Item 6. Progress in activities in 2011 and future work

a) Measurements and modelling  
(Persistent Organic Pollutants)

Victor Shatalov

on behalf of CCC and MSC-E
Main CCC/MSC-E activities on POPs in 2011

EMEP Work-Plan for 2011 [ECE/EB.AIR/2010/5]
CLRTAP long-range strategy [ECE/EB.AIR/106/add.1]
HTAP Assessment 2010

- **Routine activities**
  - Evaluation of pollution levels and transboundary transport for PAHs, PCDD/Fs and HCB (priority pollutants).

- **New developments**

Steering Body to EMEP (September 5 – 7, 2011)
Main CCC/MSC-E activities on POPs in 2011

- New developments
  - Application of integrated monitoring/modelling/emission approach.
  - Global transport of POP pollutants (oceanic transport).
  - Climate change and POP inter-linkages (influence of meteorological parameters on POP fate).
Integrated monitoring/modelling/emission approach

Step 1. Initial assessment
- Emission data – CEIP
- Model parameterization
- Monitoring data – CCC

Step 2. Evaluation of agreement between calculations and measurements

Step 3. Analysis of discrepancies (model parameterization, emission inventories, monitoring data)
- In collaboration with national experts

Step 4. Refined assessment

Steering Body to EMEP (September 5 – 7, 2011)
Integrated approach, B[a]P

Step 1: Preliminary assessment (B[a]P)

Emissions of B[a]P in the EMEP domain in 2009

Calculated B[a]P air concentrations in 2009

Evaluation of agreement (step 2)

Statistical indicators

Model calculations

Steering Body to EMEP (September 5 – 7, 2011)
<table>
<thead>
<tr>
<th>Indicator</th>
<th>Meaning</th>
<th>Threshold</th>
</tr>
</thead>
<tbody>
<tr>
<td>FAC2</td>
<td>Fraction of agreements within a factor of 2</td>
<td>&gt; 50%</td>
</tr>
<tr>
<td>Correlation coefficient</td>
<td>Agreement of variability</td>
<td>&gt; 0.6</td>
</tr>
<tr>
<td>Regression coefficient</td>
<td></td>
<td>1 ± 0.3</td>
</tr>
<tr>
<td>Normalized mean bias</td>
<td>Characterization of systematic error</td>
<td>&lt; 0.2</td>
</tr>
<tr>
<td>Student ratio</td>
<td></td>
<td>95% confidence level</td>
</tr>
</tbody>
</table>
Step 2: Evaluation of agreement

Integrated approach, B[a]P

Comparison with measurements

<table>
<thead>
<tr>
<th>Indicator</th>
<th>All sites</th>
<th>Without PL5</th>
<th>Threshold</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fac 2</td>
<td>75%</td>
<td>85.7%</td>
<td>&gt; 50%</td>
</tr>
<tr>
<td>Correlation</td>
<td>0.57</td>
<td>0.84</td>
<td>&gt; 0.6</td>
</tr>
<tr>
<td>Regr.</td>
<td>1.32</td>
<td>0.70</td>
<td>1 ± 0.3</td>
</tr>
<tr>
<td>NMB</td>
<td>0.16</td>
<td>-0.19</td>
<td>&lt; 0.2 (abs.val)</td>
</tr>
<tr>
<td>Student Ratio</td>
<td>0.56</td>
<td>-1.31</td>
<td>&lt; 2.36 (abs.val)</td>
</tr>
</tbody>
</table>

Steering Body to EMEP (September 5 – 7, 2011)
Integrated approach, B[a]P

Step 3: analysis of discrepancies

Comparison with measurements

Seasonal variations are important for PAH assessment

Emissions and measurement sites

PL5

3 times lower than at PL5

Annual averages

Non-complete year

Monthly averages

Step 3: analysis of discrepancies

Steering Body to EMEP (September 5 – 7, 2011)
Integrated approach, temporal resolution

Modification of emission seasonal variations for B[a]P

Current seasonal variations (SV) – Baart et al., 1995

Morville et al., 2011:
For air concentrations Max/Min = up to 9 times

Current and modified emission seasonal variations (SV) for B[a]P

Steering Body to EMEP (September 5 – 7, 2011)
Integrated approach, temporal resolution

Improvements resulting from emission modification (B[a]P)

Comparison of calculation results with measurements

Steering Body to EMEP (September 5 – 7, 2011)
Assessment of PCDD/Fs

The work is performed in collaboration with national experts (IVL, Stockholm University and Umeå University)

Evaluation of EMEP contamination by PCDD/F mixture in 2009
Examination of congener composition of PCDD/F mixture

Measurements used:
- congener-specific daily averages of air concentrations (SE12 and FI96) with wind direction specification
- congener-specific monthly means of deposition fluxes (SE35)

Period: 2006 – 2007
Congeners considered:
- 2,3,4,7,8-PeCDF (congeners fraction: 30 – 40% of total toxicity)
- 1,2,3,7,8,9-HxCDD
- OCDD
- OCDF

Data on emission congener composition: POPCYCLING-BALTIC project

Steering Body to EMEP (September 5 – 7, 2011)
Integrated approach, PCDD/Fs

Step 2: comparison with measurements

(2,3,4,7,8-PeCDF)

South-West (SW)

East (E)

NNE/NNW/NW

Air concentrations (site SE12)

Steering Body to EMEP (September 5 – 7, 2011)
Integrated approach, PCDD/Fs

Step 2: comparison with measurements

(2,3,4,7,8-PeCDF)

Air concentrations (site SE12)

Steering Body to EMEP (September 5 – 7, 2011)
**Integrated approach, PCDD/Fs**

**Scenario calculations (2,3,4,7,8-PeCDF)**

Correction factors:

- **emission totals:***
  - Poland: 1.5
  - Russian West: 3

- **congener fraction:** 1.7

<table>
<thead>
<tr>
<th>Indicator</th>
<th>Base Scen</th>
<th>Threshold</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fac</td>
<td>2</td>
<td>54%</td>
</tr>
<tr>
<td>Corr.</td>
<td>0.58</td>
<td>&gt; 0.6</td>
</tr>
<tr>
<td>Regr.</td>
<td>1.89</td>
<td>1 ± 0.3</td>
</tr>
<tr>
<td>NMB</td>
<td>0.63</td>
<td>&lt; 0.2</td>
</tr>
<tr>
<td>SR</td>
<td>4.77</td>
<td>&lt; 2.1</td>
</tr>
</tbody>
</table>

**Similar work was carried out for 1,2,3,7,8,9-HpCDD, OCDF and OCDD**

Steering Body to EMEP (September 5 – 7, 2011)
Integrated approach, PCDD/Fs

Scenario calculations (PCDD/Fs)

Variations of congener composition with constant toxicity

Correction factor = 1.7 (fraction of total toxicity becomes 30% \times 1.7 = 51%)

Correction factor = 3

2,3,4,7,8-PeCDF

Correction factor = 6

1,2,3,7,8,9-HxCDD

Correction factor = 6

OCDF

Requires additional consideration

OCDD

Deposition flux (site SE35)

Steering Body to EMEP (September 5 – 7, 2011)
Peculiarities of OCDD

OCDD can be generated in air by atmospheric reactions involving other contaminants (PCP) \[Baker and Hites, 2000\]

Contributions of OCDD to D&F toxicity in PCP preparations ranges from 60% to 90%. \[SEPA report, 2009\]

Simultaneous modelling of OCDD and PCP can refine the assessment

Data on congener composition in emissions in countries are one of key points for evaluation of pollution levels

A paper “Modelling the Atmospheric Transport and Deposition to the Baltic Sea” in co-authorship with Swedish experts is in preparation

Steering Body to EMEP (September 5 – 7, 2011)
Assessment of HCB contamination in EMEP

Re-volatilization from soil is one of the most important sources of HCB contamination

[Barber et al., 2005] (EuroClor Science Dossier)

Mass of HCB volatilized from soil on global level: 200 - 400 t/y

Global anthropogenic emissions in 2004 – 27 t/y

EMEP emission in 2009 – 9 t/y

Franke et al., 1996: anthropogenic emissions in Germany – 200 kg/y; re-volatilization from soil in Germany – 10 – 50 t/y

Steering Body to EMEP (September 5 – 7, 2011)
**Integrated approach, HCB**

**Step 1: Preliminary assessment**

**HCB emissions**

**EMEP domain:**
- Official data and TNO estimates for 2009

**Northern Hemisphere:**
- Official data and TNO estimates for 2009
- Historical emissions from 1990 to 2009 at hemispheric level
  - Bailey [2001]

Calculated HCB air concentrations in 2009 taking into account transport and accumulation from 1990 to 2009 at hemispheric level

*Steering Body to EMEP (September 5 – 7, 2011)*
Integrated approach, HCB

Step 2: Evaluation of agreement

MSC-E calculations made in 2011

Air concentrations

Comparison with measurements

Underestimation is about a factor of 17 (7 – 30)

Steering Body to EMEP (September 5 – 7, 2011)
Integrated approach, HCB

**Step 3: Possible reasons of discrepancies**

Underestimation is about a factor of 17 (7 – 30)

**Measurement data.**

EMEP measurements: 5 – 70 pg/m³,
other measurements: 10 – 80 pg/m³ (Barber et al., 2005)

**Model uncertainties.**

Model parameterization: sensitivity study, model intercomparison \(\rightarrow\) uncertainty may be up to a factor of 2;

**Emission uncertainties.**

Historical and contemporary emissions

Steering Body to EMEP (September 5 – 7, 2011)
Step 3: Possible reasons of discrepancies

Integrated approach, HCB

Historical emissions -> soil concentrations -> re-emission flux

MSC-E calculations made in 2011

Uncertainties in description of re-emission flux:

uncertainties in historical emissions [Bailey, 2001] used in calculations for 2009 lead to the fact that soil concentrations calculated by the model are essentially lower than measured [Barber et al., 2005].

As a result – model underestimation of air concentrations 7 – 30 times.
Main reason – underestimation of re-emission flux.
Integrated approach, HCB

Step 3: Possible reasons of discrepancies: re-emission fluxes

MSC-E calculations made in 2010

Measurements at EMEP monitoring network are in between calculation results obtained with maximum and minimum scenarios. Agreement with average scenario – factor 2 – 4

Test simulations from 1945 to 2008 for evaluation of accumulation in soil

Emission scenarios based on FAO data (taking into account agricultural use)

Steering Body to EMEP (September 5 – 7, 2011)
Step 3: Possible reasons of discrepancies: re-emission fluxes

MSC-E calculations made in 2010

Test simulations from 1945 to 2008 for evaluation of accumulation in soil

Emission scenarios based on FAO data (taking into account agricultural use)

Different rates of decay of soil and air concentrations lead to enlargement of re-emission flux
**Integrated approach, HCB**

**Step 3: usage of emission scenarios**

MSC-E calculations made in 2011 based on official EMEP data, TNO and Bailey, 2005 (global scale)

<table>
<thead>
<tr>
<th>Scenario 1</th>
<th>Anthrop. emissions × 3, re-emissions × 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scenario 2</td>
<td>...</td>
</tr>
</tbody>
</table>

**Results**

Comparison with measurements (Scenario 1)

<table>
<thead>
<tr>
<th>Indicator</th>
<th>Initial calc.</th>
<th>Scen1</th>
<th>Thresh. level</th>
</tr>
</thead>
<tbody>
<tr>
<td>FAC 2</td>
<td>11%</td>
<td>78%</td>
<td>&gt; 50%</td>
</tr>
<tr>
<td>Corr</td>
<td>0.74</td>
<td>0.73</td>
<td>&gt; 0.6</td>
</tr>
<tr>
<td>Regr.</td>
<td>3.75</td>
<td>0.96</td>
<td>1 ± 0.3</td>
</tr>
<tr>
<td>NMB</td>
<td>0.78</td>
<td>0.14</td>
<td>&lt; 0.2</td>
</tr>
<tr>
<td>SR</td>
<td>2.53</td>
<td>0.99</td>
<td>&lt; 2.3</td>
</tr>
</tbody>
</table>

Steering Body to EMEP (September 5 – 7, 2011)
Influence of global transport on POP pollution within EMEP

According to HTAP assessment 2010 and MSC-E estimates:

Contributions of non-EMEP sources to depositions to particular European countries for POPs reaches up to 50%.
Simulations of PCB-153 global transport in 2009

PCB-153 annual mean concentrations in 2009

Integrated approach, global transport

Steering Body to EMEP (September 5 – 7, 2011)
Testing the ocean model in GLEMOS

Tracer test for POP-like substance (advection, vertical and horizontal diffusion, partitioning, degradation, and sedimentation; no exchange).

After 7 months

After 12 months

Tracer ocean concentrations in the upper model layer (percent of the maximum value) from three point sources calculated by the GLEMOS ocean module.

Steering Body to EMEP (September 5 – 7, 2011)
Climate change and POP interlinkages

- Evaluate sensitivity of POP pollution levels to variation of meteorological and environmental factors.
- Investigation of climate change influence on meteo/env. parameters
- Perform modelling experiments of future changes in POP pollution using the GLEMOS and available climate change scenarios data
Sensitivity of model results to meteorological and environmental parameters

Target parameters:
- Transport distance (considered earlier)
- Mean air concentrations in a country
- Total deposition flux to a country

Factors:
- Temperature
- Precipitation intensity
- Wind speed
- Wind direction
- Outflow through boundaries
- Coverage by vegetation
- ...

Steering Body to EMEP (September 5 – 7, 2011)
Integrated approach: influence of meteo/env. parameters

Ranking of factors: air concentrations over Europe

particulate, degradable (B[a]P)

Most important – temperature, precipitation and wind direction

Highest priority – temperature

Steering Body to EMEP (September 5 – 7, 2011)
Integrated approach: influence of meteo/env. parameters

Ranking of factors: different locations

PCB-153

<table>
<thead>
<tr>
<th>Regions</th>
<th>Priority parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Northern Europe</td>
<td>Vegetation cover, precipitation</td>
</tr>
<tr>
<td>Western Europe</td>
<td>Precipitation, wind speed and direction</td>
</tr>
<tr>
<td>Central and Eastern Europe</td>
<td>Temperature, precipitation</td>
</tr>
<tr>
<td>Southern Europe</td>
<td></td>
</tr>
</tbody>
</table>
Modelling of POP fate using climate change scenarios data

Climate change leads to the change of meteorological and environmental parameters

Selection of climate change scenarios data:
GCM model output for a number of scenarios is used to prepare meteorological input for GLEMOS (2010-2100)

Planning of modelling experiments:
Explore effect of changes of climate and emissions on POP long-range transport, source-receptor relationships, and distribution of POPs in media and re-emissions (PAHs, PCDD/Fs, …)
Future activities

CCC

Review, store and make available EMEP monitoring data for the modelling centres and Parties.

Evaluate new measurements data of POPs from Eastern Europe, the Caucasus and Central Asia.

Maintain close interaction with relevant organizations and bodies in relation to integration of observations.

...
Future activities

MSC-E

Model assessment of transboundary pollution on regional and global scale.

Model parameterization of air/vegetation exchange.

Implementation of the integrated approach for POPs, including adjoint modelling.

Model investigation of climate change effects on POP transport and fate.

Pilot calculations of POP pollution on a local scale.

...
Thank you for your attention!
Integrated approach, HCB

**Step 3: Possible reasons of discrepancies: re-emission fluxes**

*Historical emissions -> re-emission flux*

**Uncertainties in description of re-emission flux:**

Uncertainties in historical emissions (Bailey, 2001) lead to the fact that soil concentrations calculated by the model are essentially lower than measured (Barber et al., 2005). The model reasonably describes accumulation in media and re-volatilization for pollutants with similar behavior (PCB-153).

Measurements at EMEP monitoring network are in between calculation results obtained with maximum and minimum scenarios. Agreement with average scenario – factor 2 – 4

Test simulations from 1945 to 2008 for evaluation of accumulation in soil

Emission scenarios based on FAO data and MSC-E estimates (taking into account agricultural use)

Steering Body to EMEP (September 5 – 7, 2011)