On the estimation of solute transport parameters for rivers

Steve Wallis	**Heriot-Watt University, UK**
Marzena Osuch	**Institute of Geophysics, Poland**
Russell Manson	**Richard Stockton College, USA**
Renata Romanowicz	**Institute of Geophysics, Poland**
Benoit Demars	**James Hutton Institute, UK**

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Background

- **Predicting the impact of pollution incidents requires knowledge of physical transport parameters**
- **The parameter values need to be estimated over a wide range of flow rates for an extensive range of rivers**
- **Ultimately, would like (empirical / theoretical) equations**
  - **$PV_1 = f_1$ (hydraulics, geomorpholgy, etc)**
  - **$PV_2 = f_2$ (hydraulics, geomorpholgy, etc)**
  - **$PV_3 = f_3$ (hydraulics, geomorpholgy, etc)**
- **But, initially, require reliable estimates of parameter values in order to derive the equations**

Background

- A few techniques are available, but the most popular one involves the analysis of tracer experiment data
  - Method of moments (discredited – unfairly?)
  - Optimisation of mathematical model
    - Analytical solution
    - Numerical solution
    - Routing solution

    - Several traditional optimisation algorithms

      Levenberg-Marquardt
    - Several newer approaches

      neural networks, genetic & evolutionary algorithms, particle swarm

Background

- **But are the results reliable?**

  - **model validity**
  - **numerical scheme**
  - **locally or globally optimised**
  - **equifinality**
  - **quality of data**

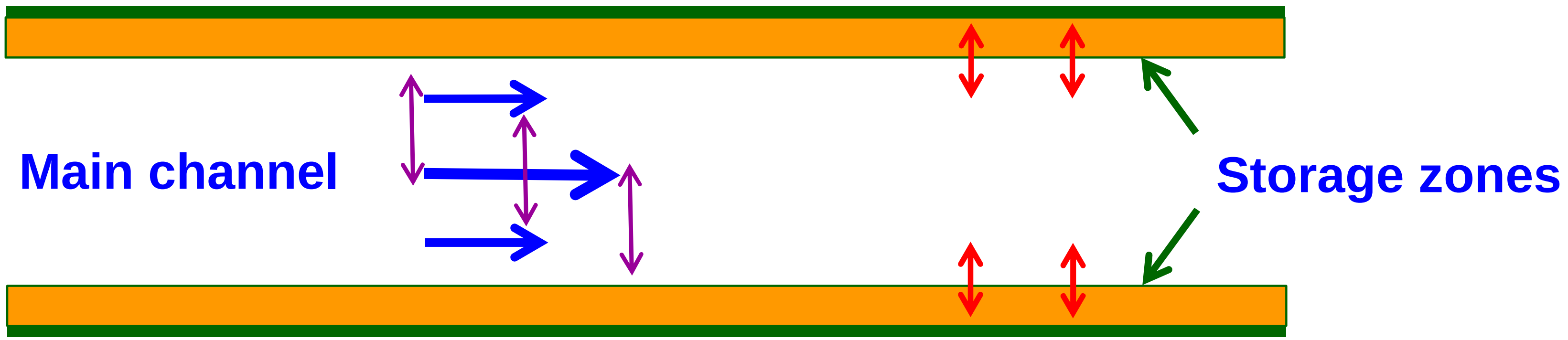
Background

- **Aim of work**
  - **To explore a very simple question:**

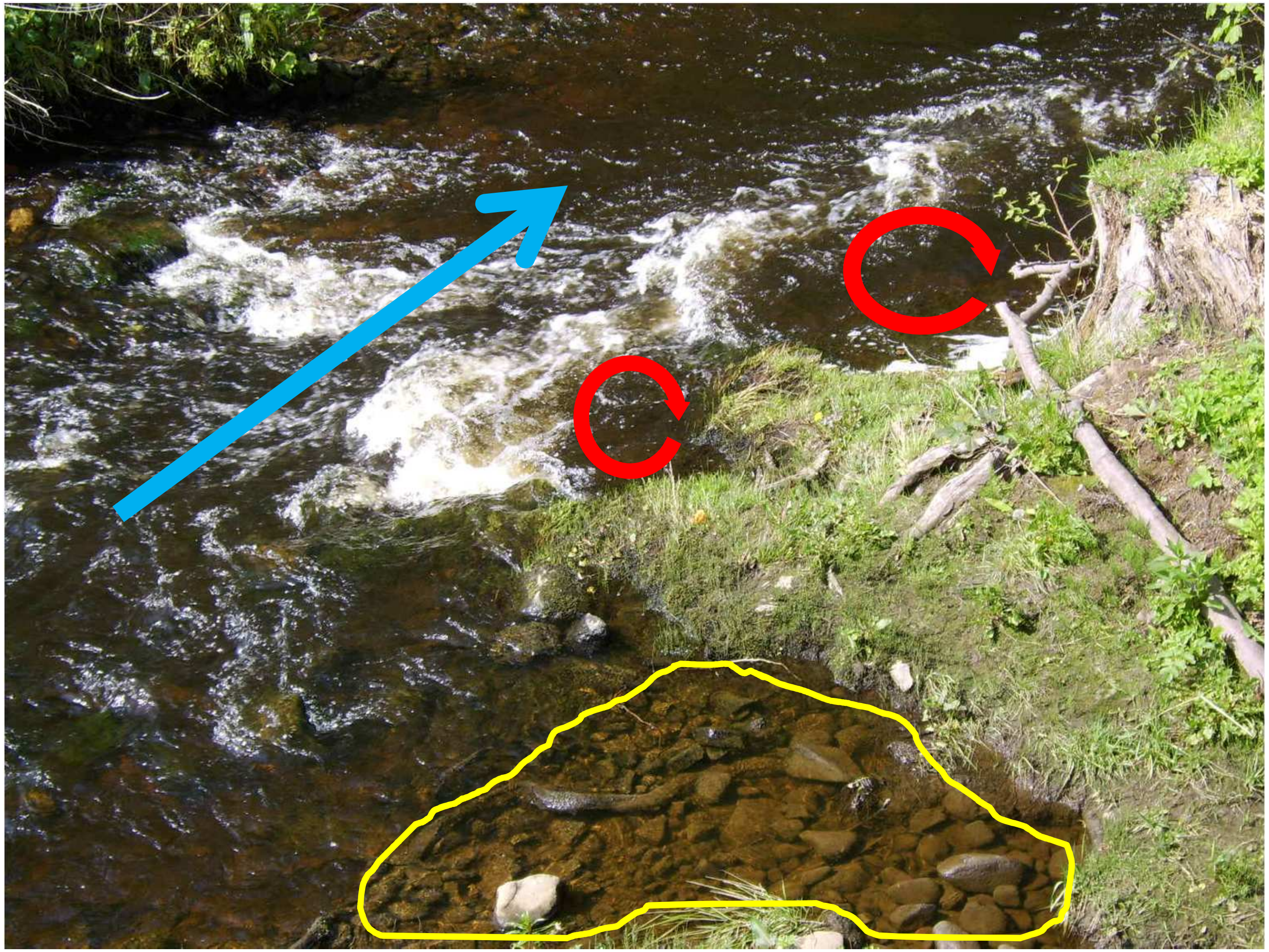
"Do we get the same, or different, parameter values when applying different model/optimisation systems to the same data?"

Models & Processes

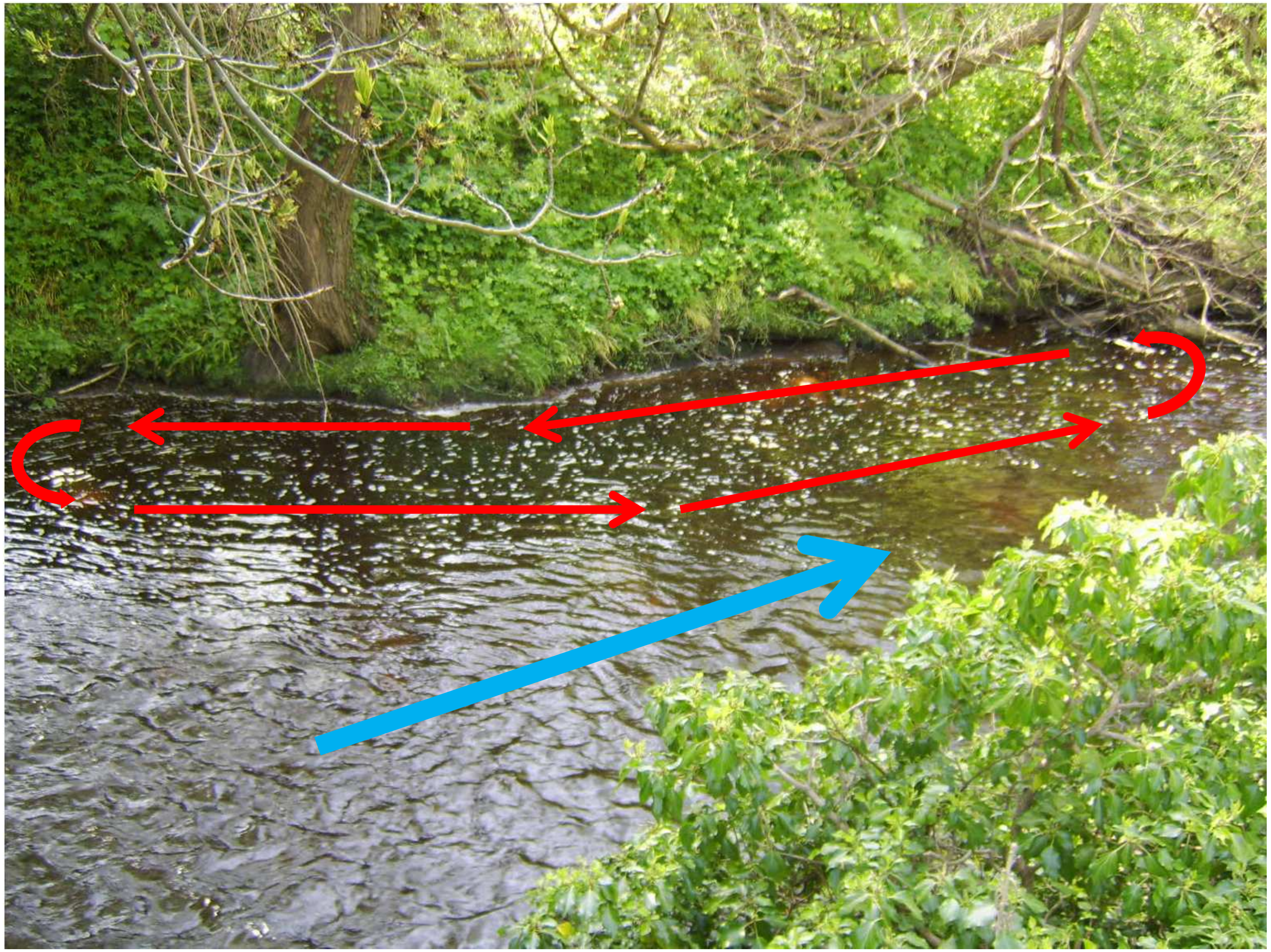
- **Numerical solutions of the transient storage equations**
- **Four parameters to be optimised**
  - **Velocity in (or cross-sectional area of) main channel**
  - **Dispersion coefficient in main channel**
  - **Size of transient storage zones**
  - **Exchange rate between main channel and storage zones**



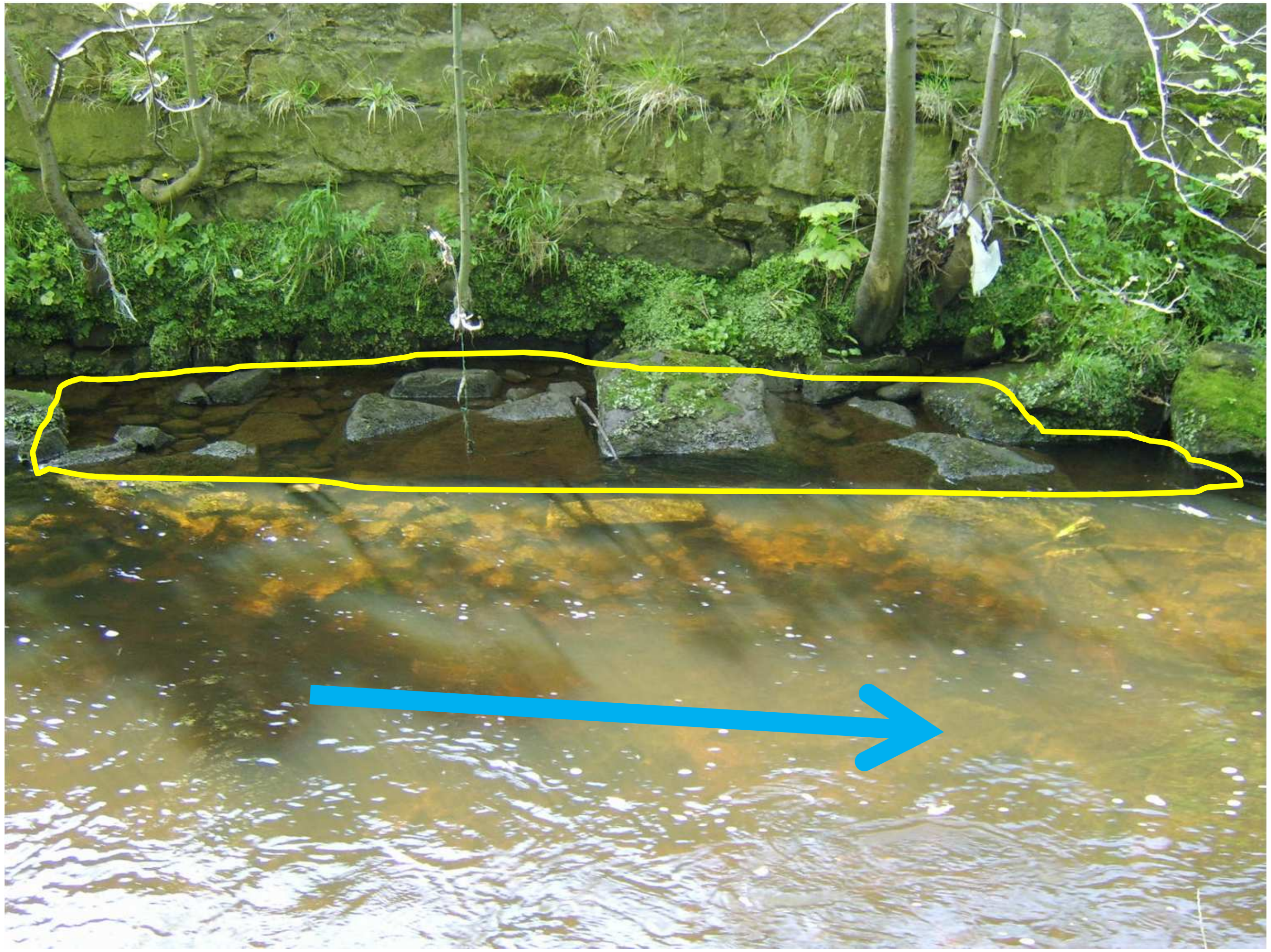
Models & Processes



Models & Processes



Models & Processes

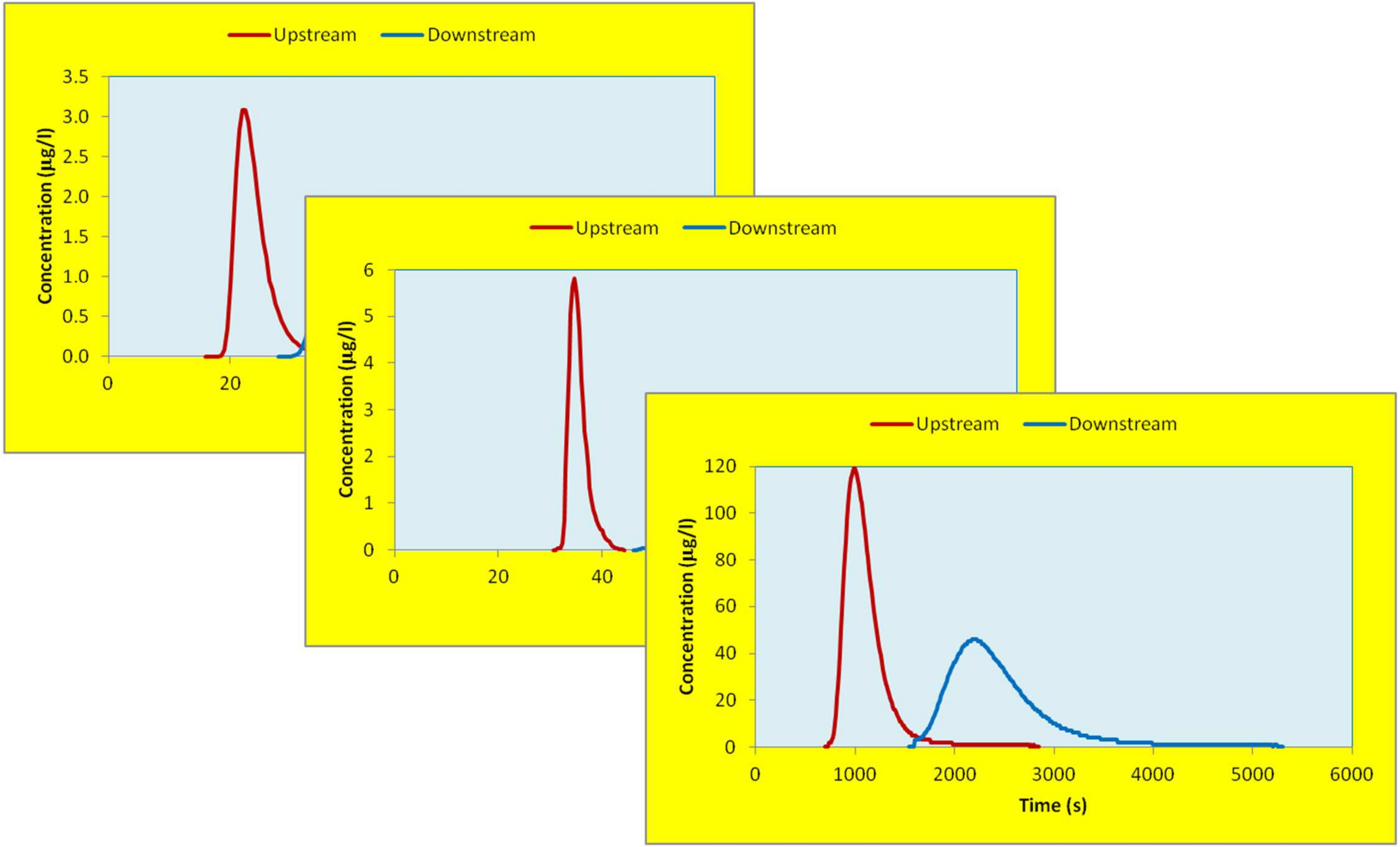


Data

- **Observed temporal solute concentration profiles at both ends of 7 experimental reaches**

Case	Reach	Length (m)	Flow (L/s)	Time step (s)
1	Murray Burn	184	145	30
2	River Rhine	47150	1169000	600
3	River Rhine	73800	1169000	1200
4	Cairn Burn	91	10.2	10
5	Uvas Creek	152	13.6	600
6	Uvas Creek	186	14.0	600
7	Analytical	250	1000	1

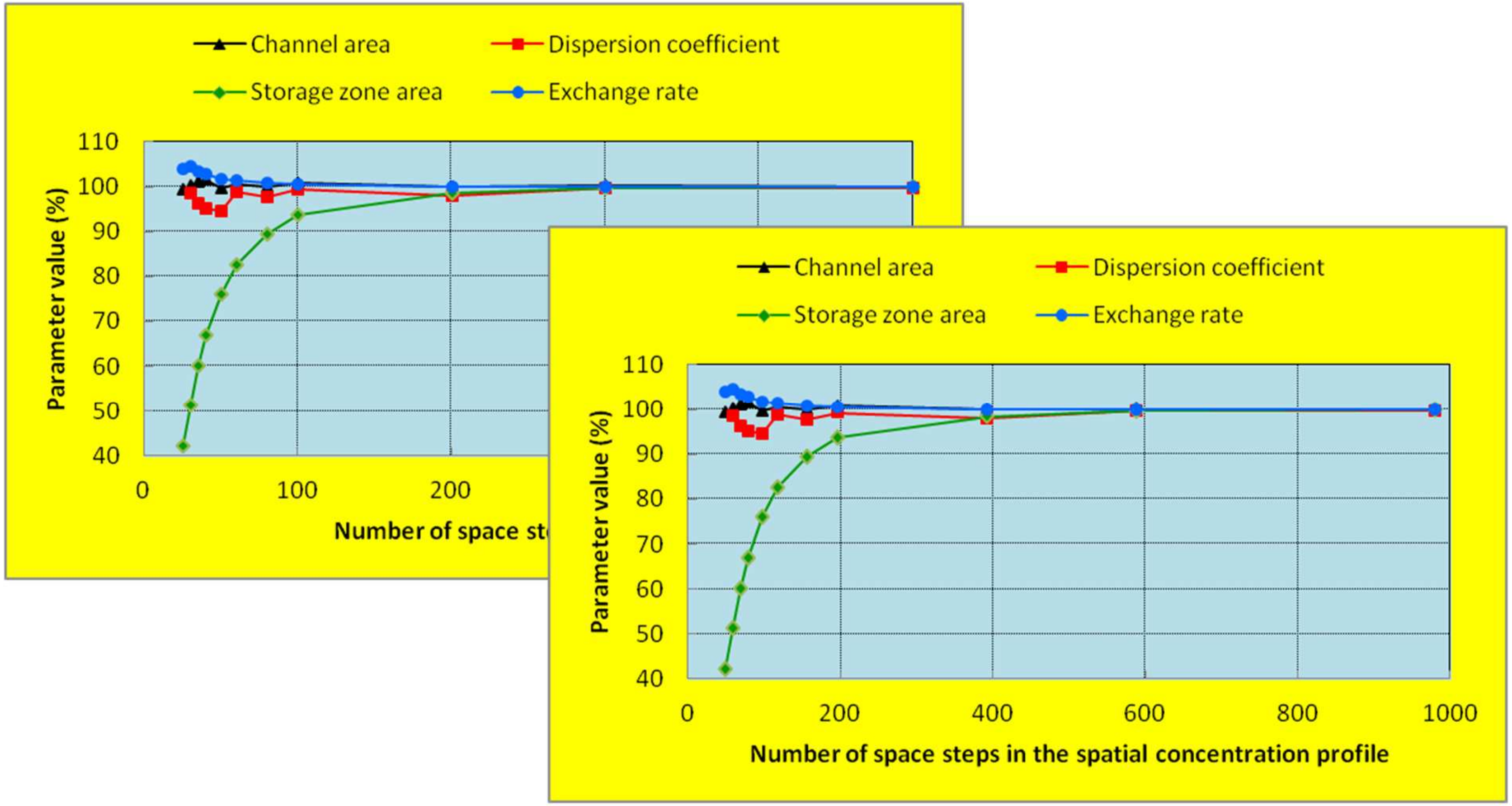
Data



Upstream
Downstream
Concentration (μg/l)
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
Upstream
Downstream
Concentration (μg/l)
6
5
4
3
2
1
0
0
20
40
Upstream
Downstream
Concentration (μg/l)
120
100
80
60
40
20
0
0
1000
2000
3000
4000
5000
6000
Time (s)

Results

- **Spatial resolution**
  - **Case 7**



Results

- **Optimised parameter values**
  - **Highest spatial resolution**

Reach	Model	A (m^2)	D (m^2/s)	α (1/s)	A_s (m^2)
Murray Burn	Polish	0.688	0.361	0.00100	0.083
Murray Burn	UK	0.737	0.564	0.00025	0.039
River Rhine	Polish	1418	22.5	0.00002	86.3
River Rhine	UK	1367	46.0	0.00062	112.8
River Rhine	Polish	1284	299	0.00001	380
River Rhine	UK	1336	743	0.00013	16.8

A – main channel area; D – dispersion coefficient; α – exchange rate; A_s – storage zone area

Results

- **Optimised parameter values**
  - **Highest spatial resolution**

Reach	Model	A (m^2)	D (m^2/s)	α (1/s)	A_s (m^2)
Cairn Burn	Polish	0.137	0.187	0.00018	0.017
Cairn Burn	UK	0.145	0.235	0.00031	0.661
Uvas Creek	Polish	0.451	0.204	0.00003	0.919
Uvas Creek	UK	0.460	0.250	0.00003	1.892
Uvas Creek	Polish	0.513	0.153	0.00005	4.710
Uvas Creek	UK	0.694	1.383	0.00075	0.053
Analytical	Polish	2.020	1.110	0.00035	3.722
Analytical	UK	2.019	1.097	0.00038	3.230
		2	1	0.00025	0.1

Discussion

- **Influence of Damkohler number, DaI**
  - **Reliable parameter values: 0.1 < DaI < 1.0**

Reach	Model	DaI
Murray Burn	Polish	>5
Murray Burn	UK	>5
River Rhine	Polish	>5
River Rhine	UK	>5
River Rhine	Polish	1 – 5
River Rhine	UK	>5

Reach	Model	DaI
Cairn Burn	Polish	1 – 5
Cairn Burn	UK	0.2 – 1
Uvas Creek	Polish	0.2 – 1
Uvas Creek	UK	0.2 – 1
Uvas Creek	Polish	0.2 – 1
Uvas Creek	UK	>5
Analytical	Polish	0.2 – 1
Analytical	UK	0.2 – 1

But DaI values based on optimised parameter values

Discussion

- Other issues
  - Model equations
  - Numerical schemes
  - Optimisation

Discussion

- **Model equations**

Polish model

$$\frac{\partial c}{\partial t}+\frac{Q}{A}\frac{\partial c}{\partial x}=\frac{1}{A}\frac{\partial}{\partial x}\left(AD\frac{\partial c}{\partial x}\right)+\alpha(s-c)$$

$$\frac{\partial s}{\partial t}=-\alpha\frac{A}{A_s}(s-c)$$

UK model

$$\frac{\partial(cA)}{\partial t}+\frac{\partial(cAU)}{\partial x}=\frac{\partial}{\partial x}\left(AD\frac{\partial c}{\partial x}\right)+k_1A(s-c)$$

$$\frac{\partial s}{\partial t}=-k_2(s-c)$$

c – main channel concentration; Q – flow rate; s – storage zone concentration; t – time; x – spatial co-ordinate; U – main channel velocity; k_1 – exchange rate; k_2 – $\alpha A/A_s$

Discussion

- **Numerical schemes**

Polish model

OTIS (Eulerian; finite difference; Crank-Nicolson)

Runkel & Broshears (1991)

UK model

DISCUS (Semi-Lagrangian; finite volume; Quickest & backward implicit)

Manson et el (2001)

Same boundary and initial conditions in both models

Discussion

- **Optimisation**

Polish model	UK model
Parameters – D, A, α, A_s	Parameters – D, U, k_1, k_2
	($A = Q/U$; $\alpha = k_1$; $A_s = \alpha A/k_2$)
Method – differential evolution	Method – genetic algorithm
Storn & Price (1997)	Yang et al (1998)
Population size – 40; scaling factor – 0.85; inheritance probability – 0.8	Population size – 5; mutation probability – 0.2; crossover rate – 0.5

Conclusions

- Different optimised parameter values obtained from the two modelling systems
- Some comfort from (a) results of analytical solution case and (b) robust main channel areas
- Several issues identified which might explain differences between results
- Further work needed.

Acknowledgement

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