Role of dispersion in interpretation of differences between FOCUS leaching models

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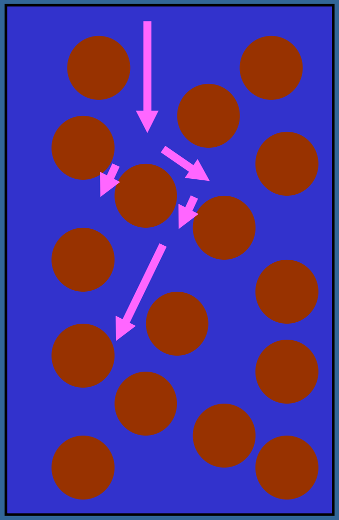
- introduction to dispersion
- description of dispersion in FOCUS scenarios
- effect of dispersion length in FOCUS scenarios
- conclusions

Introduction to dispersion



soil column

Dispersion: mixing process for solutes resulting from local differences in water flow rates

dispersion flux in PEARL:

$$J_{DIS} = - L_{DIS} \, | q | \, \partial c / \partial z$$

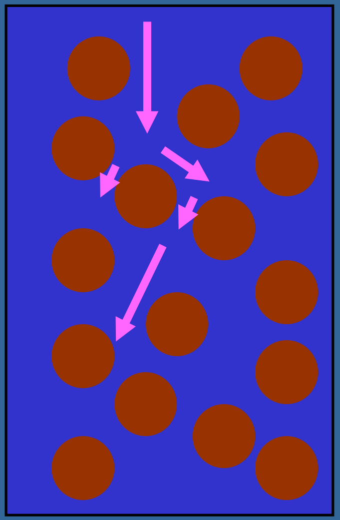
L_{DIS} = dispersion length
q = flow rate of water
c = concentration in liquid phase
z = depth in soil

- dispersion caused by local differences in water flow rates

- dispersion is weak form of preferential flow: normally distributed water flow rates

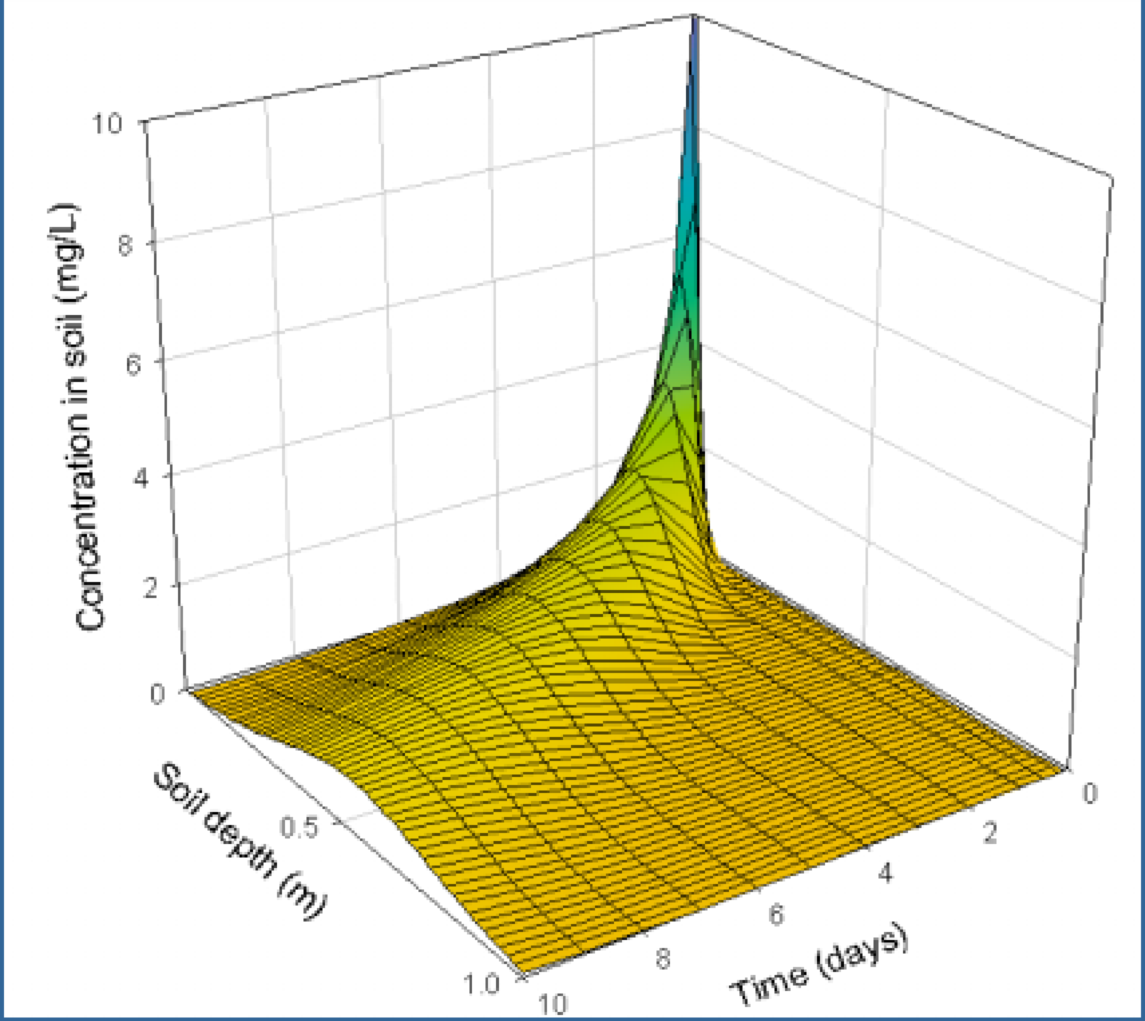
- preferential flow: water flow rates with a bimodal distribution

- chromatographic theory (1975): weak preferential flow can be simulated by appropriate dispersion length

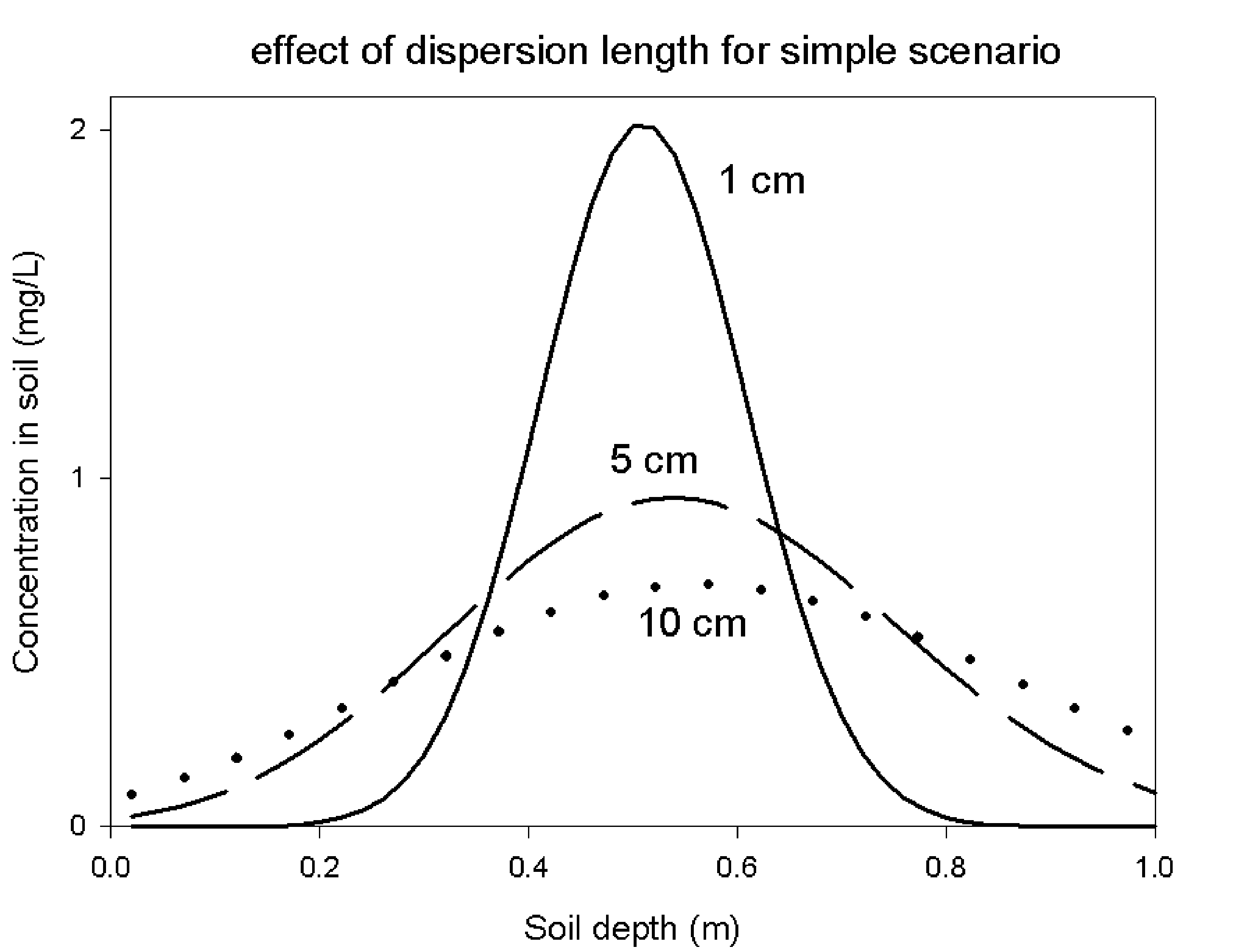


soil column

What happens to a surface-applied pulse ?

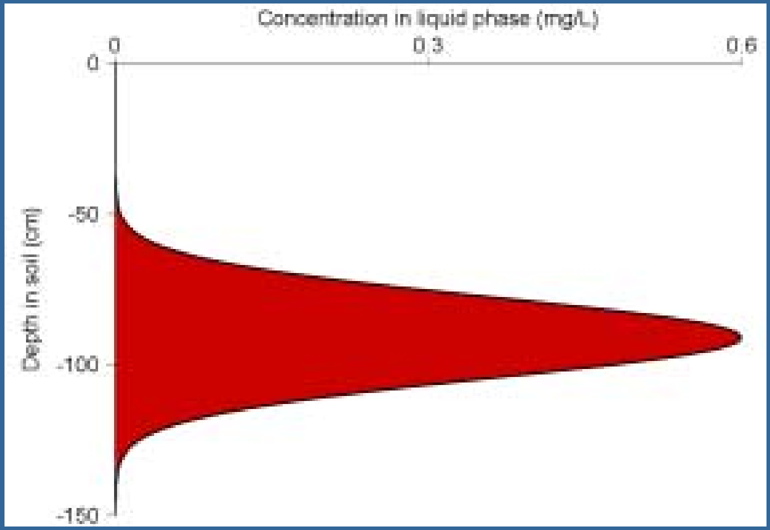


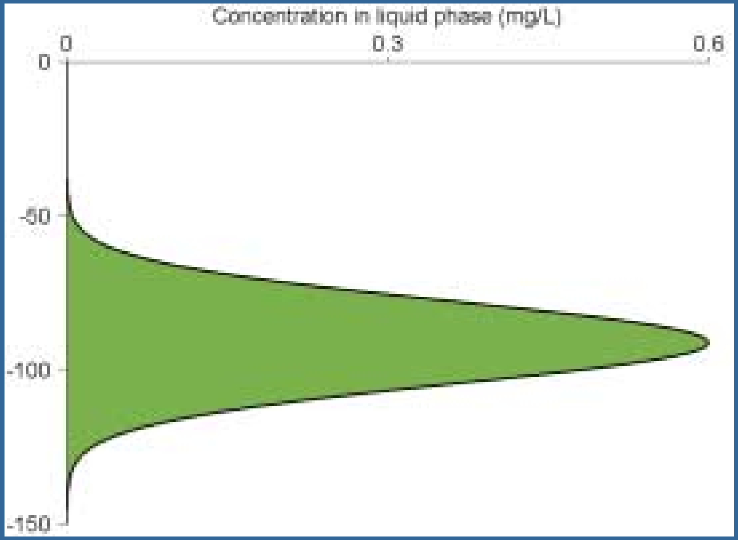
calculations with PEARL for simple scenario



calculated with PEARL

concept implies no effect of water flux on dispersion: different water flow rates but same total infiltration gives identical concentration profiles





45 d
1 cm/d

4.5 d
10 cm/d

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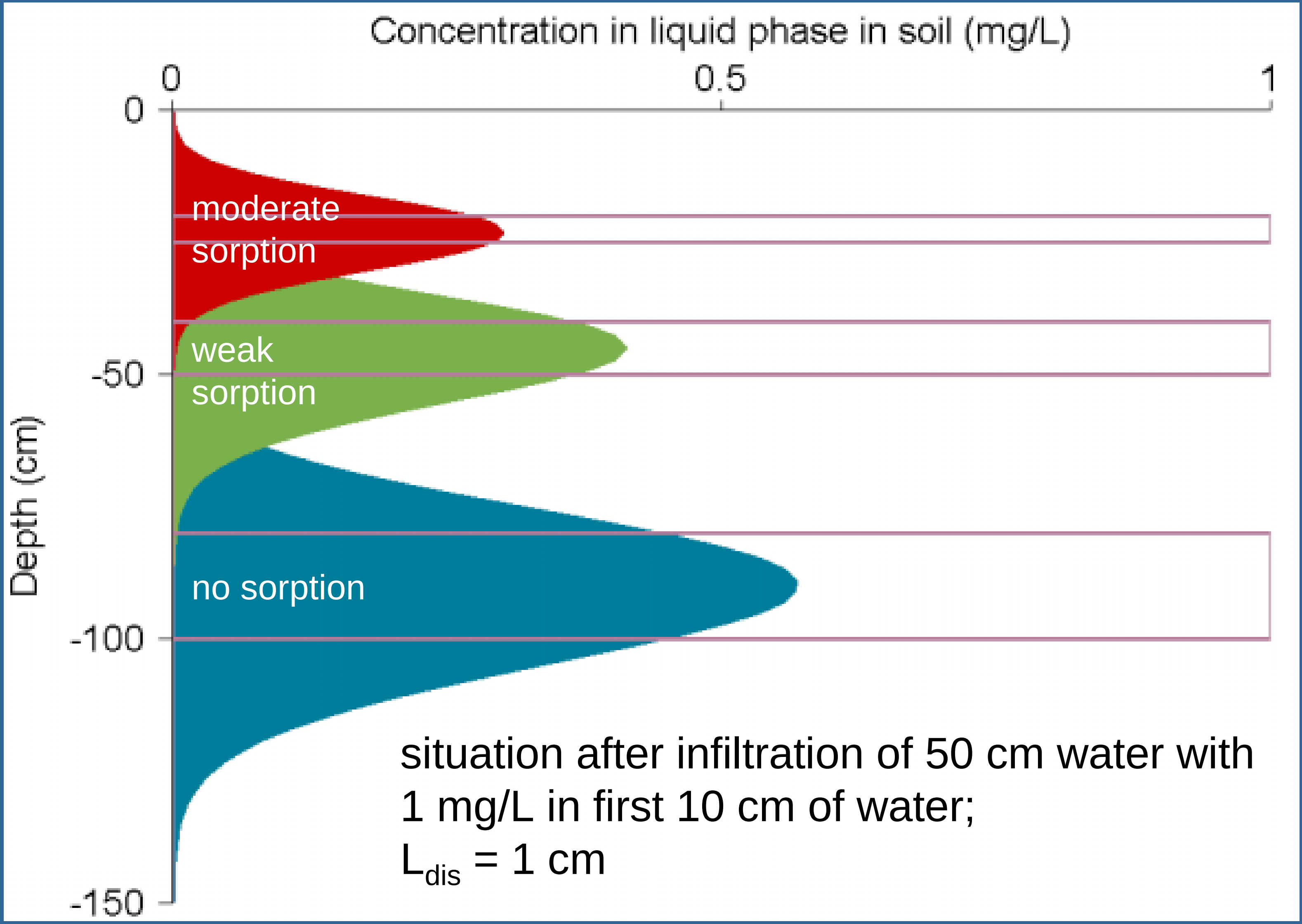
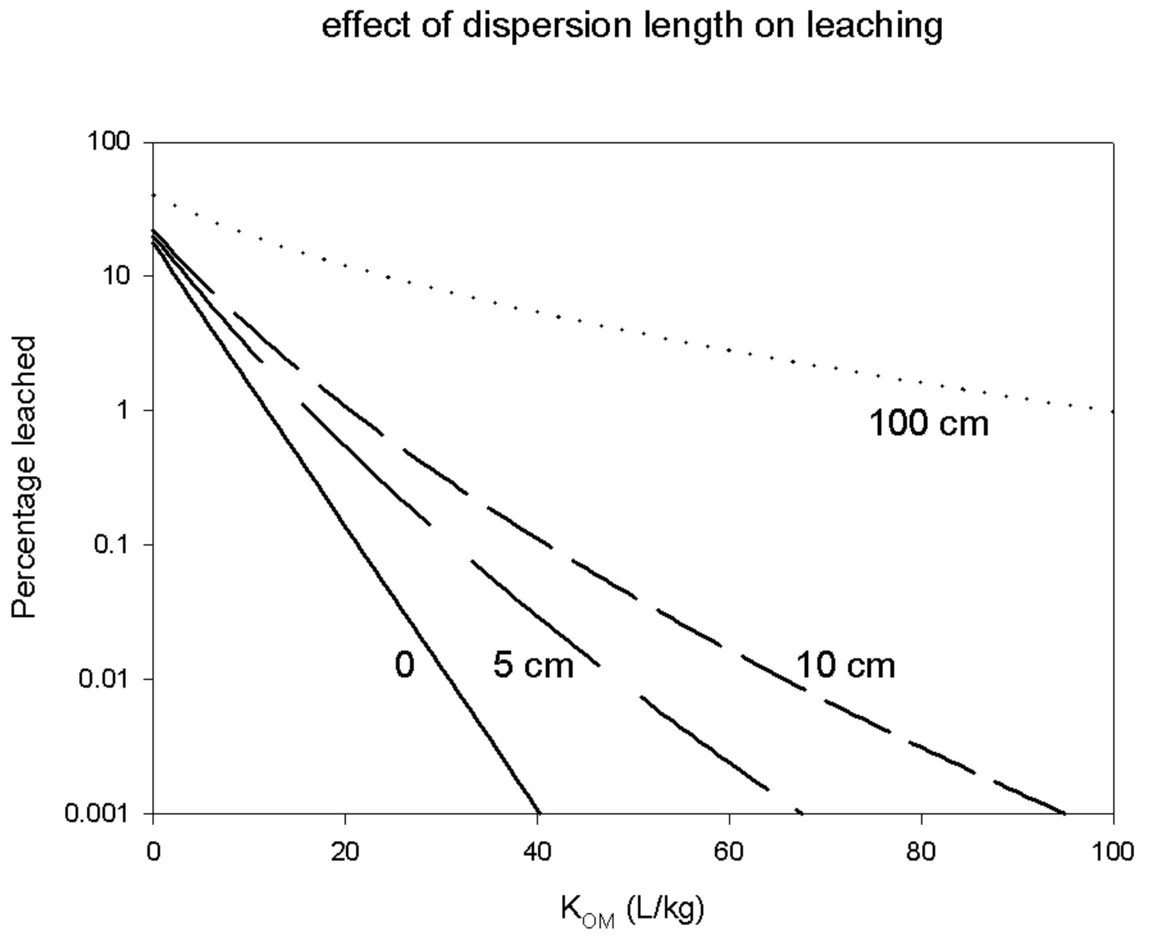

Concentration in liquid phase in soil (mg/L)
0
0.5
1
0
-50
-100
-150
Depth (cm)
moderate sorption
weak sorption
no sorption
situation after infiltration of 50 cm water with
1 mg/L in first 10 cm of water;
L_{dis} = 1 cm

Effect of dispersion on leaching calculated with PEARL for simple scenario



System properties:
2% org. matter
half-life of 40 d
water flux of 2 mm/d
soil column of 1 m
vol. fract. of water of 0.2
bulk density of 1.4 kg/L

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Description of dispersion in FOCUS scenarios

FOCUS: L_{DIS} = 5 cm (Vanderboght et al., 2000)

PEARL: $J_{DIS} = - L_{DIS} \; | q | \; \partial c / \partial z$

PRZM and PELMO:

- dispersion not described via flux but generated implicitly by numerical solution

- L_{DIS} equal to 0.5 times thickness of compartments

Thickness of compartments:

- PELMO: 5 cm for whole profile
- PRZM: 5 cm below 10 cm depth (1 mm in top 10 cm)

Effective dispersion lenghts used within FOCUS:

PEARL	5 cm
PELMO	2.5 cm
PRZM	2.5 cm (0.5 mm in top 10 cm)

Comparison of other concepts in PEARL, PELMO and PRZM

- Freundlich equilibrium sorption: almost identical

- plant uptake: identical

- transformation kinetics: almost identical

- water flow: different concepts
    - tipping bucket versus Darcian water flow
    - run-off based on different approaches

Comparison of calculated leaching for FOCUS scenarios:

- good correspondence at leaching levels above 1%

- at lower levels, PEARL gives always more leaching than PELMO and PRZM

- the lower the concentration level, the larger the difference

- illustration: substance D (DT_{50} = 20 d, K_{OM} = 35 L/kg) for standard FOCUS autumn application

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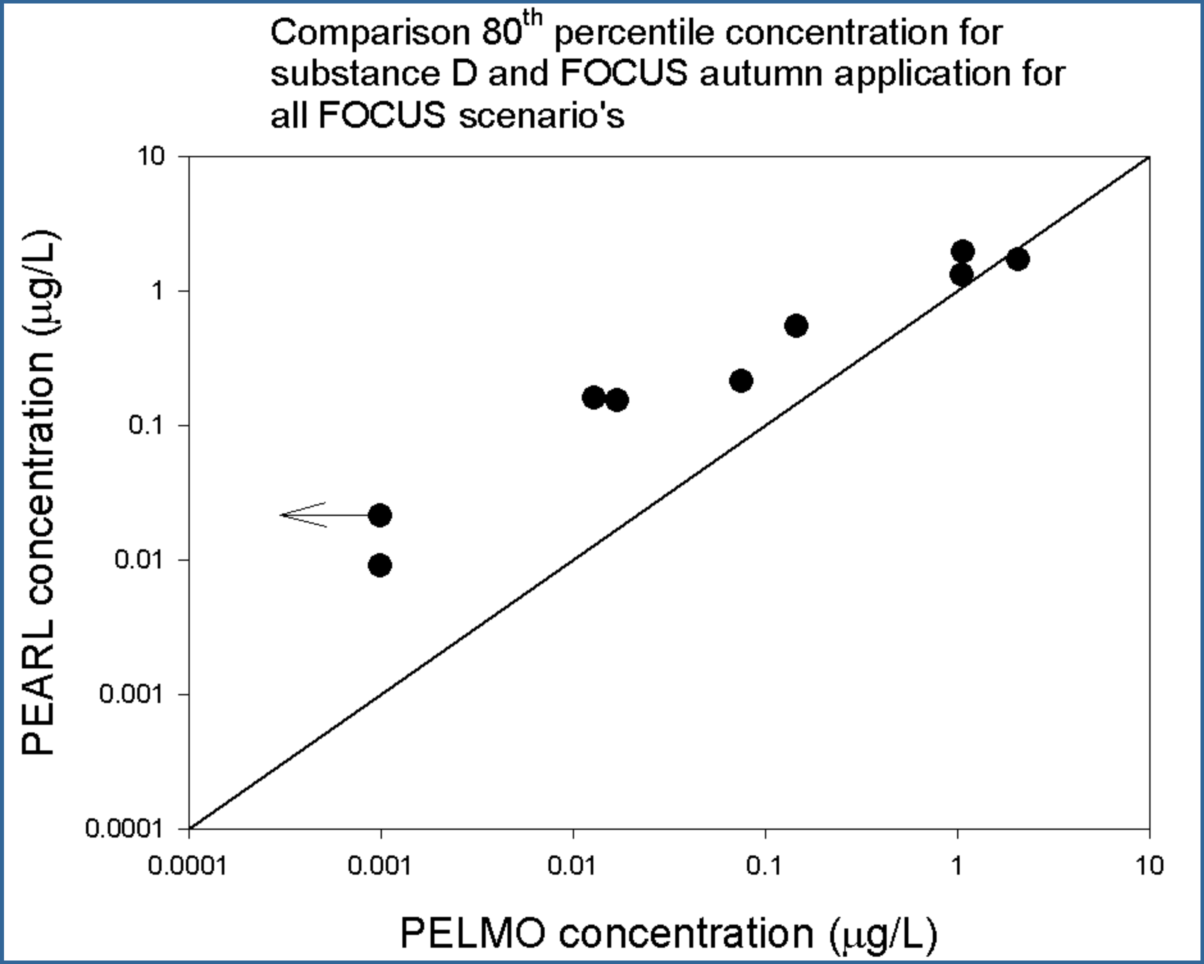
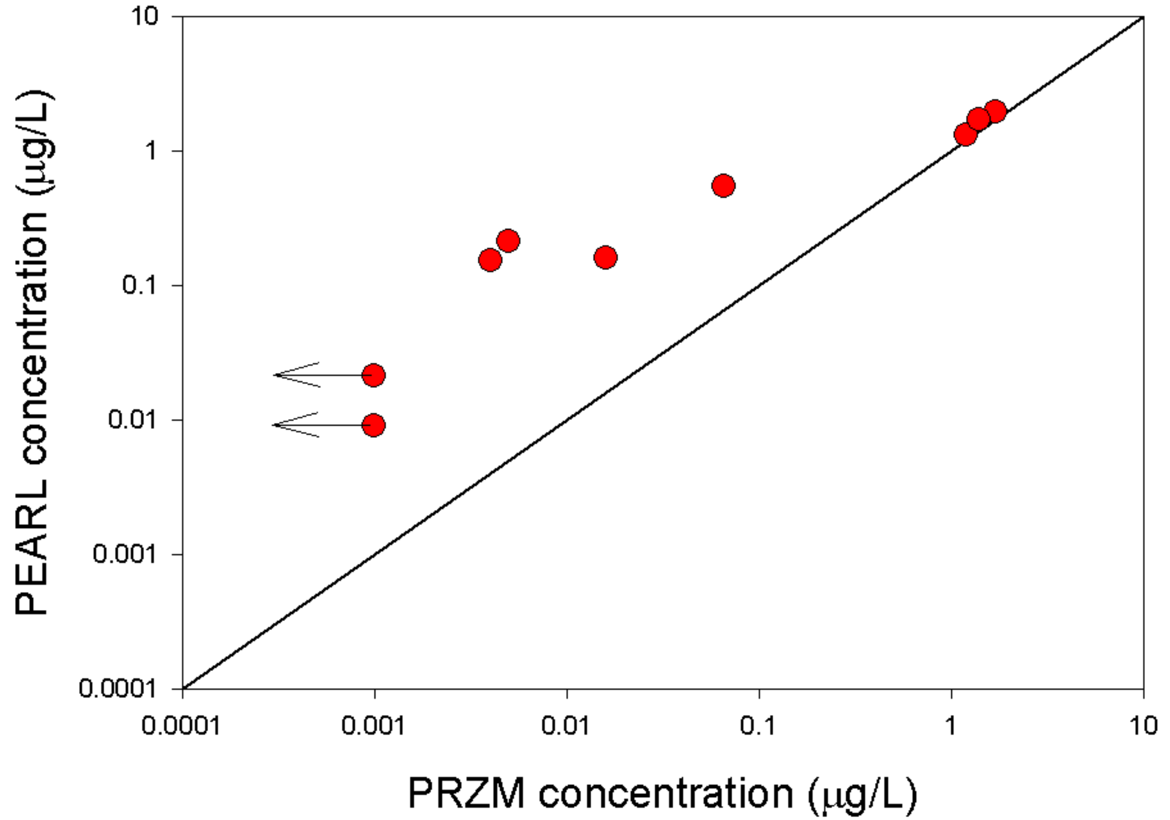

Comparison 80th percentile concentration for substance D and FOCUS autumn application for all FOCUS scenario's
PEARL concentration (μg/L)
10
1
0.1
0.01
0.001
0.0001
0.0001
0.001
0.01
0.1
1
10
PELMO concentration (μg/L)

Comparison 80th percentile concentration for substance D and FOCUS autumn application for all FOCUS scenario's



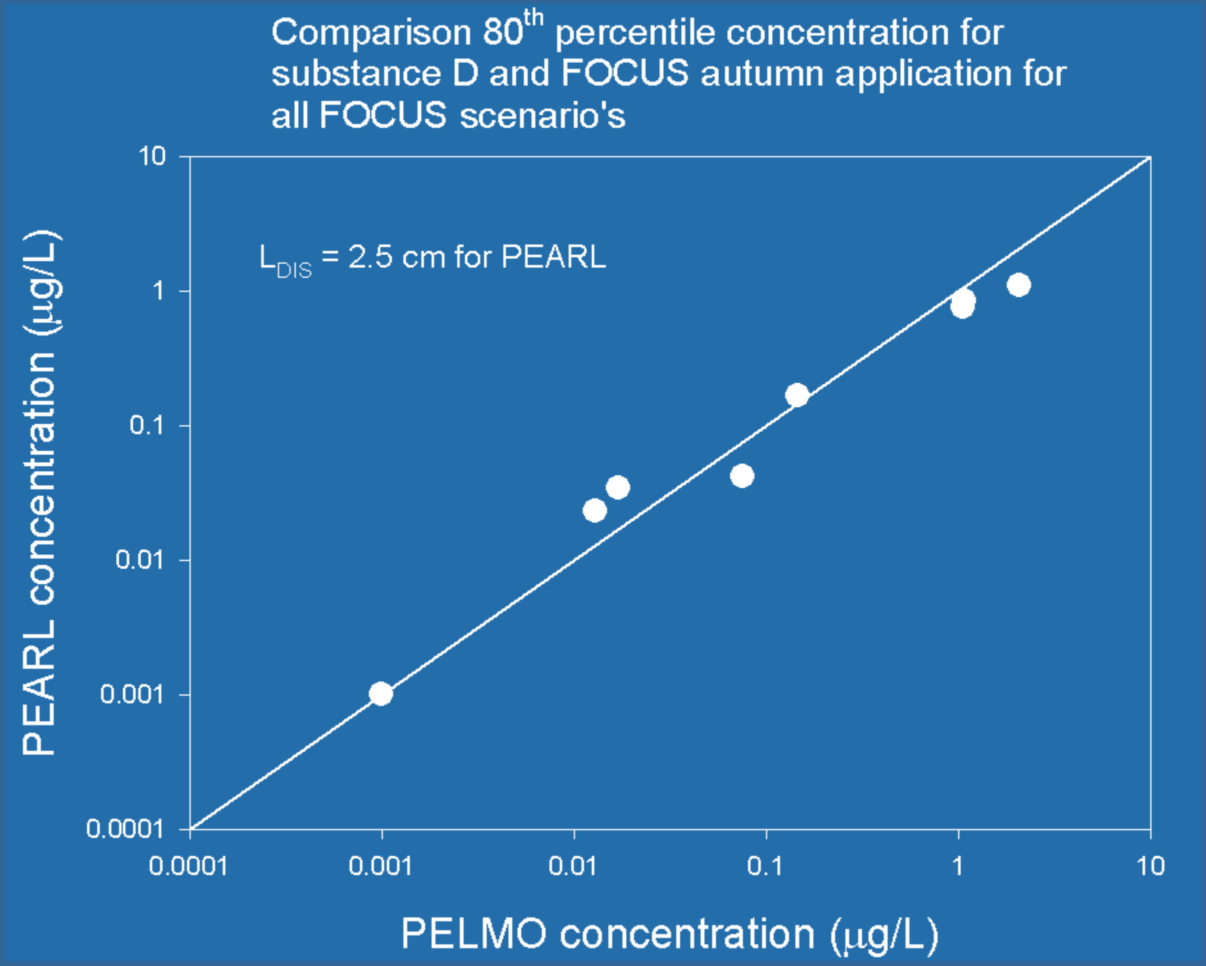
Effect of dispersion length in FOCUS scenarios

Hypothesis:
difference in effective dispersion length is major cause of differences in calculated leaching between PELMO/PRZM and PEARL

Test of hypothesis:
calculations with equal dispersion length (so also 2.5 cm for PEARL) for

1. all FOCUS scenarios and one substance
2. one FOCUS scenario and range of substances

PEARL - PELMO but now L_{DIS} = 2.5 cm for PEARL



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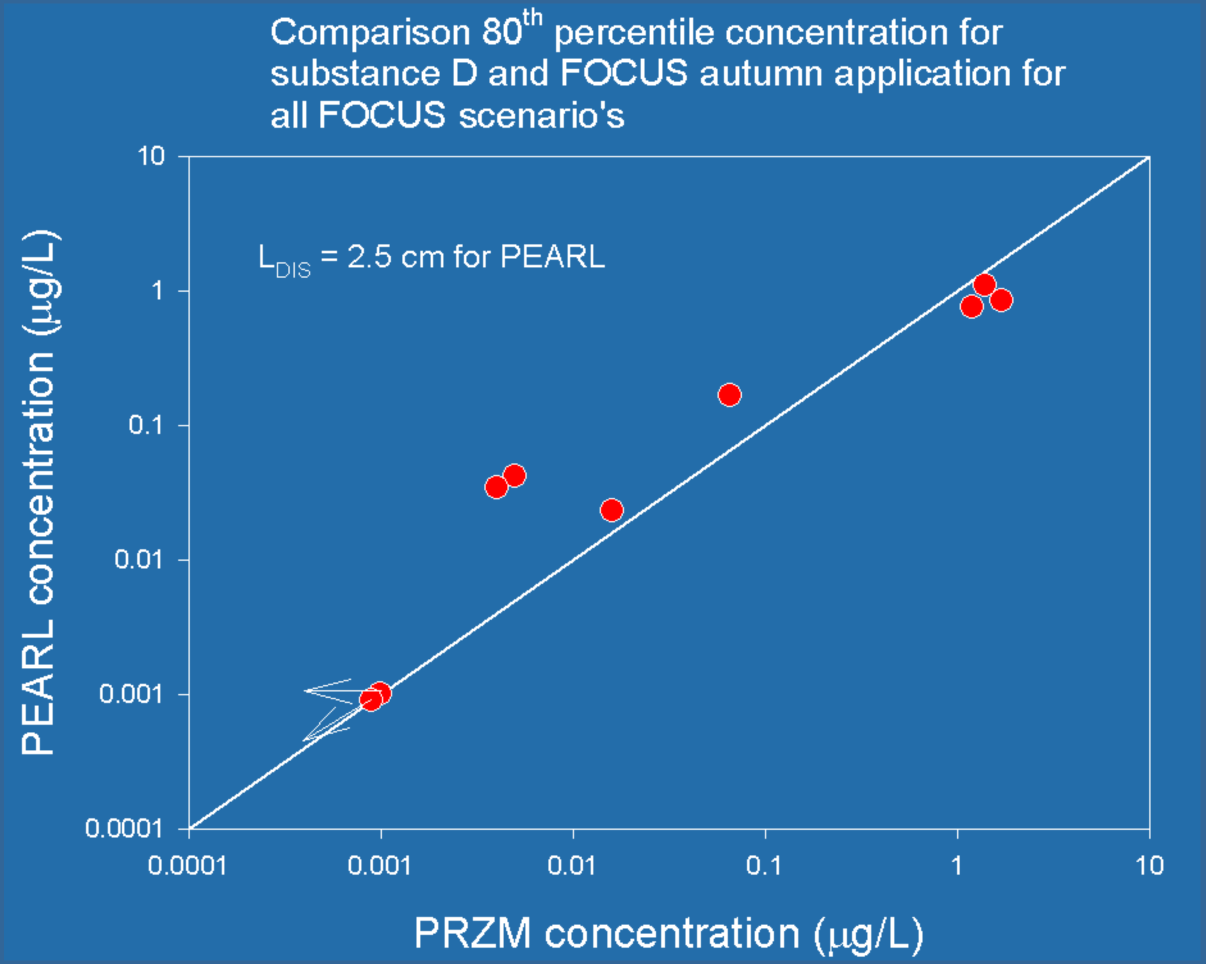
PRZM - PEARL but now L_{DIS} = 2.5 cm for PEARL



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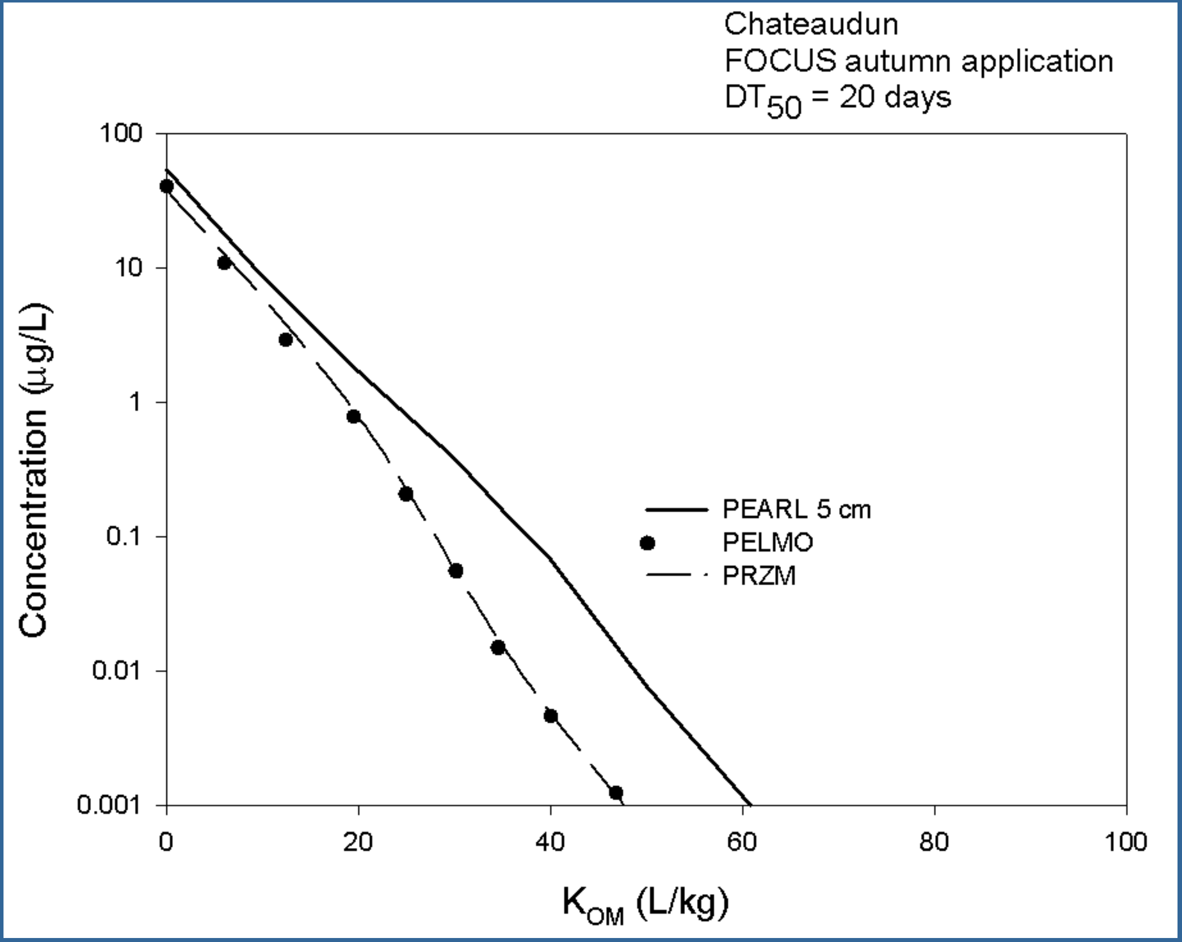
Now second part of test:

- one scenario (Chateaudun)

- variable substance properties:
  leaching as a function of K_{OM}
  (other properties equal to substance D)

standard FOCUS calculations



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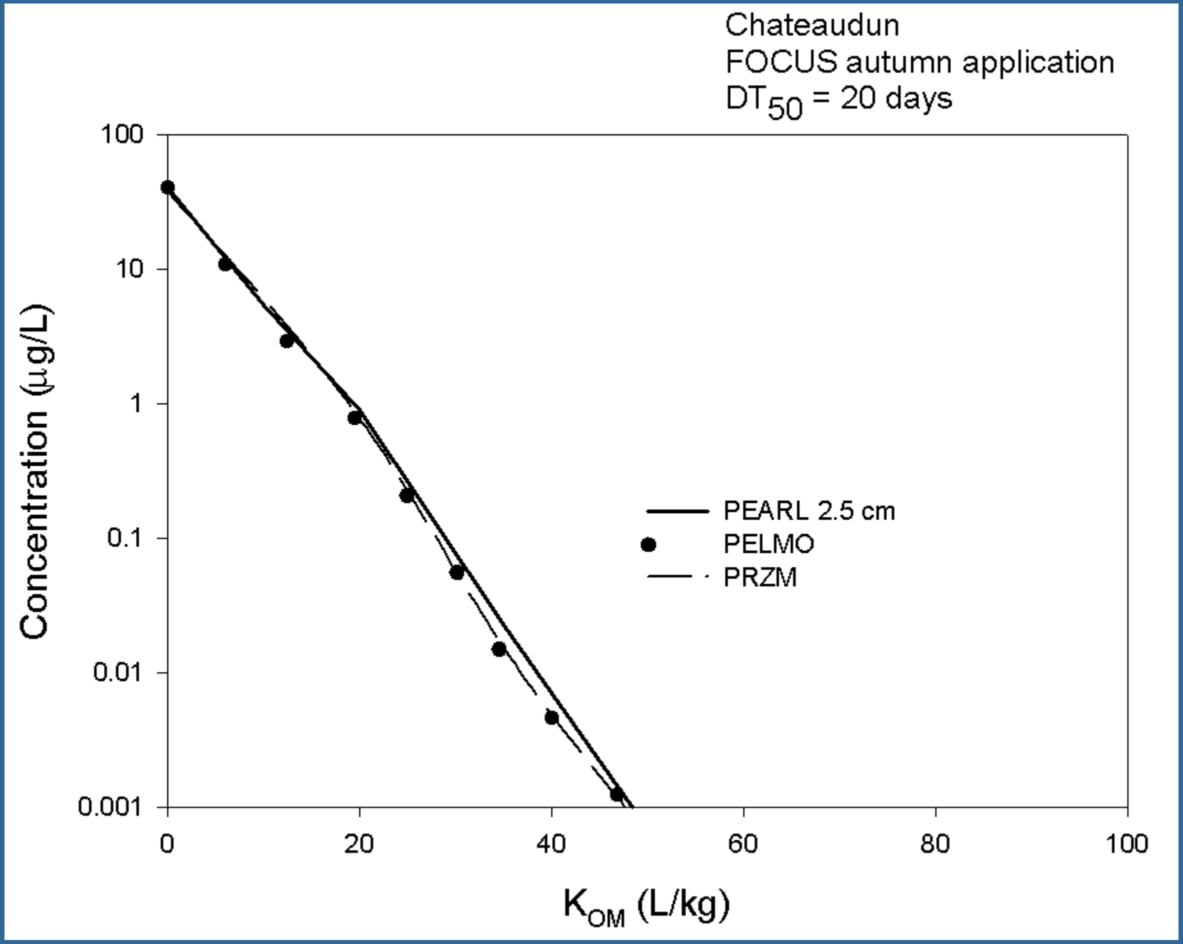
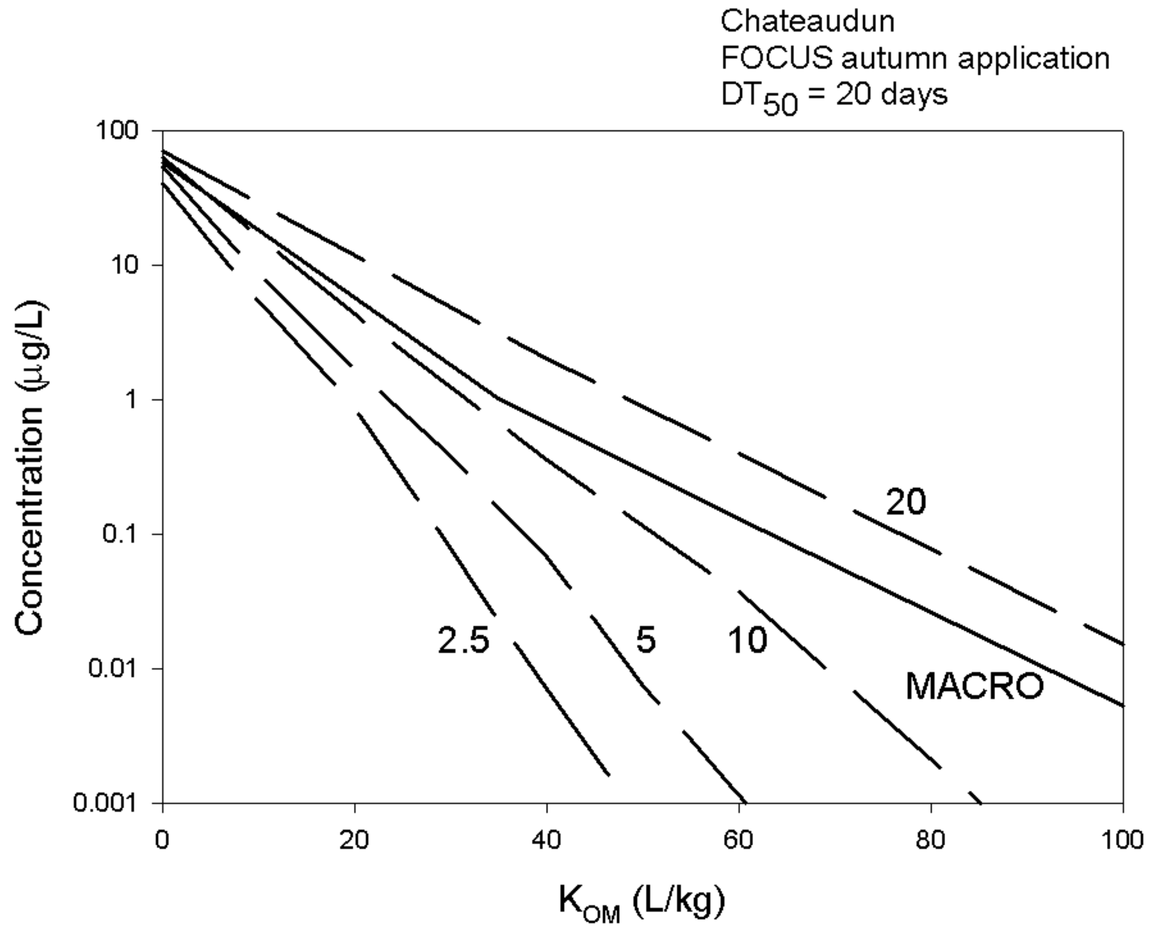
now L_{DIS} = 2.5 cm for PEARL



effect of dispersion length (cm) in PEARL compared to MACRO



Conclusions

- difference in dispersion length is major cause of differences between PELMO/PRZM and PEARL

- harmonisation of dispersion concept would reduce differences between PELMO/PRZM and PEARL considerably

- disclaimer: not all relevant cases considered: significant differences will remain between models (e.g. resulting from differences in runoff)