# Pharmaceutical transport through turf/soil systems: field and modeling results

Michael H. Young[1], Dale A. Devitt[2], Lena Wright[2]

[1]Bureau of Economic Geology, Jackson School of Geosciences, University of Texas at Austin, TX

[2]School of Life Sciences, University of Nevada Las Vegas, NV

## Background and Motivation

- Recycled water is quickly becoming accepted as an asset for augmenting water supplies during periods of shortages.
- Lingering questions on the transport and fate of pharmaceutical compounds in recycled water raise public concerns about long-term safety of this resource.
- We monitored mass flux of selected pharmaceuticals in irrigated turf/soil systems that relied solely on recycled water.

## Goal and Questions

- To monitor water flow and selected compound concentrations at lysimeter scale with different soil, irrigation and upper boundary treatment.
- To better understand potential attenuation of selected pharmaceuticals through turf/soil systems.
- To simulate flow and transport of compounds to predict future behavior in different soils.
- The overall objective was to use the modeling to evaluate the question: What is the overall risk to humans and the environment from inadvertent application of compounds we studied?

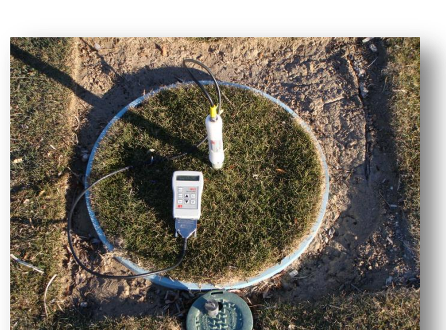
## Experimental Location and Design

- Soil was collected from experimental facilities in Boulder City NV (loamy sand) and North Las Vegas NV (sandy loam).
- Experimental design consisted of eight combinations of three independent variables (soil, leaching fraction, upper boundary), randomized in space, in triplicate (24 total).

| Soil Type | Leaching Fraction | Turf / Bare |
|---|---|---|
| Loamy Sand | 0.05 | B |
| Loamy Sand | 0.05 | G |
| Loamy Sand | 0.25 | B |
| Loamy Sand | 0.25 | G |
| Sandy Loam | 0.05 | B |
| Sandy Loam | 0.05 | G |
| Sandy Loam | 0.25 | B |
| Sandy Loam | 0.25 | G |



- Instrumentation included ceramic drainage samplers, water content profiler, and redox probes. Sites were irrigated with reclaimed water for 745 days.

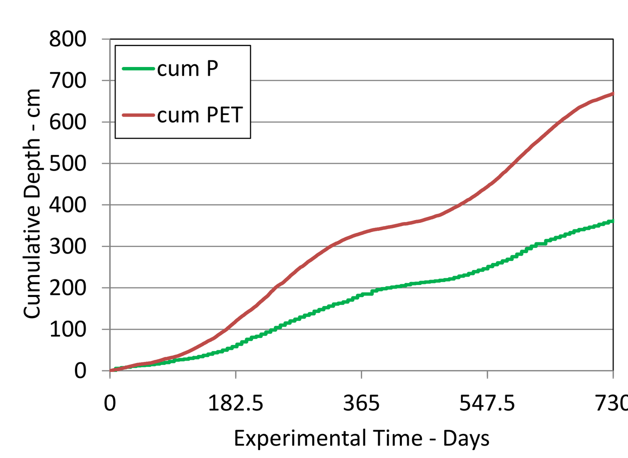

## Compounds Studied

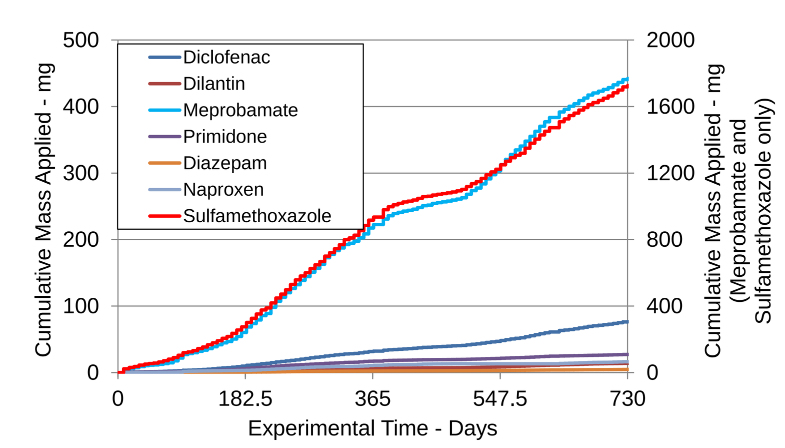
| Compound | Human Usage | Human Health Threshold*† | pKa | Log $K_{ow}$ |
|---|---|---|---|---|
| Atenolol | β-Blocker; cardiovascular disease; hypertension | 70,000 | 9.48[a] | 0.16[a] |
| Atorvastatin | Lower blood pressure (Lipitor) | 5,000 | 4.46[d] | 6.36[b] |
| Carbamazepine | Anti-convulsant | 1,000 | <2[c] | 2.30[a] |
| Diazepam | Sedative and anti-convulsant | N/A | 3.3[c] | 2.82[a] |
| Diclofenac | Anti-inflammatory | N/A | 4.15[b] | 4.51[b] |
| Fluoxetine | Anti-depressant (Prozac) | 10,000 | 9.62[a] | 4.60[b] |
| Gemfibrozil | Lower lipid levels | 45,000 | 4.7[c] | 4.77[b] |
| Ibuprofen | Anti-inflammatory | 34,000 | 4.91[a] | 3.50[a] |
| Meprobamate | Tranquilizer | 260,000 | <2[c] | 0.70[a] |
| Naproxen | Anti-inflammatory (Aleve) | 220,000 | 4.15[ab] | 3.18[ab] |
| Primidone | Anti-convulsant | N/A | 11.62 | 0.91 |
| Sulfamethoxazole | Anti-biotic | 35,000 | 5.7[c] | 0.89[a] |
| Triclosan | Anti-biotic | 350 | 7.9[c] | 4.53[a] |
| Trimethoprim | Anti-biotic | 61,000 | 7.1[c] | 0.91[a] |

a – Sangster, 2012; b – SRC PhysProp Database, 2012; c – Yoon et al., 2007; d – Wu et al., 2000; * - Monitoring Triggering Levels (Anderson et al., 2010); † - concentrations in ng/L

## Model Setup and Boundary Conditions

- Model: HYDRUS-1D v. 4.xx
- Soil column thickness – 120 cm
- Grid spacing: variable – 10x higher at surface
- Root zone distribution – max at surface, 0 at 50 cm (when used)
- Initial conditions:
  - $\psi$ profile: uniform at -30 kPa ($\theta_v$ = 0.04)
  - solute concentration: 0 ng/L
- Boundary conditions:
  - Lower boundary: -60 kPa (constant)
  - Upper boundary: Measured temperature and water input (P + I); PET calculated using onsite micrometeorological data and Penman Eqn.; solute mass based on species concentration and known water input

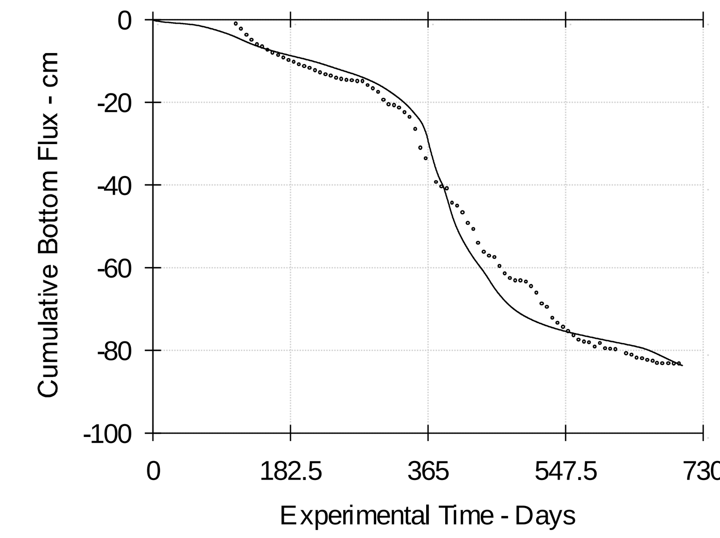


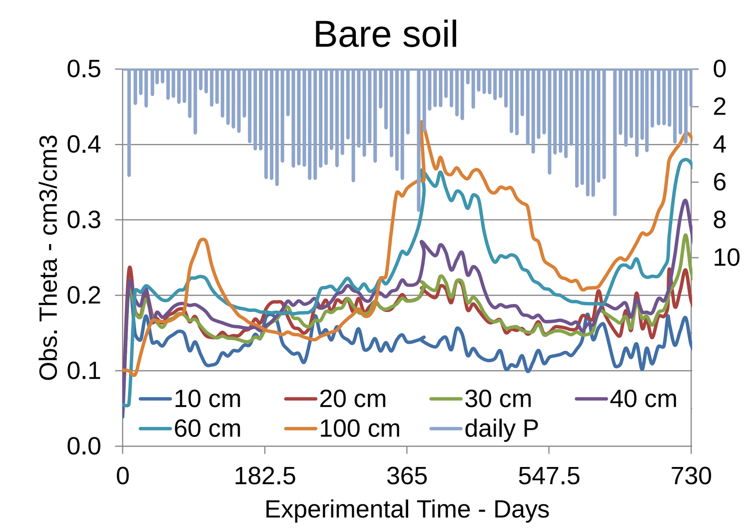

## Field Experimental Results

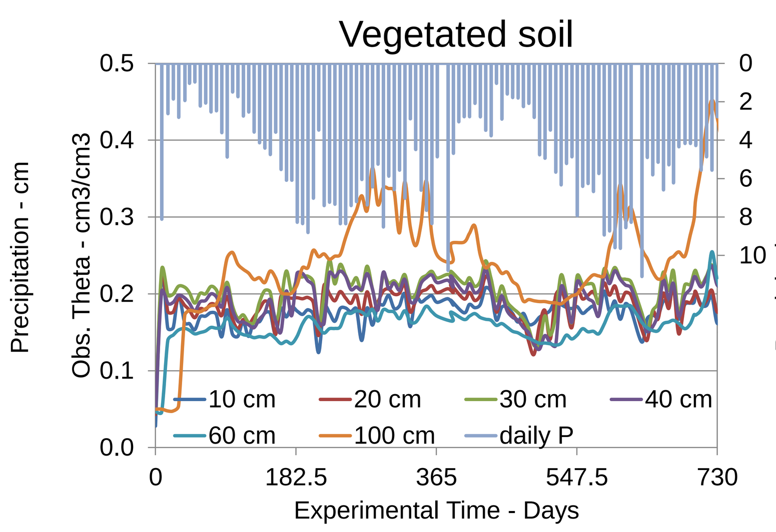
| Loamy Sand | | | | Sandy Loam | | | |
|---|---|---|---|---|---|---|---|
| **0.05 Bare Soil** | | | | **0.05 Bare Soil** | | | |
| Analyte | Avg | SD | CV | Analyte | Avg | SD | CV |
| Carbamazepine | 1.84 | 3.19 | 1.73 | Carbamazepine | <RL | <RL | <RL |
| Primidone | 25.99 | 20.39 | 0.78 | Primidone | 0.25 | 0.44 | 1.73 |
| Sulfamethoxazole | 84.89 | 74.66 | 0.88 | Sulfamethoxazole | 7.29 | 12.63 | 1.73 |
| **0.05 Turf** | | | | **0.05 Turf** | | | |
| Analyte | Avg | SD | CV | Analyte | Avg | SD | CV |
| Carbamazepine | <RL | <RL | <RL | Carbamazepine | <RL | <RL | <RL |
| Primidone | 44.26 | 19.32 | 0.44 | Primidone | 0.53 | 0.55 | 1.04 |
| Sulfamethoxazole | 93.64 | 29.39 | 0.31 | Sulfamethoxazole | 1.93 | 3.34 | 1.73 |
| **0.25 Bare Soil** | | | | **0.25 Bare Soil** | | | |
| Analyte | Avg | SD | CV | Analyte | Avg | SD | CV |
| Carbamazepine | 26.84 | 27.53 | 1.03 | Carbamazepine | <RL | <RL | <RL |
| Primidone | 98.35 | 17.87 | 0.18 | Primidone | 6.53 | 9.35 | 1.43 |
| Sulfamethoxazole | 253.93 | 90.78 | 0.36 | Sulfamethoxazole | 88.80 | 117.94 | 1.33 |
| **0.25 Turf** | | | | **0.25 Turf** | | | |
| Analyte | Avg | SD | CV | Analyte | Avg | SD | CV |
| Carbamazepine | 100.60 | 23.52 | 0.23 | Carbamazepine | <RL | <RL | <RL |
| Primidone | 102.29 | 14.65 | 0.14 | Primidone | 8.09 | 3.01 | 0.37 |
| Sulfamethoxazole | 130.97 | 21.72 | 0.17 | Sulfamethoxazole | 5.66 | 9.81 | 1.73 |

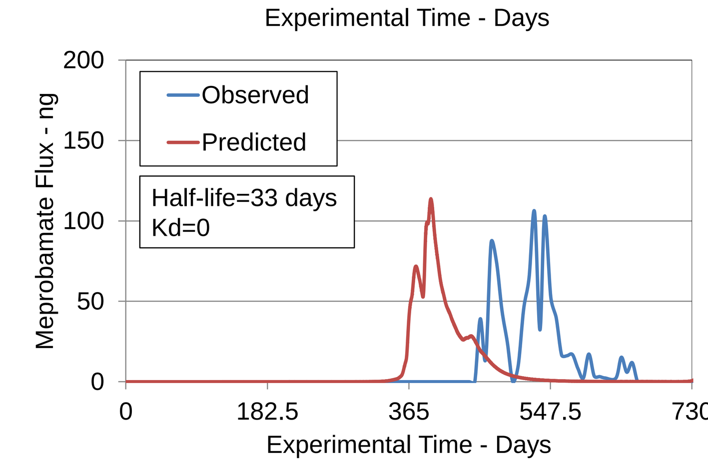
## Preliminary Modeling Results

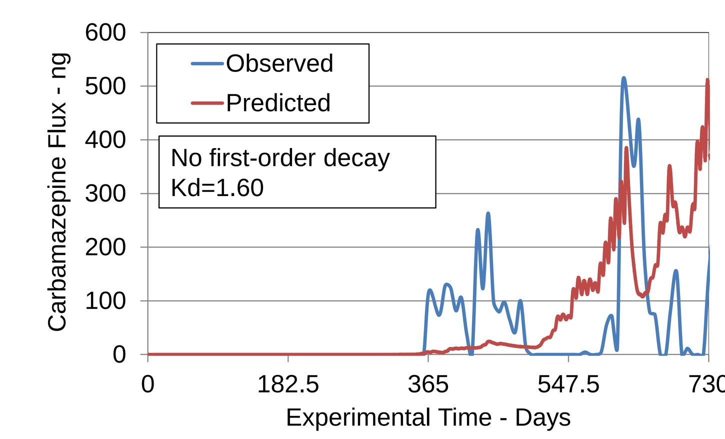



- Hydraulic property estimation done using bottom flux and water content at 2 depths in bare, loamy sand soil.
- Water arrival occurred sooner in model, but total flux differed by ~0.25 cm.
- Water content trend similar but model was less responsive than observed data at depth.




- Example outputs of modeled versus observed mass flux.
- Cyclical behavior of observed flux caused by higher irrigation rates during overseeding of cool, winter turf.
- Laboratory sorption data (Lin et al., 2012) reasonably well described solute/soil interaction, but boundary conditions were difficult to fully represent in the model.

## Conclusions

- 9 of 14 tested PPCPs detected in drainage. Sulfamethoxazole had the highest mass discharge (~250 mg/ha/yr) and Primidone had the highest average % mass discharge in drainage (25%).
- Field results showed no influence of vegetative boundary on flux—influence strongest on soil texture and leaching fraction.
- Observed release at 120 cm depth depends on compound, soil material and aerobic status–no simple relationships exist.
- Combination of solute retardation and half-life significantly affected predicted flux.

- Highest mass discharge associated with sandy soils with high LF—combination should be avoided in the field.

## References and Acknowledgments

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