Risk assessment for mixtures of agricultural chemicals in surface water; a SETAC Pellston workshop update

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Introduction

- In March of 2015, a SETAC Pellston workshop was held to help inform decision making around aquatic mixture risk assessments of chemicals using exposure scenarios and decision trees
- The efforts were broadly grouped into three areas of chemical origination: agriculture, domestic, and urban influences (a separate integration group was charged with looking at overarching issues)

Agricultural work group

- The agricultural land use combined effect measures with exposure scenarios of chemical mixtures for field and catchment-scale
- Exposure estimates were generated using an existing regulatory modeling framework for consistency with current practice
- However, results not intended for regulatory decision making
- Generated a daily concentration series that assesses the co-occurrence of potential mixture components
- Chemicals modeled were those used in crop protection and livestock production, and were considered to occur as mixtures (in time and space)
- Use of case studies to demonstrate approach

Case Study 1: Problem formulation

- Pesticide risk assessments are product based (either individual active substances or co-formulated mixtures of active substances)
- Is there any additional risk associated with exposure of the aquatic environment to any mixtures that arise from the full suite of plant protection products applied to a crop?
- The risk assessment relates to a single crop and risk is expected to be greatest at field-scale where there is limited potential for dilution within the receiving water body.
- The approach is illustrated in Case Study 1: winter wheat in the UK.

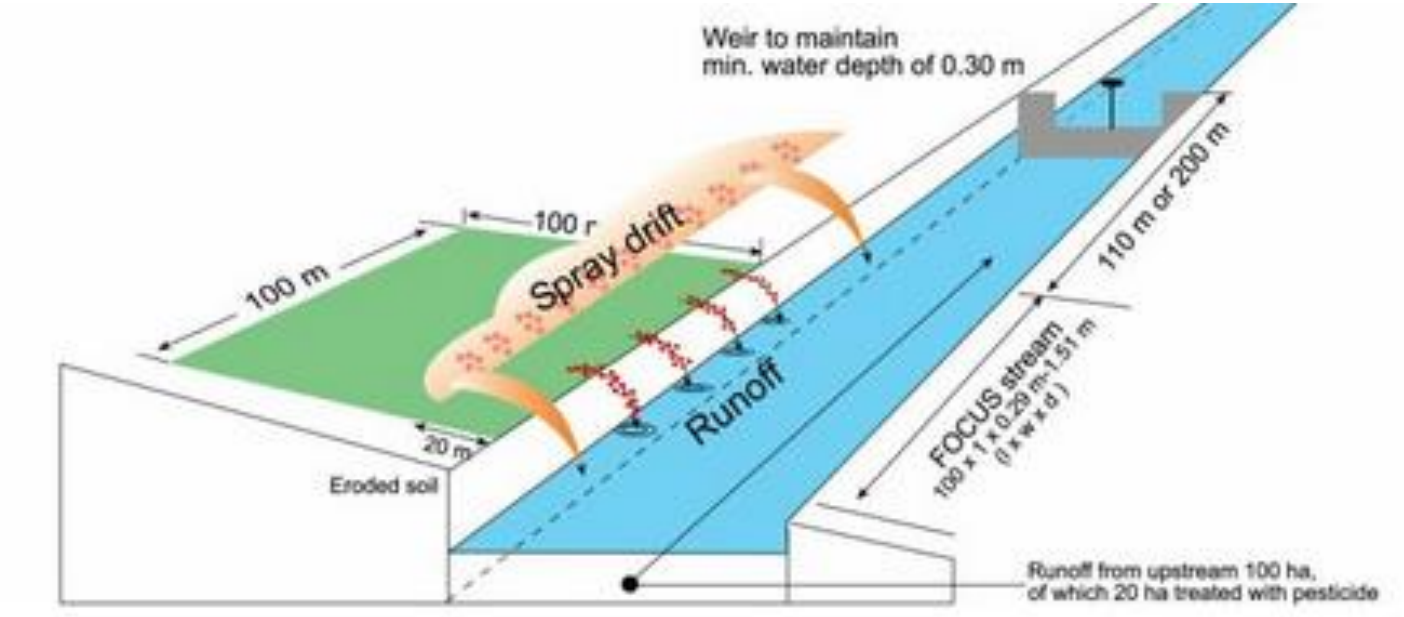
Case Study 1: Scenario definition

- Modeled as a wheat field in Eastern UK, consisting of crop protection applications of 13 substances over the course of the year
- This scenario used standard FOCUS soil, weather and receiving water body information
- Modeled over 20 years

Chemical name	Group	Application date
Flufenacet	Herbicide	14 October
Pendimethalin	Herbicide	14 October
Cypermethrin	Insecticide	6 November
		9 April
Iodosulfuron-methyl	Herbicide	9 April
Mesosulfuron-methyl	Herbicide	9 April
Epoxiconazole	Fungicide	14 April
		27 April
		19 May
Boscalid	Fungicide	27 April
Chlorothalonil	Fungicide	27 April
		19 May
Proquinazid	Fungicide	27 April
Prochloraz	Fungicide	19 May
Pyraclostrobin	Fungicide	19 May
Fluoxastrobin	Fungicide	18 June
Prothioconazole	Fungicide	18 June

Case Study 1: Modeling details

- Concentrations based on the stream in the FOCUS R1 scenario, most applicable scenario for this area in UK
- The loadings to water were calculated with FOCUS SWASH/PRZM, then the water fate part with STEPS1234
- Edge-of-field model with UK LERAP (Local Environment Risk Assessment for Pesticides) no-spray buffer of 5 m



Case Study 2: Problem formulation

- Agricultural fields don't exist in isolation within the landscape
- What is the risk associated with the potential environmental combination of plant protection products and veterinary medicines applied in the same watershed?
- The risk assessment relates to multiple sources of chemical inputs, where risk is expected to be greatest at watershed-scale where there is greater potential for aggregation within a low-flow water body
- The approach is illustrated in Case Study 2: Corn in Iowa, US

Case Study 2: Scenario definition

- Simulates a multi-unit watershed scenario consisting of a combination of corn fields, pasture, and feedlot inputs based in part on the US EPA Iowa corn scenario used in pesticide registration evaluations
- Twelve different active substances for crop protection were modeled on the corn field
  - These applications ranged from a pre-plant herbicide to a late-year fungicide application
- Manure from treated cattle containing two different pharmaceutical substances (parasiticide and antibiotic) was applied to corn fields as fertilizer
  - As well as direct runoff input from pasture and feedlot

Case Study 2: Scenario definition

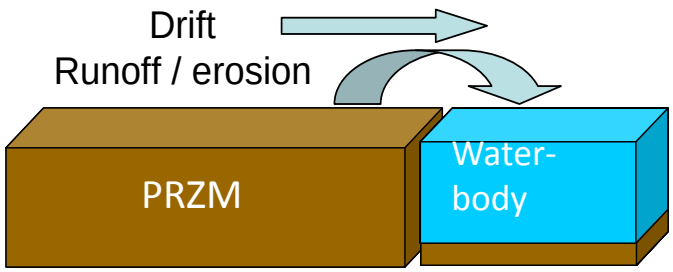
- Crop protection (left table) and veterinary medicines (right table)

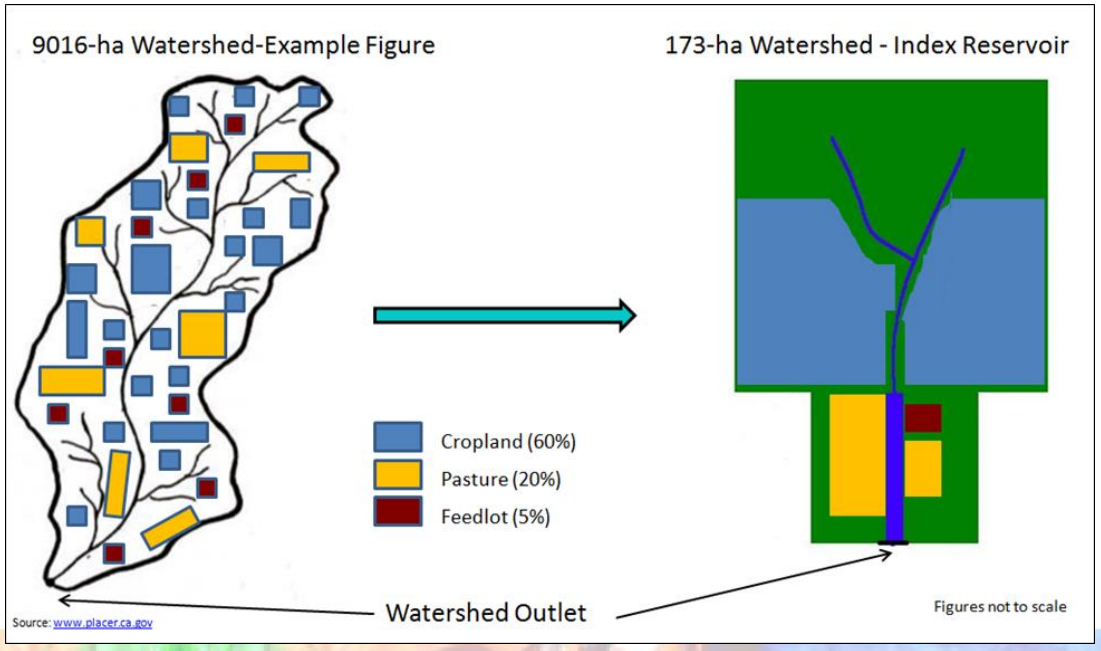
Crop Protection Chemical name	Group	Application date
Acetochlor	Pre-herbicide	1 wk before plant
Flumetsulam	Pre-herbicide	1 wk before plant
Clopyralid	Pre-herbicide	1 wk before plant
Atrazine	Pre-herbicide	1 wk before plant
Clothianidin	Seed treatment	At planting
Ipconazole	Seed treatment	At planting
Trifloxystrobin	Seed treatment	At planting
Metalaxyl	Seed treatment	At planting
Tefluthrin	Soil insecticide	At planting
Glyphosate	Post-herbicide	28 d after emerge
Pyraclostrobin	Fungicide	65 d after emerge
Metconazole	Fungicide	65 d after emerge

Veterinary Medicine Chemical name	"Application" date
Tilmicosin	
Manured cropland (solid manure)	May 8, Oct 26
Manured cropland (liquid manure)	May 30, June 30, July 30, Aug 30
Pasture	Apr 1 – 14 (14 day excretion)
Feedlot	Apr 15 – 29 (14 day excretion)
Moxidectin	
Manured cropland (solid manure)	May 8, Oct 26
Manured cropland (liquid manure)	May 30, June 30, July 30, Aug 30
Pasture	Apr 1 – 20 (20 day excretion)
Feedlot	Apr 1 – 20 (20 day excretion)

Case Study 2: Modeling details

- Based on US EPA's Index Reservoir scenario as modeled with EPA's Surface Water Concentration calculator (SWCC)
- Soil, weather and other parameters based on US EPA Tier II Iowa corn scenario
- Watershed composition: 56.6% corn, 2.3% pasture, 0.09% feedlot
- Modeled for 30 years
- Crop modeling still 'edge-of-field' and adhered to most stringent label buffer requirement





Aquatic toxicity endpoints

- Acute and chronic endpoints for primary producers, invertebrates and fish were collected from available registration documents
  - Most sensitive endpoint was selected
- Standard assessment factors were applied to obtain regulatory acceptable concentrations
- UK scenario:
  - EU review reports and EFSA conclusions
  - Acute assessment factor: 100, chronic assessment factor: 10, mesocosm assessment factor 3 on NOEC/NOAEC
- US scenario:
  - aquatic benchmark values and the related EPA documents, registration reports for veterinary medicines
  - Crop protection - Acute assessment factor: 2, chronic assessment factor: 1
  - Veterinary Medicines– Acute assessment factor as given in registration reports : 100 or 1000

Evaluating mixtures

- Daily concentration output from each chemical modelled were brought together into a single output file
- Concentrations were compared to toxicity outputs to create RQ for each compound (on a daily basis)
- Daily ∑RQ were calculated across all compounds
- Initial summarization of daily data:
  - How many days ∑RQ > 1?
  - How many days ∑RQ > 1 driven by only one compound? More than one?
  - How many days ∑RQ > 1 due to a mixture, when otherwise would not > 1?
  - Maximum number of consecutive days ∑RQ > 1?

Results – UK Case Study

- Of the 7,519 days modeled, the ∑RQ > 1 for 391 days (5.2%)
- Of the 13 compounds modeled, RQ exceedances were primarily driven by two compounds
- For days ∑RQ > 1, 38% of time only one compound had RQ > 1
- For days ∑RQ > 1, 39% of time more than one compound had RQ > 1
  - I.e., these would be covered by normal risk assessment process
- The remainder 23% of days ∑RQ > 1 (1.2% of days overall), no single compound had RQ > 1
  - I.e., the effects of the mixture would exceed the effect(s) of an individual
- The maximum number of consecutive days ∑RQ > 1 = 4 days
- Mitigation on label used in modeling (LERAP 5m buffer)
  - But there may be additional mitigation on label for individual compounds (e.g., drift reduction technology) that were not taken into account

Results – US Case Study

- Of the 10,957 days modeled, the ∑RQ > 1 for 11.8% of days
- Of the 13 compounds modeled, RQ exceedances were primarily driven by three compounds
- For days ∑RQ > 1, 24% of time only one compound had RQ > 1
- For days ∑RQ > 1, 38% of time more than one compound had RQ > 1
  - I.e., these would be covered by normal risk assessment process
- The remainder 38% of days ∑RQ > 1, no single compound had RQ > 1
  - I.e., the effects of the mixture would exceed the effect(s) of an individual
- The maximum number of consecutive days ∑RQ > 1 was much higher than UK scenario which reflects the receiving water body used in modelling – reservoir with very low flow
- US scenario combined crop protection and veterinary medicines, however these may have very different safety factors when determining LOC. E.g., vet med AF = 100, crop protection AF = 2

Conclusions (1)

This study demonstrates situations in both case studies where the sum of the mixture toxicity may produce effects that individual compounds may not.

Some considerations:

- We used most sensitive endpoint for each compound
  - This spanned multiple taxonomic groups
  - E.g., effects to both primary producers and fish taxa combined
  - Concentration addition may not be appropriate in these cases
- Combined both chronic and acute toxicity endpoints across all compounds
- Chronic endpoints should be examined over time
  - We looked at daily peak concentrations
  - TWA using a comparable timeframe to testing (e.g., 21 day, 60 day) may be more appropriate

Conclusions (2)

- Does it make sense to use concentration addition?
  - For screening level assessments such as this, CA is ok
  - But it may combine different endpoints for within & across taxonomic groups
  - At higher tier this should be re-examined when indicated
- The receiving water body heavily influences exposure patterns (stream, reservoir)
- For UK case study, the mixture effects were small and are likely to be covered by the safety factors used in determining the RAC
- For US case study, a higher tier assessment may be warranted; e.g.,
  - Separate acute and chronic assessments
  - Separate assessments for taxa

Summary

- We have developed a methodology for estimating concentrations of mixtures that could be occurring in headwater streams or reservoirs in agricultural areas
  - This has been based on current regulatory modeling scenarios
  - Encompasses temporal relevance of exposures from mixtures
- We have estimated the effects that these mixtures may have on aquatic organisms
  - Using conservative assumptions about effects endpoints in combination with each other (e.g., across taxonomic groups, acute & chronic)
- When toxicity to aquatic organisms was present, it was often due to only one or two compounds
  - Which would likely be covered individually in the current risk assessment process
- These results will be combined with those of other working groups (urban and municipal) as part of the integration process

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Thank You