: 1271

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### Table

<table>
<thead>
<tr>
<th>Medium</th>
<th>Volume (m³)</th>
<th>Concentration 2000 (pg/m³)</th>
<th>Mass Balance Estimates (kg)</th>
<th>Changes in Inventory (kg/yr)</th>
<th>Mass Balances for Individual Media (kg/yr)</th>
<th>Mass Budget (kg/yr)</th>
<th>Intermedia Flow (kg/yr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>air</td>
<td>1.26E+17</td>
<td>0.44</td>
<td>107</td>
<td>-35</td>
<td>-40</td>
<td>586</td>
<td>35</td>
</tr>
<tr>
<td>water</td>
<td>9.69E+14</td>
<td>3.7</td>
<td>1258</td>
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<td>-40</td>
<td>584</td>
<td>40</td>
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<td>604</td>
<td>20</td>
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<td>-702</td>
<td>-25</td>
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<td>101</td>
<td>-0</td>
<td>-0.1%</td>
<td>101</td>
<td>0</td>
</tr>
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</table>

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### Footnotes

- **C**: Concentration
- **kg**: Kilograms
- **mg**: Milligrams
- **pg**: Picograms
- **L**: Liters
- **g**: Grams

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8
References


