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Defining
Deriving
Validating
Pov and LRTP
of chemical substances
for POP and PBT assessment

National Institute
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and the Environment

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Pov and LRTP

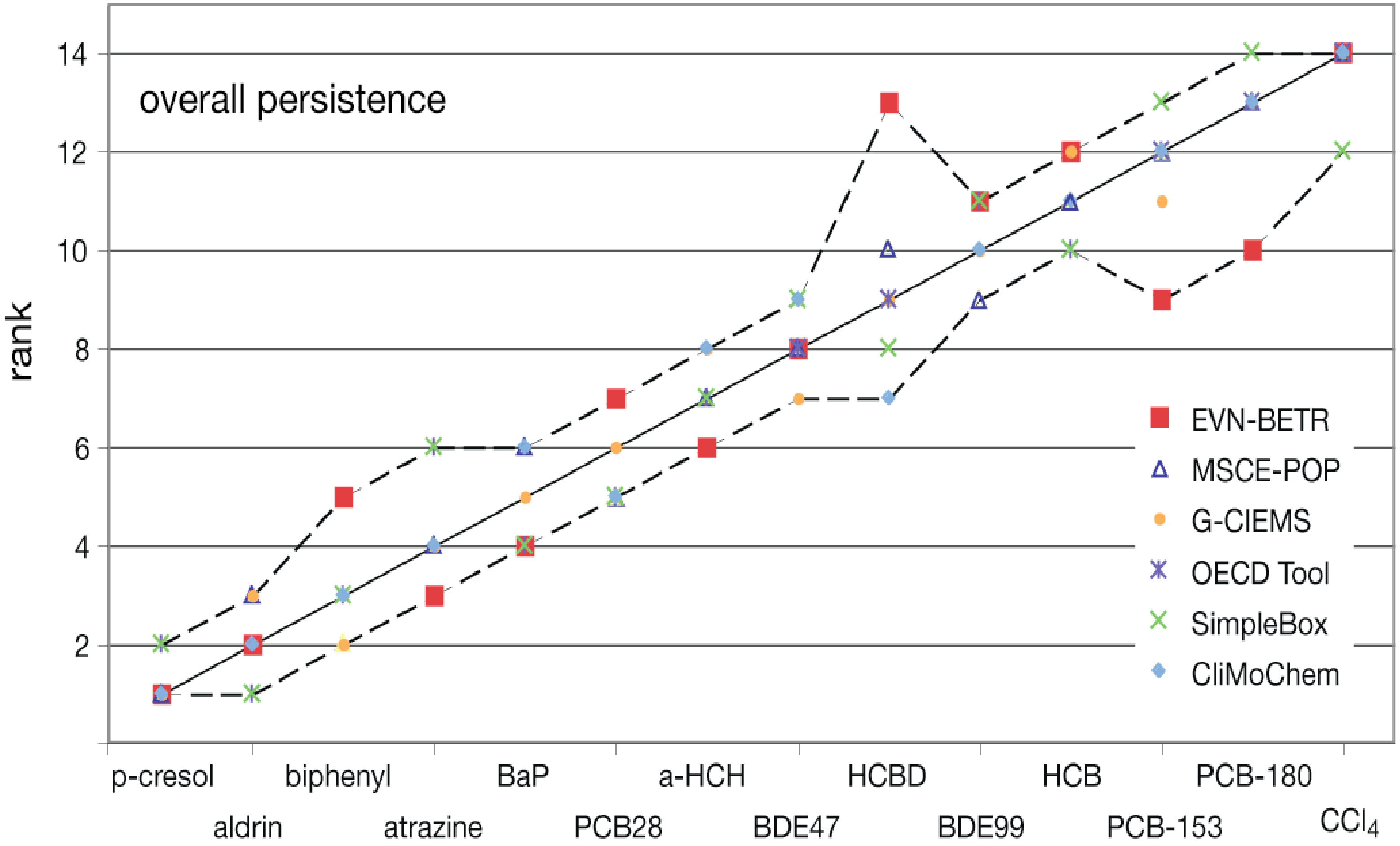
- International conventions
  - UNEP Stockholm Convention
  - UNECE CRLRTAP
  - Substance “POP” of “PBT”?
  - Then measures
- How are POP- or PBT-ness assessed?
  - Expert decision
  - Supported by scienific evidence
  - Model computations
  - Use of Pov and LRTP
- Modeling assumptions important?
  - MSC-East: POP models intercomparison study
  - SETAC Pellston conference January 2008, Pensacola, FL

Disadvantage of Pov and LRTP

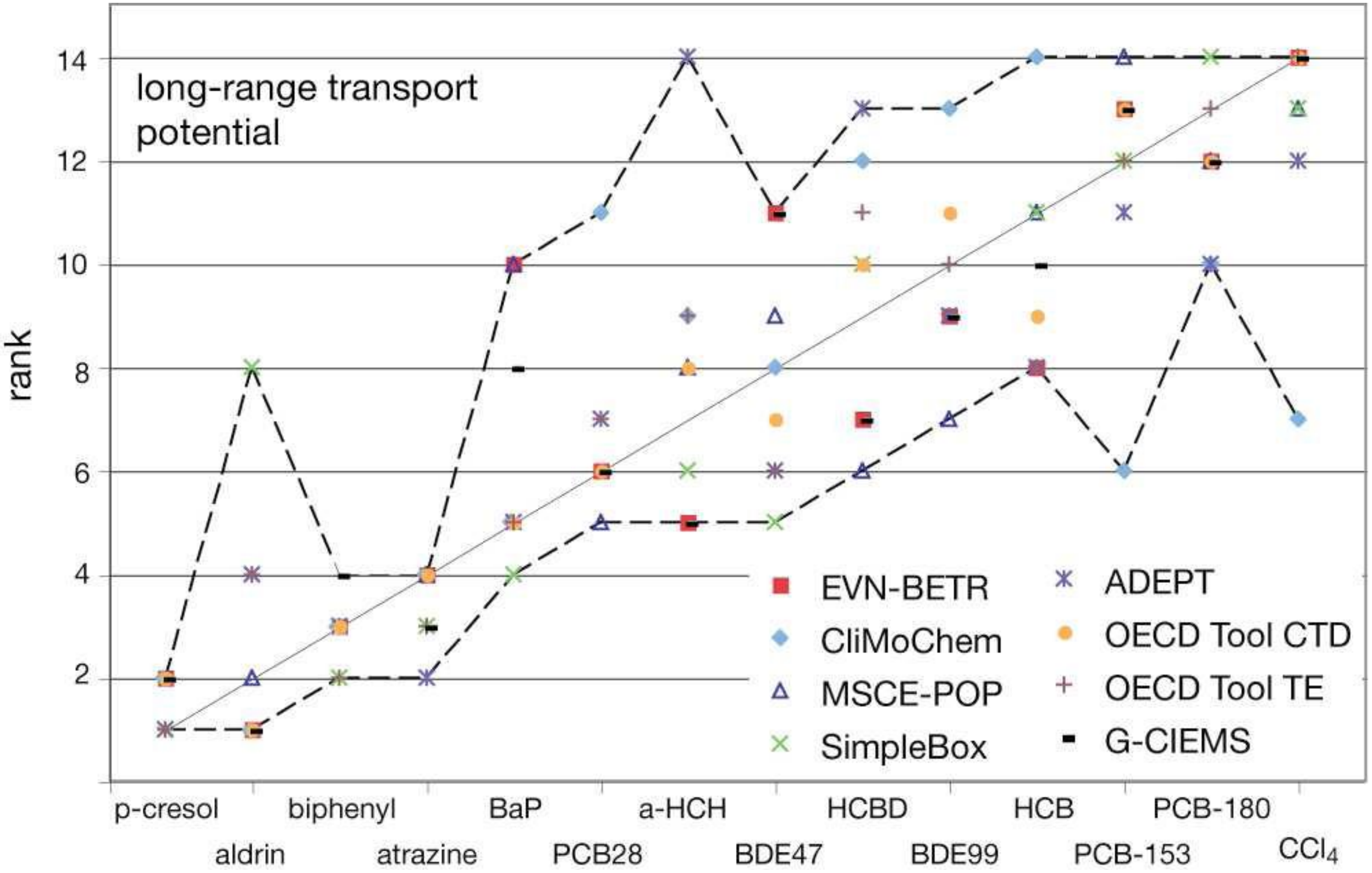
- Not directly measurable in field or laboratory, so always derived from modeling:
  - No validation
  - Different model approaches

  - Fortunately, model approaches yield similar results…

MSC-East study



MSC-East study



SETAC conference

- SETAC Pellston conference on POP- and PBT assessment
  - January 26-Feb 1, 2008, Pensacola, FL
  - 50 experts
- Open questions about Pov and LRTP
  - Meaningful definitions: what do Pov and LRTP express?
  - Assessment: how to find Pov en LRTP from substance properties?
  - Criteria: which Pov and LRTP values should not be exceeded?
  - Validation: can Pov and LRTP be derived from field data?
- Consensus reached
  - Answers proposed
- Publication in preparation IEAM

Meaning of Pov and LRTP

- Different metrics for Pov
  - Residence time at steady state
  - Clearance time
  - Remote state
- Different metrics for LRTP
  - Characteristic travel distance
    - In air
    - In water
  - Fraction transported out of system
  - Artic … Potential
  - Great Lakes Transfer Efficiency

Meaning of Pov and LRTP

- Proposed by SETAC group

$$P_{OV} = \text{average lifetime of molecules in environment}$$

$$LRTP = \text{average lifetime displacement of molecules}$$

Assessment of Pov and LRTP

- Theoretical derivation of Pov

$$P_{OV} = \langle \text{time} \rangle = \frac{1}{k_{OV}}$$

$$k_{OV} = \varphi_A k_A + \varphi_W k_W + \varphi_S k_S$$

Assessment of Pov and LRTP

- Theoretical derivation of LRTP

$$LRTP = \langle \text{length} \rangle = \sqrt{\frac{D_{OV}}{k_{OV}}} = \sqrt{D_{OV} \cdot P_{OV}}$$

$$D_{OV} = \varphi_A D_A + \varphi_W D_W$$

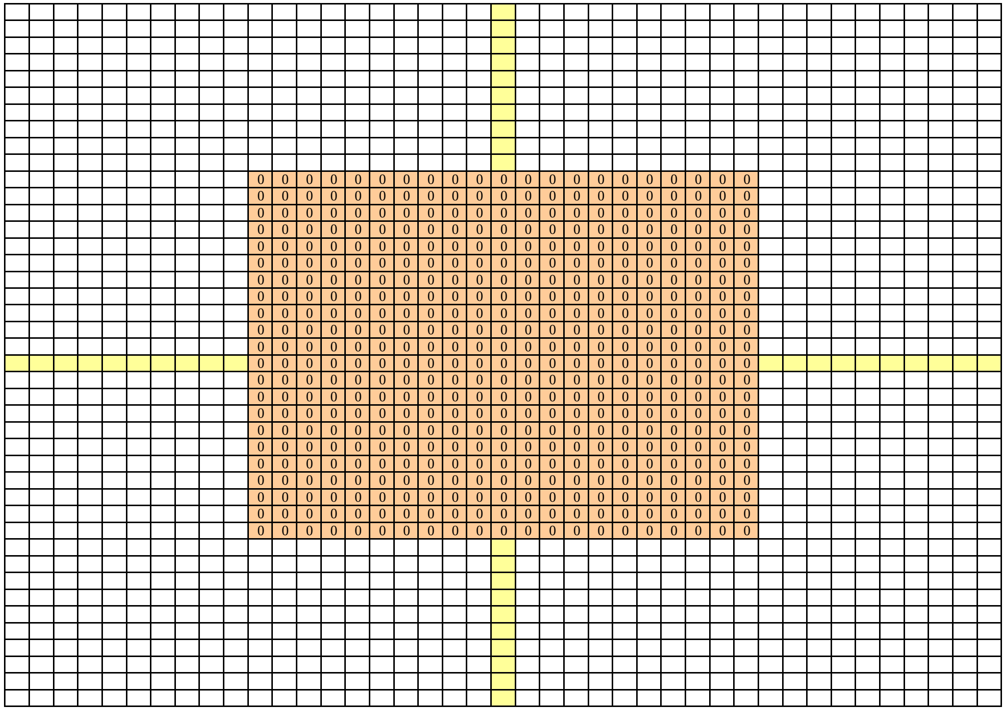
$$k_{OV} = \varphi_A k_A + \varphi_W k_W + \varphi_S k_S$$

Simulation model

- Degradation spatially and temporally constant
  - k_{OV} = 0.1 yr^{-1}
- Dispersion directionally, spatially and temporally constant
  - 2-dimensional
  - D = 3.10^4 $km^2.yr^{-1}$
- $P_{OV} = \frac{1}{k_{OV}} = 10\ yr$
- $LRTP = \sqrt{D/k} = 548\,\mathrm{km}$

Simulation

- 100 km x 100 km grid
- emission in 2000 x 2000 km square
- between 1950 and 1990
- record m''(x,t)



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										0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0										
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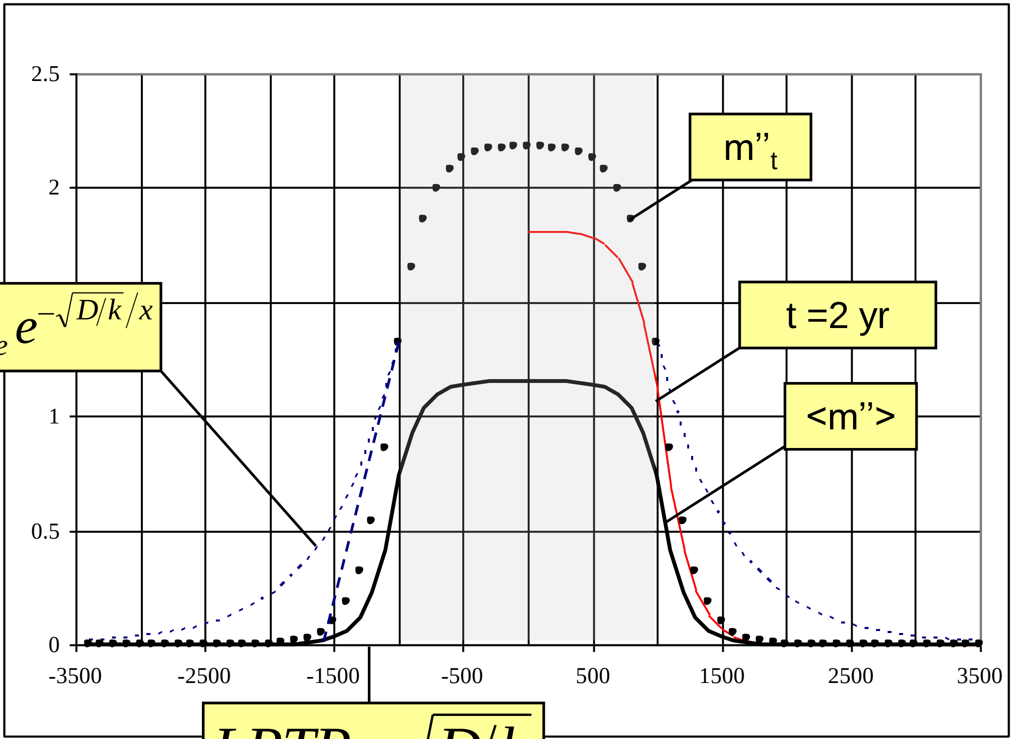
Simulation

- m’’(x,t)



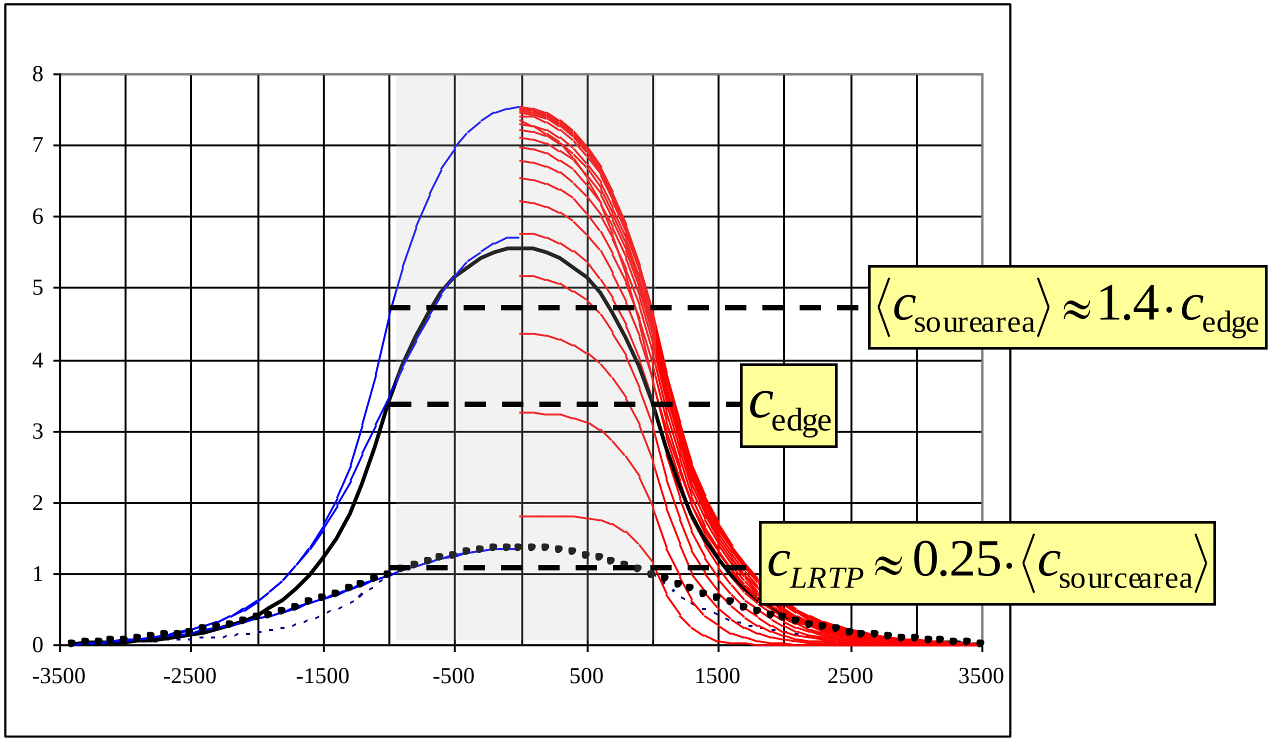
$$c(x,t) = c_{edge}\, e^{-\sqrt{D/k}/x}$$

$$LRTP = \sqrt{D/k}$$

Simulating ……

Simulation

- From simulated m’’(x,t) values
- Deduce Pov and LRTP

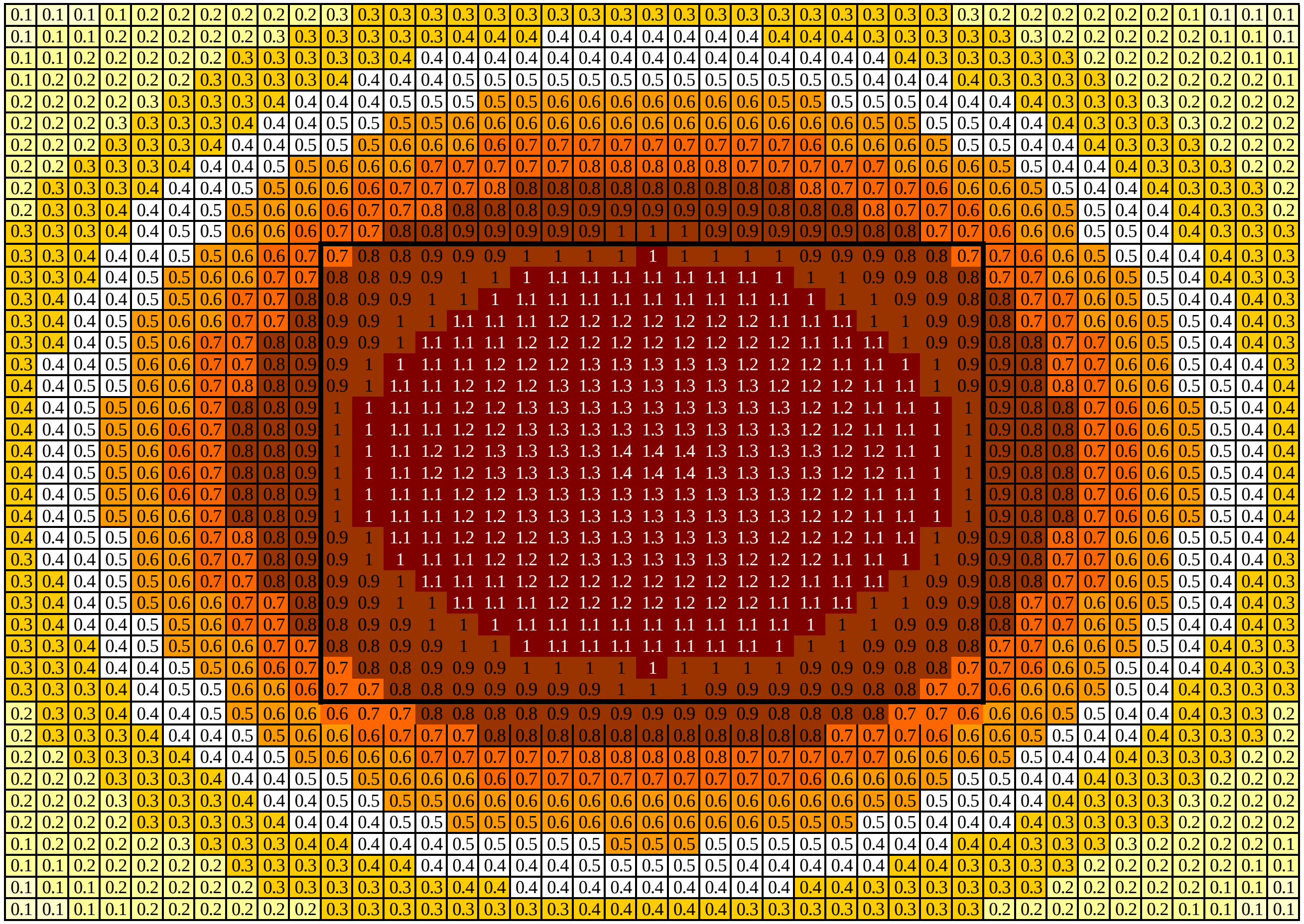


$\langle c_{\text{sourearea}} \rangle \approx 1.4 \cdot c_{\text{edge}}$

c_{edge}

$c_{LRTP} \approx 0.25 \cdot \langle c_{\text{sourcearea}} \rangle$

Simulation result at t = 50 yr



0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.2	0.2	0.2	0.2	0.2	0.2	0.1	0.1	0.1	0.1
0.1	0.1	0.1	0.2	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.3	0.3	0.2	0.2	0.2	0.2	0.2	0.1	0.1	0.1
0.1	0.1	0.2	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.3	0.2	0.2	0.2	0.2	0.2	0.1	0.1
0.1	0.2	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.2	0.2	0.2	0.2	0.2	0.1
0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.5	0.5	0.5	0.5	0.5	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.5	0.5	0.5	0.5	0.5	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.2	0.2	0.2	0.2
0.2	0.2	0.2	0.3	0.3	0.3	0.3	0.4	0.4	0.4	0.5	0.5	0.5	0.5	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.5	0.5	0.5	0.5	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.2	0.2	0.2
0.2	0.2	0.2	0.3	0.3	0.3	0.4	0.4	0.4	0.5	0.5	0.5	0.6	0.6	0.6	0.6	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.6	0.6	0.6	0.6	0.5	0.5	0.5	0.4	0.4	0.4	0.3	0.3	0.3	0.2	0.2	0.2
0.2	0.2	0.3	0.3	0.3	0.4	0.4	0.4	0.5	0.5	0.6	0.6	0.6	0.7	0.7	0.7	0.7	0.7	0.8	0.8	0.8	0.8	0.8	0.7	0.7	0.7	0.7	0.7	0.6	0.6	0.6	0.5	0.5	0.4	0.4	0.4	0.3	0.3	0.3	0.2	0.2
0.2	0.3	0.3	0.3	0.4	0.4	0.4	0.5	0.5	0.6	0.6	0.6	0.7	0.7	0.7	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.7	0.7	0.7	0.6	0.6	0.6	0.5	0.5	0.4	0.4	0.4	0.3	0.3	0.3	0.2
0.2	0.3	0.3	0.4	0.4	0.4	0.5	0.5	0.6	0.6	0.6	0.7	0.7	0.8	0.8	0.8	0.8	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.8	0.8	0.8	0.8	0.7	0.7	0.6	0.6	0.6	0.5	0.5	0.4	0.4	0.4	0.3	0.3	0.2
0.3	0.3	0.3	0.4	0.4	0.5	0.5	0.6	0.6	0.6	0.7	0.7	0.8	0.8	0.9	0.9	0.9	0.9	0.9	1	1	1	0.9	0.9	0.9	0.9	0.9	0.8	0.8	0.7	0.7	0.6	0.6	0.6	0.5	0.5	0.4	0.4	0.3	0.3	0.3
0.3	0.3	0.4	0.4	0.4	0.5	0.5	0.6	0.6	0.7	0.7	0.8	0.8	0.9	0.9	0.9	1	1	1	1	1	1	1	1	1	0.9	0.9	0.9	0.8	0.8	0.7	0.7	0.6	0.6	0.5	0.5	0.4	0.4	0.4	0.3	0.3
0.3	0.3	0.4	0.4	0.5	0.5	0.6	0.6	0.7	0.7	0.8	0.8	0.9	0.9	1	1	1	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1	1	1	0.9	0.9	0.8	0.8	0.7	0.7	0.6	0.6	0.5	0.5	0.4	0.4	0.3	0.3
0.3	0.4	0.4	0.4	0.5	0.5	0.6	0.7	0.7	0.8	0.8	0.9	0.9	1	1	1	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1	1	1	0.9	0.9	0.8	0.8	0.7	0.7	0.6	0.5	0.5	0.4	0.4	0.4	0.3
0.3	0.4	0.4	0.5	0.5	0.6	0.6	0.7	0.7	0.8	0.9	0.9	1	1	1.1	1.1	1.1	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.1	1.1	1.1	1	1	0.9	0.9	0.8	0.7	0.7	0.6	0.6	0.5	0.5	0.4	0.4	0.3
0.3	0.4	0.4	0.5	0.5	0.6	0.7	0.7	0.8	0.8	0.9	0.9	1	1.1	1.1	1.1	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.1	1.1	1.1	1	0.9	0.9	0.8	0.8	0.7	0.7	0.6	0.5	0.5	0.4	0.4	0.3
0.3	0.4	0.4	0.5	0.6	0.6	0.7	0.7	0.8	0.9	0.9	1	1	1.1	1.1	1.2	1.2	1.2	1.3	1.3	1.3	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1	1	0.9	0.9	0.8	0.7	0.7	0.6	0.6	0.5	0.4	0.4	0.3
0.4	0.4	0.5	0.5	0.6	0.6	0.7	0.8	0.8	0.9	0.9	1	1.1	1.1	1.2	1.2	1.2	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1	0.9	0.9	0.8	0.8	0.7	0.6	0.6	0.5	0.5	0.4	0.4
0.4	0.4	0.5	0.5	0.6	0.6	0.7	0.8	0.8	0.9	1	1	1.1	1.1	1.2	1.2	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.2	1.2	1.1	1.1	1	1	0.9	0.8	0.8	0.7	0.6	0.6	0.5	0.5	0.4	0.4
0.4	0.4	0.5	0.5	0.6	0.6	0.7	0.8	0.8	0.9	1	1	1.1	1.1	1.2	1.2	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.2	1.2	1.1	1.1	1	1	0.9	0.8	0.8	0.7	0.6	0.6	0.5	0.5	0.4	0.4
0.4	0.4	0.5	0.5	0.6	0.6	0.7	0.8	0.8	0.9	1	1	1.1	1.2	1.2	1.3	1.3	1.3	1.3	1.4	1.4	1.4	1.3	1.3	1.3	1.3	1.2	1.2	1.1	1	1	0.9	0.8	0.8	0.7	0.6	0.6	0.5	0.5	0.4	0.4
0.4	0.4	0.5	0.5	0.6	0.6	0.7	0.8	0.8	0.9	1	1	1.1	1.2	1.2	1.3	1.3	1.3	1.3	1.4	1.4	1.4	1.3	1.3	1.3	1.3	1.2	1.2	1.1	1	1	0.9	0.8	0.8	0.7	0.6	0.6	0.5	0.5	0.4	0.4
0.4	0.4	0.5	0.5	0.6	0.6	0.7	0.8	0.8	0.9	1	1	1.1	1.1	1.2	1.2	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.2	1.2	1.1	1.1	1	1	0.9	0.8	0.8	0.7	0.6	0.6	0.5	0.5	0.4	0.4
0.4	0.4	0.5	0.5	0.6	0.6	0.7	0.8	0.8	0.9	1	1	1.1	1.1	1.2	1.2	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.2	1.2	1.1	1.1	1	1	0.9	0.8	0.8	0.7	0.6	0.6	0.5	0.5	0.4	0.4
0.4	0.4	0.5	0.5	0.6	0.6	0.7	0.8	0.8	0.9	0.9	1	1.1	1.1	1.2	1.2	1.2	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1	0.9	0.9	0.8	0.8	0.7	0.6	0.6	0.5	0.5	0.4	0.4
0.3	0.4	0.4	0.5	0.6	0.6	0.7	0.7	0.8	0.9	0.9	1	1	1.1	1.1	1.2	1.2	1.2	1.3	1.3	1.3	1.3	1.3	1.2	1.2	1.2	1.1	1.1	1	1	0.9	0.9	0.8	0.7	0.7	0.6	0.6	0.5	0.4	0.4	0.3
0.3	0.4	0.4	0.5	0.5	0.6	0.7	0.7	0.8	0.8	0.9	0.9	1	1.1	1.1	1.1	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.1	1.1	1.1	1	0.9	0.9	0.8	0.8	0.7	0.7	0.6	0.5	0.5	0.4	0.4	0.3
0.3	0.4	0.4	0.5	0.5	0.6	0.6	0.7	0.7	0.8	0.9	0.9	1	1	1.1	1.1	1.1	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.1	1.1	1.1	1	1	0.9	0.9	0.8	0.7	0.7	0.6	0.6	0.5	0.5	0.4	0.4	0.3
0.3	0.4	0.4	0.4	0.5	0.5	0.6	0.7	0.7	0.8	0.8	0.9	0.9	1	1	1	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1	1	1	0.9	0.9	0.8	0.8	0.7	0.7	0.6	0.5	0.5	0.4	0.4	0.4	0.3
0.3	0.3	0.4	0.4	0.5	0.5	0.6	0.6	0.7	0.7	0.8	0.8	0.9	0.9	1	1	1	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1	1	1	0.9	0.9	0.8	0.8	0.7	0.7	0.6	0.6	0.5	0.5	0.4	0.4	0.3	0.3
0.3	0.3	0.4	0.4	0.4	0.5	0.5	0.6	0.6	0.7	0.7	0.8	0.8	0.9	0.9	0.9	1	1	1	1	1	1	1	1	1	0.9	0.9	0.9	0.8	0.8	0.7	0.7	0.6	0.6	0.5	0.5	0.4	0.4	0.4	0.3	0.3
0.3	0.3	0.3	0.4	0.4	0.5	0.5	0.6	0.6	0.6	0.7	0.7	0.8	0.8	0.9	0.9	0.9	0.9	0.9	1	1	1	0.9	0.9	0.9	0.9	0.9	0.8	0.8	0.7	0.7	0.6	0.6	0.6	0.5	0.5	0.4	0.4	0.3	0.3	0.3
0.2	0.3	0.3	0.4	0.4	0.4	0.5	0.5	0.6	0.6	0.6	0.7	0.7	0.8	0.8	0.8	0.8	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.8	0.8	0.8	0.8	0.7	0.7	0.6	0.6	0.6	0.5	0.5	0.4	0.4	0.4	0.3	0.3	0.2
0.2	0.3	0.3	0.3	0.4	0.4	0.4	0.5	0.5	0.6	0.6	0.6	0.7	0.7	0.7	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.7	0.7	0.7	0.6	0.6	0.6	0.5	0.5	0.4	0.4	0.4	0.3	0.3	0.3	0.2
0.2	0.2	0.3	0.3	0.3	0.4	0.4	0.4	0.5	0.5	0.6	0.6	0.6	0.7	0.7	0.7	0.7	0.7	0.8	0.8	0.8	0.8	0.8	0.7	0.7	0.7	0.7	0.7	0.6	0.6	0.6	0.5	0.5	0.4	0.4	0.4	0.3	0.3	0.3	0.2	0.2
0.2	0.2	0.2	0.3	0.3	0.3	0.4	0.4	0.4	0.5	0.5	0.5	0.6	0.6	0.6	0.6	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.6	0.6	0.6	0.6	0.5	0.5	0.5	0.4	0.4	0.4	0.3	0.3	0.3	0.2	0.2	0.2
0.2	0.2	0.2	0.3	0.3	0.3	0.3	0.4	0.4	0.4	0.5	0.5	0.5	0.5	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.5	0.5	0.5	0.5	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.2	0.2	0.2
0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.5	0.5	0.5	0.5	0.5	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.5	0.5	0.5	0.5	0.5	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.2	0.2	0.2	0.2
0.1	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.4	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.2	0.2	0.2	0.2	0.1
0.1	0.1	0.2	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.5	0.5	0.5	0.5	0.5	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.2	0.2	0.2	0.2	0.2	0.1	0.1
0.1	0.1	0.1	0.2	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.3	0.3	0.2	0.2	0.2	0.2	0.2	0.1	0.1	0.1
0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.2	0.2	0.2	0.2	0.2	0.2	0.1	0.1	0.1	0.1

Pov and LRTP from field data

- From theory and model simulations, it follows that

$$P_{OV} = \langle \mathrm{time} \rangle = \frac{\int_0^{\infty} m''(x,y,t)\,dxdydt}{\int_0^{\infty} e''(x,y,t)\,dxdydt} = \frac{\langle m \rangle \cdot t}{e_{tot}}$$

$$LRTP = \langle \mathrm{length} \rangle = \sqrt{\frac{A_{0.25}}{\pi}} - \sqrt{\frac{A_{source}}{\pi}}$$

Limitations

- Still lots of limitations:

- Strict emission source area
- LRTP can only be derived from ongoing, continuous emissions
- Pov can only be derived from total mass and emission data

- However, this concept can be refined…

Conclusions

- Meaningful definitions of Pov and LRTP
- Values of Pov en LRTP related to properties
  - substance
  - system
- Values deducable from field data

Future

- Expand these concepts mathematically

- Compare with real measurement data and emission data
  - Existing?
  - Measurement campaign?