Continuous modeling of VFS for pesticide removal under PWC scenarios

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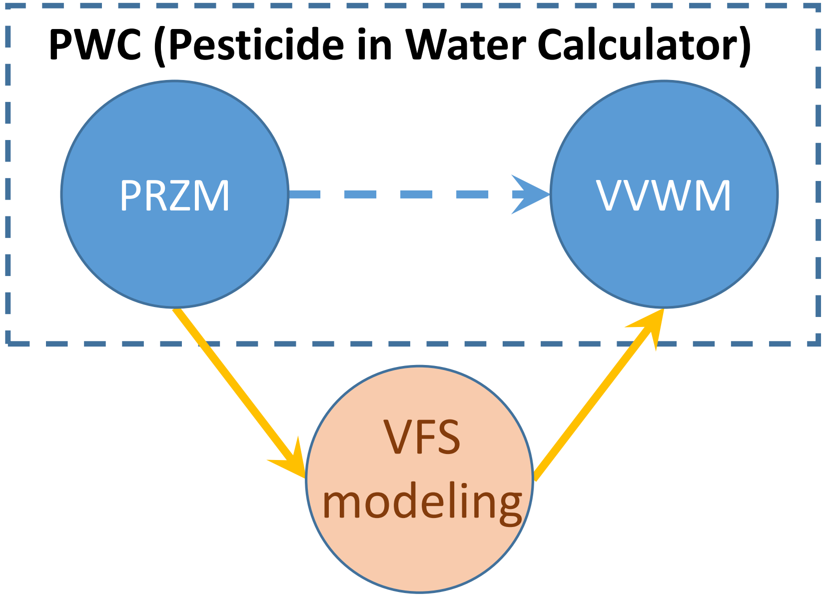
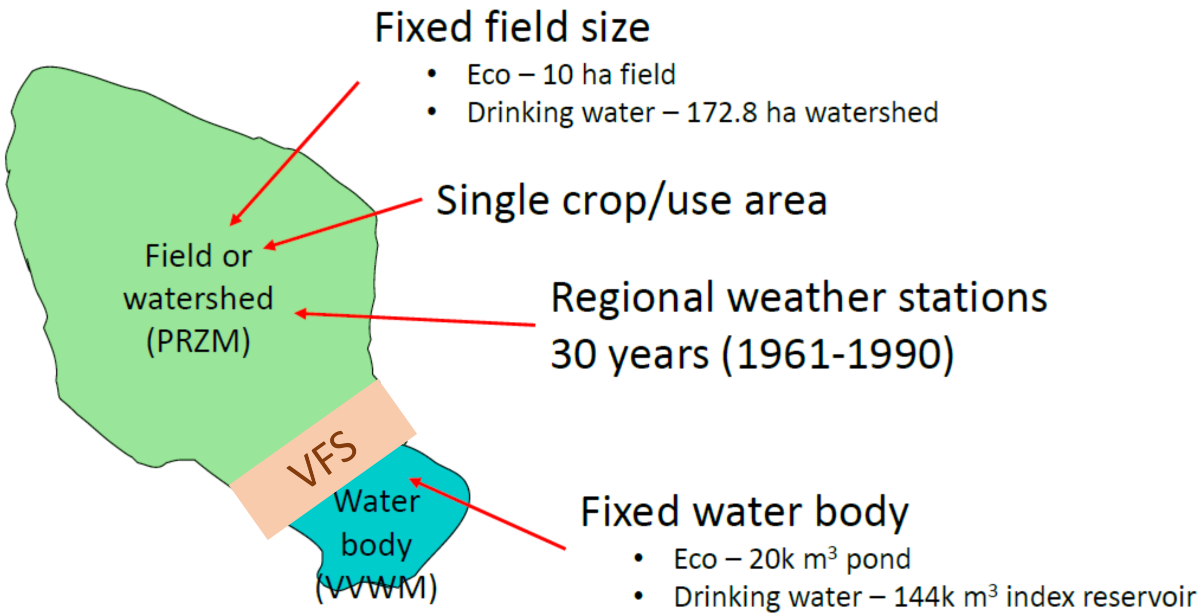
Continuous modeling of VFS

- PWC-VFS modeling system





Modified based on:
EPA-HQ-OPP-2015-0424-0036

Introduction

- VFS is required/recommended for some pesticide products, e.g., agricultural applications of pyrethroids and neonics
- USEPA/OPP does not have an official modeling approach for VFS
  - e.g., ERA (ecological risk assessment) on pyrethroids (USEPA, 2016a) did not consider the label-required 10-ft VFS
- VFS has been modeled with various approaches, e.g., by PWG (Pyrethroid Working Group) (Giddings et al., 2015)
- DPR’s SWPP started review and development of VFS modeling in 2016

Modeling approaches for VFS

- VFSMOD (Muñoz-Carpena et al., 1999), originally developed for hydrology (water and sediment) only
  - Trapping effects for water flow (ΔQ) and suspended sediment (ΔE)
- *Regression* equations for pesticide (ΔP)
  - (Sabbagh et al., 2009): $\Delta P = f(\Delta Q, \Delta E, F_{ph}, \%clay)$, where F_{ph} is a phase distribution factor for incoming pesticide, $F_{ph}=Q_{in}/E_{in}/K_d$
  - Integrated into VSFMOD
  - Initially calibrated with 47 field data sets, recently improved with 244 data (Reichenberger et al., 2019)

Modeling approaches for VFS

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- *Regression* equations for pesticide (ΔP)
  - (Sabbagh et al., 2009): $\Delta P = f(\Delta Q, \Delta E, F_{ph}, \%clay)$
  - Other regression-based methods, e.g., Chen et al., (2016):

$$\Delta P = f(\Delta Q, \Delta E, K_{OC}, \%clay)$$

Modeling approaches for VFS

- VFSMOD (Muñoz-Carpena et al., 1999), originally developed for hydrology (water and sediment) only
  - Trapping effects for water flow (ΔQ) and suspended sediment (ΔE)
- *Regression* equations for pesticide (ΔP)
- *Semi-mechanistic* method for pesticide: $\Delta P_d = \Delta Q$, $\Delta P_s = \Delta E$ (Neitsch et al., 2009)
  - ΔP_d: removal efficiency for dissolved pesticide
  - ΔP_s: removal efficiency for sorbed pesticide

Modeling approaches for VFS: summary

- Actually, TWO modeling components
  - Hydrological simulation (ΔQ and ΔE), and
  - Pesticide simulation (ΔP)

Hydrologic simulation	Pesticide simulation	Example of "VFS modeling"
N/A	Empirical (ΔP=a*WIDTH^b)	Early SWAT (Neitsch et al., 2005)
Empirical	Semi-mechanistic ($\Delta P_d=\Delta Q$, $\Delta P_s=\Delta E$)	SWAT 2009 (Neitsch et al., 2009)
Mechanistic (VFSMOD)	Empirical (regression equation)	(Sabbagh et al., 2009)
Mechanistic (VFSMOD)	Semi-mechanistic	(Luo, 2017; Reichenberger et al., 2019)
Mechanistic (VFSMOD)	Mechanistic	CDPR approach (this talk)

SWAT = Soil-Water Assessment Tool

CDPR model review

- VFSMOD: the best available mechanistic model for hydrological simulation in a VFS
- Limitations in existing approaches for pesticide simulation
  - Regression equation
  - Semi-mechanistic method

Limitations in the existing approaches for pesticide simulation

- Range of pesticide properties in field experiments
  - In the 244 field measurements used to calibrate the regression equation (Reichenberger et al., 2019): 98% are associated with $K_d<1000$ and 93% with $K_d<200$
  - Not appropriate for pesticides with high/moderate hydrophobicity

Limitations in the existing approaches for pesticide simulation

- Range of pesticide properties in field experiments
- Use of “total” (i.e., whole-water) concentration, and assumption of instantaneous equilibrium in incoming flow
  - In fact, edge-of-field pesticide masses are not necessarily in equilibrium according to measured data or PRZM predictions

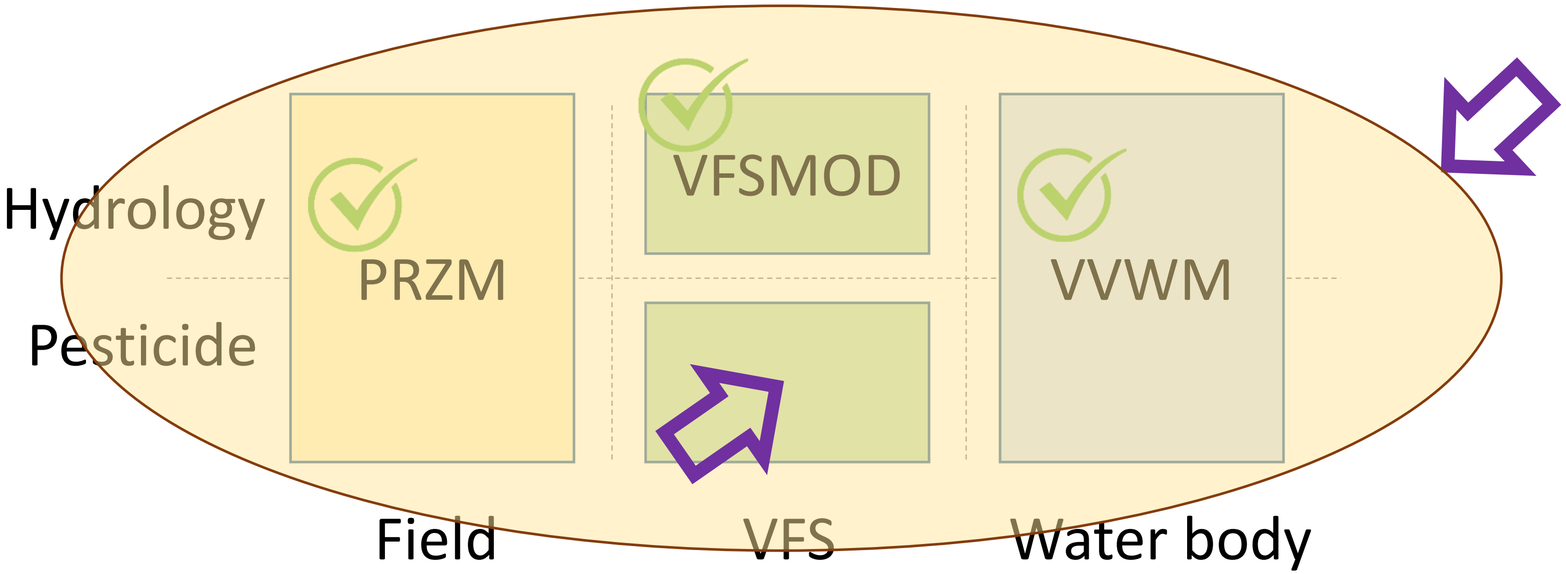
  - Recall the phase distribution factor (F_{ph}) used in regression equations
  - Bifenthrin and the PWC scenario for “California almond” as an example
    - $F_{ph}= Q_{in}/E_{in}/K_d= 4.4$ (this value is used in regression equations)

Limitations in the existing approaches for pesticide simulation

- Range of pesticide properties in field experiments
- Use of "total" (i.e., whole-water) concentration, and assumption of instantaneous equilibrium in incoming flow
- Pesticide removal efficiency (ΔP) is independent to incoming pesticide loadings (in terms of total mass or phase distribution)
  - Regression: $\Delta P = f(\Delta Q, \Delta E, F_{ph}, \%clay)$ where $F_{ph}=Q_{in}/E_{in}/K_d$
  - Semi-mechanistic: $\Delta P_d = \Delta Q$, $\Delta P_s = \Delta E$
  - Irrelevant to incoming pesticides in dissolved (RLFX) or sorbed (ELFX) phases

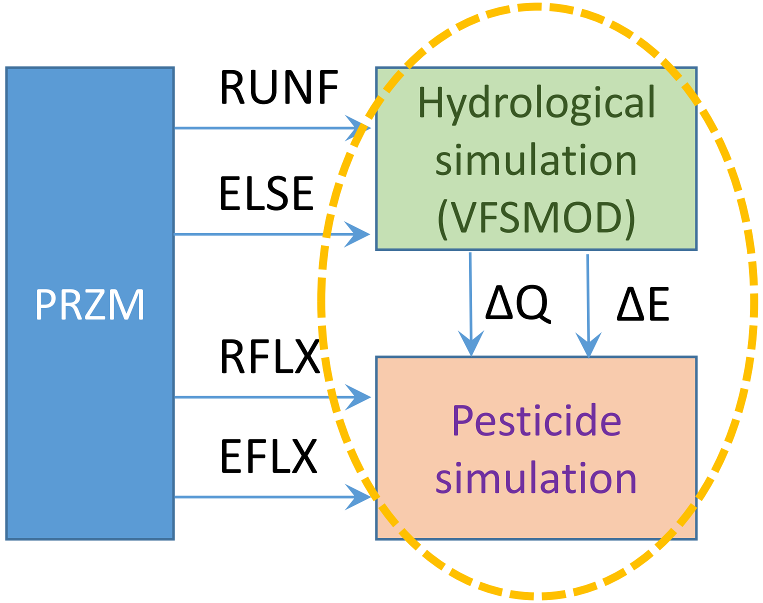
DPR’s approach: overview

- VFSMOD for hydrological simulation (ΔQ and ΔE)
- CDPR development for pesticide simulation (ΔP)
- Interpolation over field measurements for model validation
- Integrated modeling system for continuous modeling



Model development by CDPR

1. To separate hydrological simulation vs. pesticide simulation
   - Use VFSMOD for hydrological simulation (ΔQ and ΔE)
   - Develop our own approach for pesticide simulation

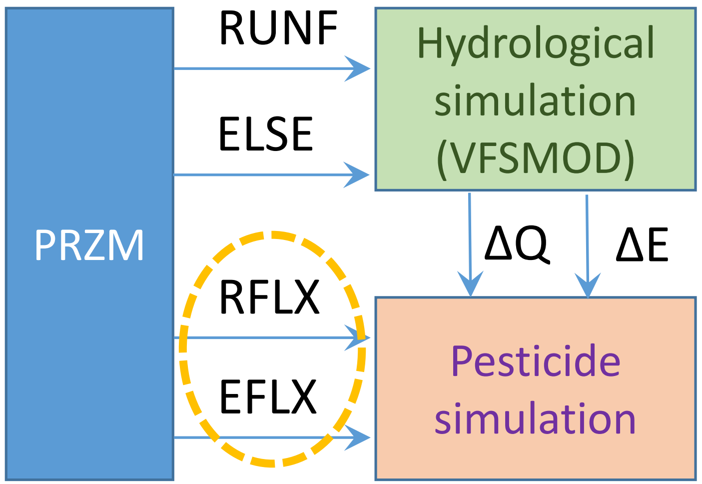


PRZM outputs:

- RUNF = water, Q_{in}
- ELSE = sediment, E_{in}
- RFLX = pesticide (dissolved)
- EFLX = pesticide (sorbed)

Model development by CDPR

2. To separate pesticide mass in dissolved vs. sorbed phases
   - Directly use PRZM-predicted pesticide fluxes (not assume instantaneous *equilibrium* and *mixing* between RFLX and EFLX)

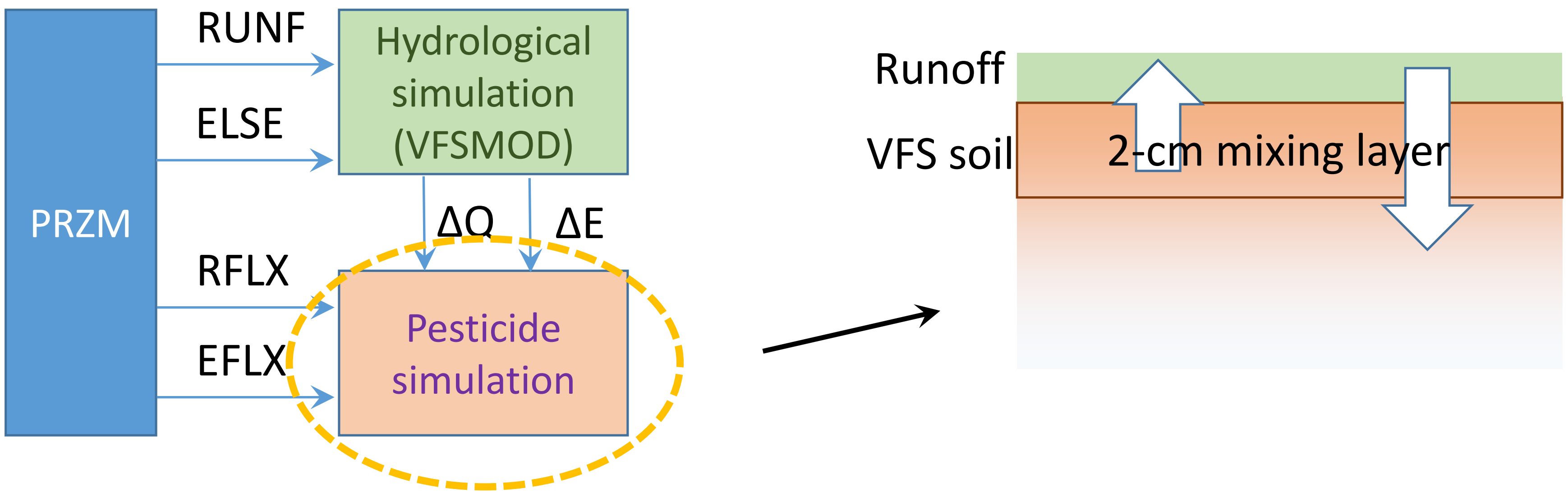


PRZM outputs:

- RUNF = water, Q_{in}
- ELSE = sediment, E_{in}
- RFLX = pesticide (dissolved)
- EFLX = pesticide (sorbed)

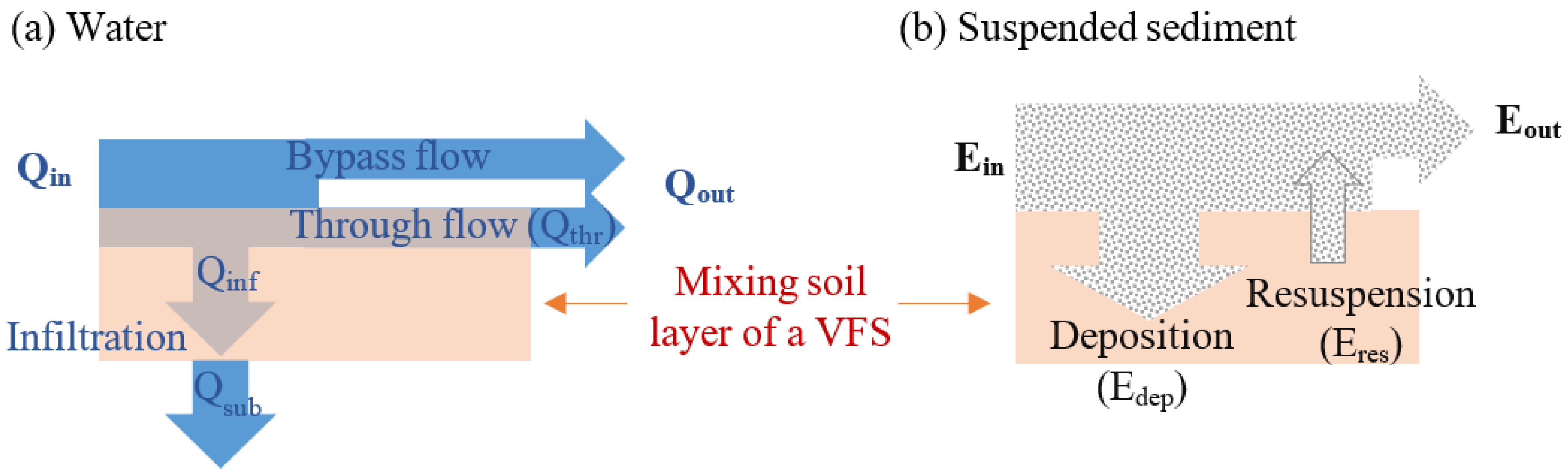
Model development by CDPR

3. To formulate two processes for pesticide simulation
   - From runoff to filter: trapping (dissolved and sorbed phases)
   - From filter to runoff: extraction (dissolved) and resuspension (sorbed)



Mechanistic approach for pesticide simulation

- Based on soil-water interaction



Mechanistic approach for pesticide simulation

- Based on soil-water interaction
- Equations for pesticide removal

$$\begin{cases} \Delta P_d = \Delta Q + f_{thr}(1 - \frac{C}{C_i}) \\ \Delta P_s = \Delta E + f_{res}(1 - \frac{S}{S_i}) \end{cases}$$

Recall the semi-mechanistic approach (Neitsch et al., 2009)

$$\begin{cases} \Delta P_d = \Delta Q \\ \Delta P_s = \Delta E \end{cases}$$

- f_{thr} = runoff interacting factor (through flow)
- f_{res} = resuspension ratio
- C = dissolved pesticide concentration (L/kg)
- S = particle-bound pesticide concentration (kg/kg[soil])
  - C and S are calculated by solving mass balance equations

Mechanistic approach for pesticide simulation

- Based on soil-water interaction
- Equations for pesticide removal
- "Through" flow (Q_{thr}) and runff interacting factor (f_{thr})
  - A concept from PRZM, where "*runoff flow is conceptualized as partially flowing through … and interacts with the soil*" (Young, 2016)
  - Specified as $f_{thr} = Q_{thr}/Q_i$, or "runoff interacting factor"
  - For agricultural fields, f_{thr} = 0.26 (PRZM default); and re-calibrated 0.19 (Young and Fry, 2017)
  - A higher value is expected for VFS, and to be calibrated with field data

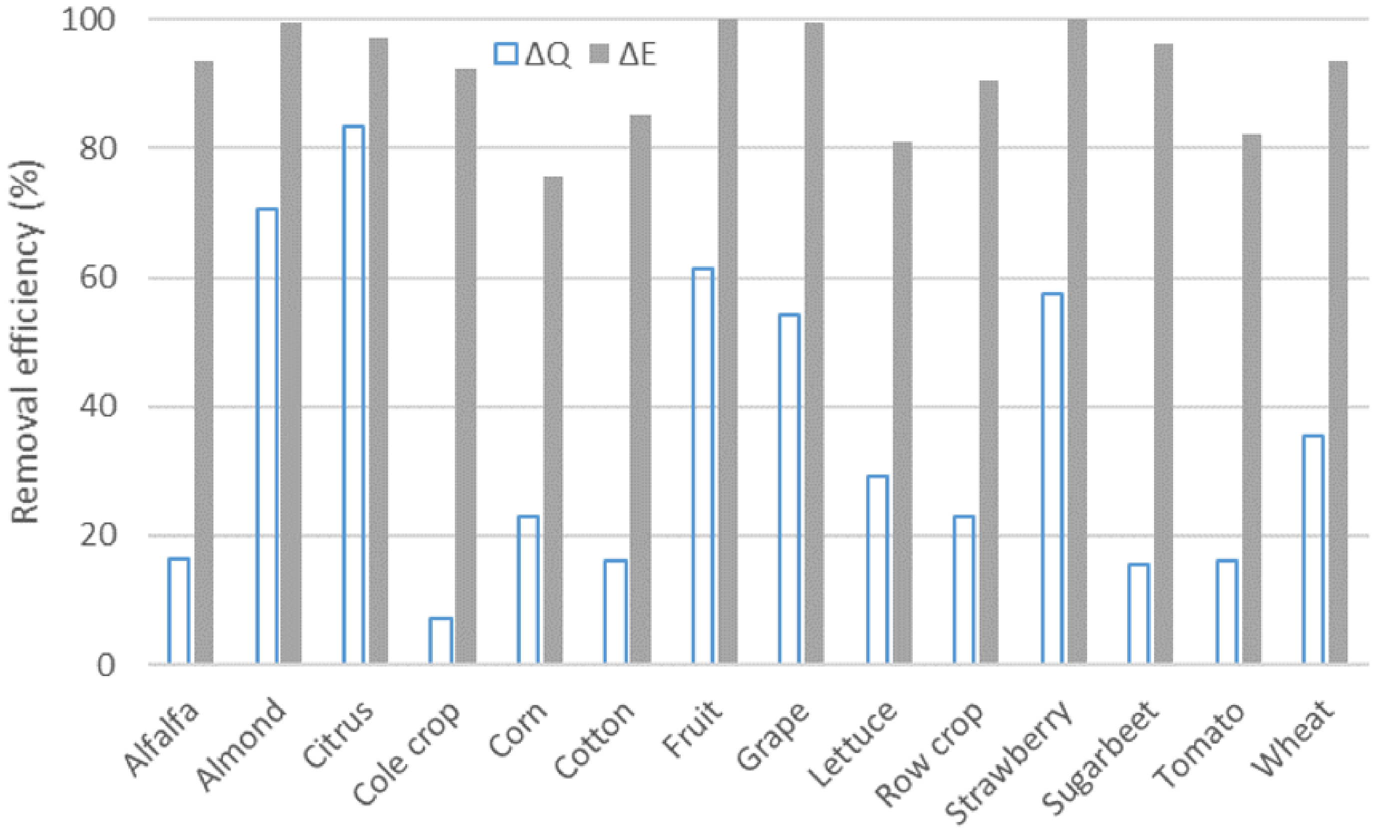
Model demonstration

- 4 pesticides
  - bifenthrin, chlorpyrifos, imidacloprid, permethrin
  - Representing pesticides with KOC in the orders of 10^2, 10^3, 10^4, and 10^5
- Input data from ERAs (USEPA, 2010, 2011, 2016, 2017)
  - Physiochemical properties
  - Label review (use pattern, application method/rate/frequency, PWC scenario)
  - In summary, 14 PWC scenarios in California are tested
    - “alfalfa”, “almond”, “citrus”, “cole crop”, “corn”, “cotton”, “fruit”, “grape”, “lettuce”, “row crop”, “strawberry”, “sugarbeet”, “tomato”, and “wheat”
- Assumption: the VFS has the same *soil properties* and *weather data* as defined in the PWC scenario

Model demonstration: other inputs

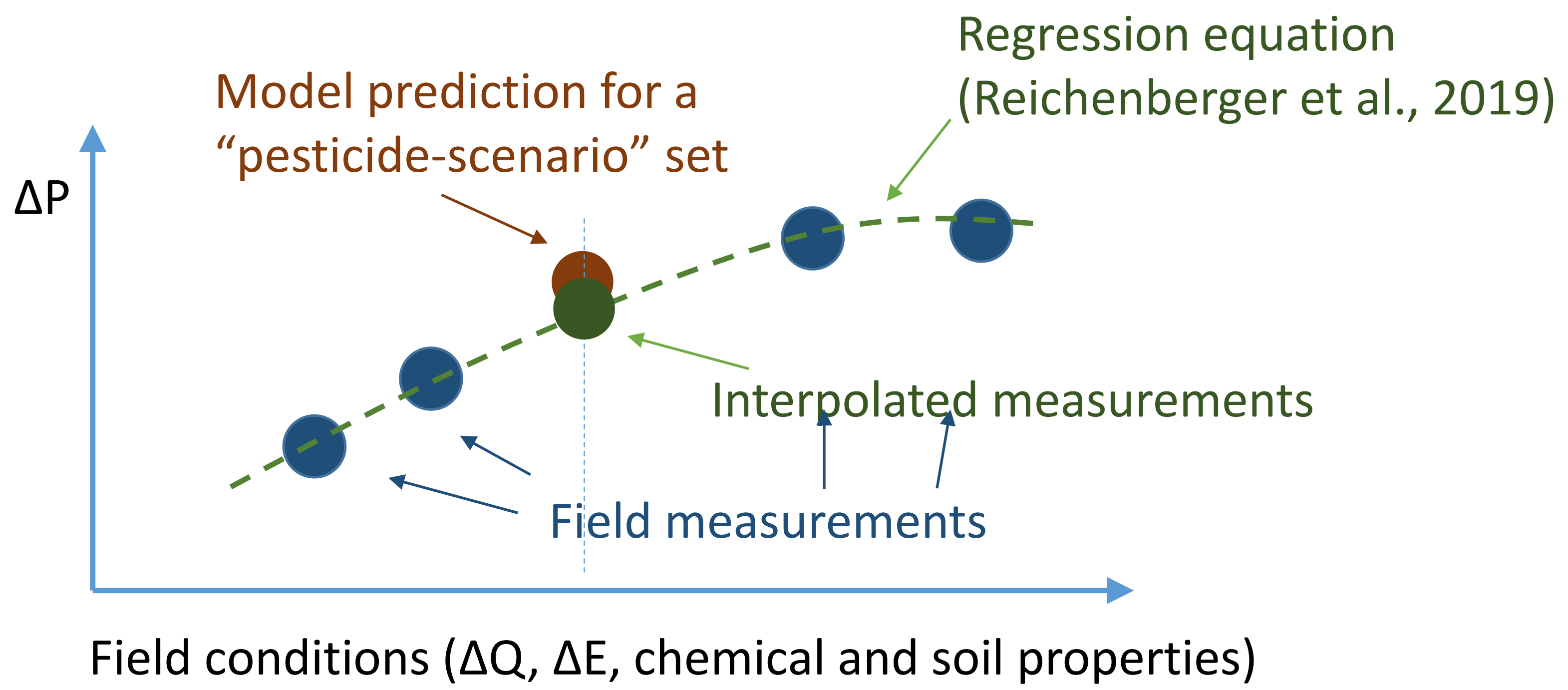
- Manning's roughness coefficient (N): 0.40 in the case study
  - Grass (bluegrass sod) N= 0.45; Bermuda grass N=0.41 (PRZM5 user's manual, Young, 2016)
- VFS width: 10 ft
- VFSMOD default values, e.g., buffer properties (".igr" input file)

Hydrological simulation (VFSMOD) results



Build a database to validate pesticide simulation results

- No sufficient data for direct comparison between observed and predicted removal efficiency
- Build validation data from the regression equation: $\Delta P = f(\Delta Q, \Delta E, F_{ph}, \%clay)$



Build a database to validate pesticide simulation results

Scenario	Bifenthrin	Chlorpyrifos	Imidacloprid	Permethrin
Alfalfa	NA	51.4	44.7	56.4
Almond	82.9	72.8	68.7	93
Citrus	76.4	67.5	66.9	87
Cole crop	45.8	44.6	43.4	45.4
Corn	44.6	51.3	57	66.7
Cotton	65.2	60.3	60.2	72.5
…	…	…	…	…

Removal efficiency (%) interpolated from field measurements for select PWC scenarios in California, showing results for the first 6 scenarios as example.

- "NA" for "pesticide-scenario" sets not modeled in USEPA's ERAs
- Orange numbers indicate the corresponding $K_d \geq 1000$ (extrapolation).

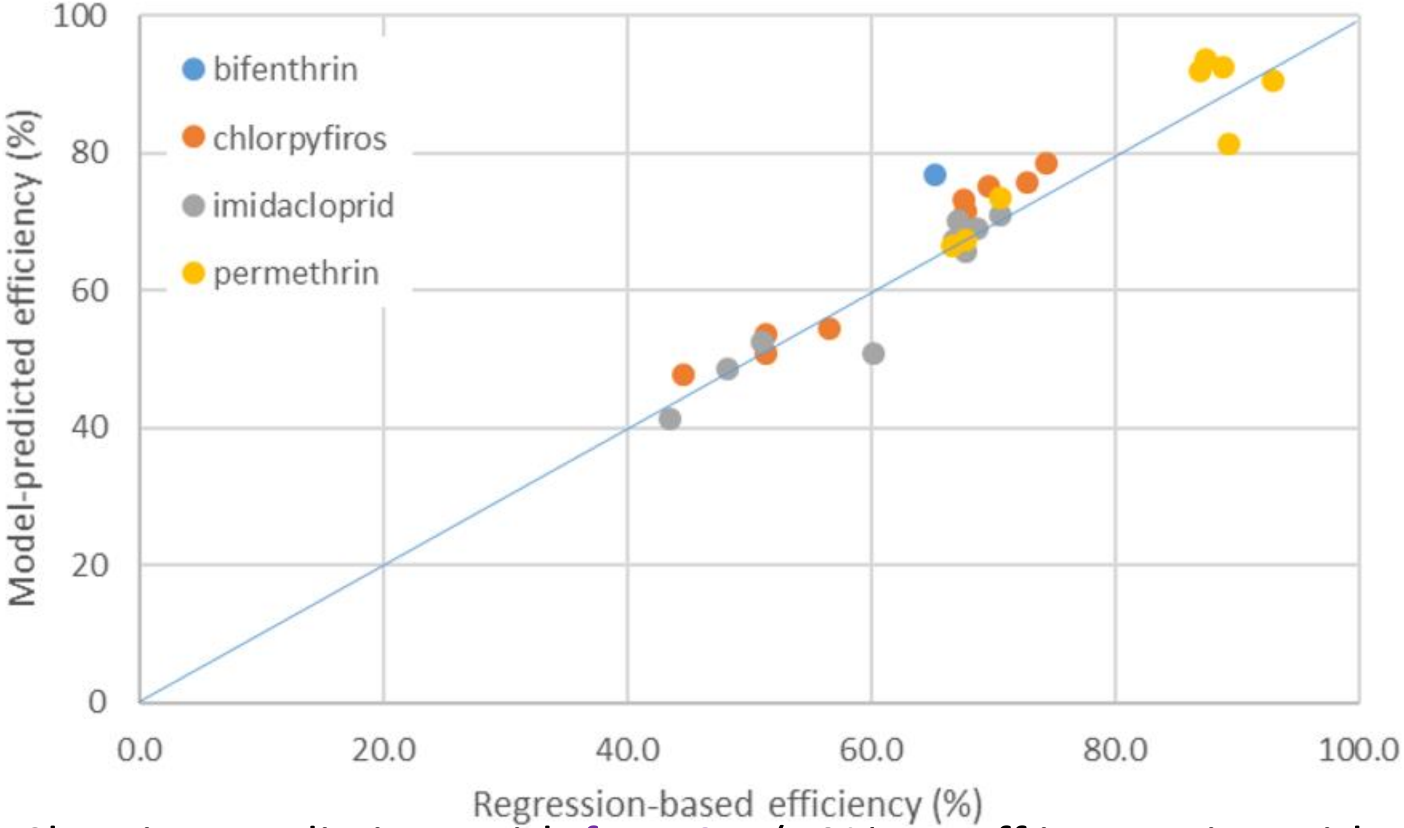
Build a database to validate pesticide simulation results

- No sufficient data for direct comparison between observed and predicted removal efficiency
- Build validation data from the regression equation
- Compare *processed measurements* vs. *model predictions*
  - For K_d<1000: results are used to evaluate model performance
  - For K_d≥1000: to demonstrate the modeling capability

Note: K_d is calculated from K_{OC} (chemical property) and soil OC content (PWC scenario), i.e., pesticide-scenario specific.

Pesticide simulation results

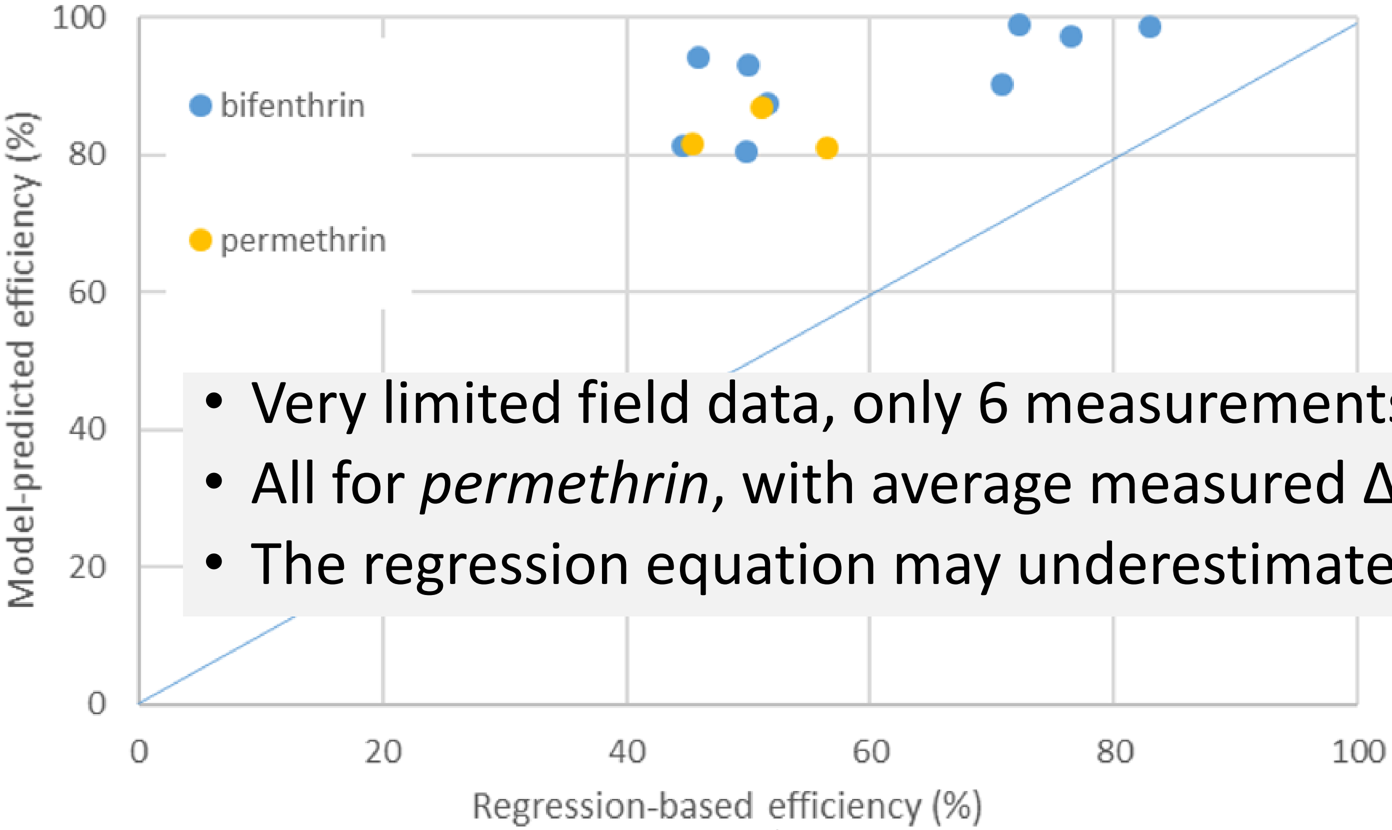
- For "pesticide-scenario" sets with K_d<1000



Showing predictions with f_{thr} = 0.4 (40% runoff interacting with soil) and f_{res}=0 (no effective resuspension)

Pesticide simulation results

- For “pesticide-scenario” sets with K_d≥1000

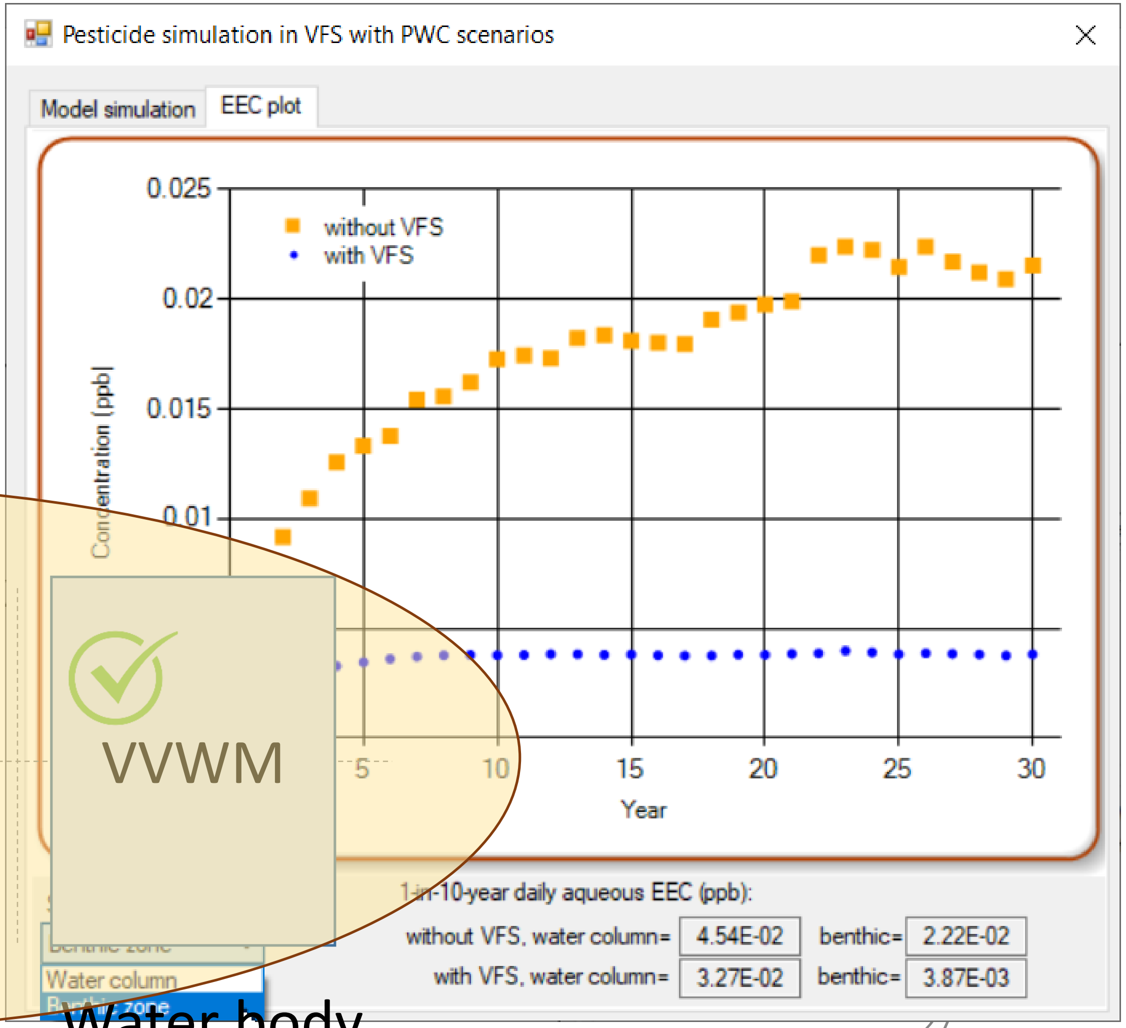


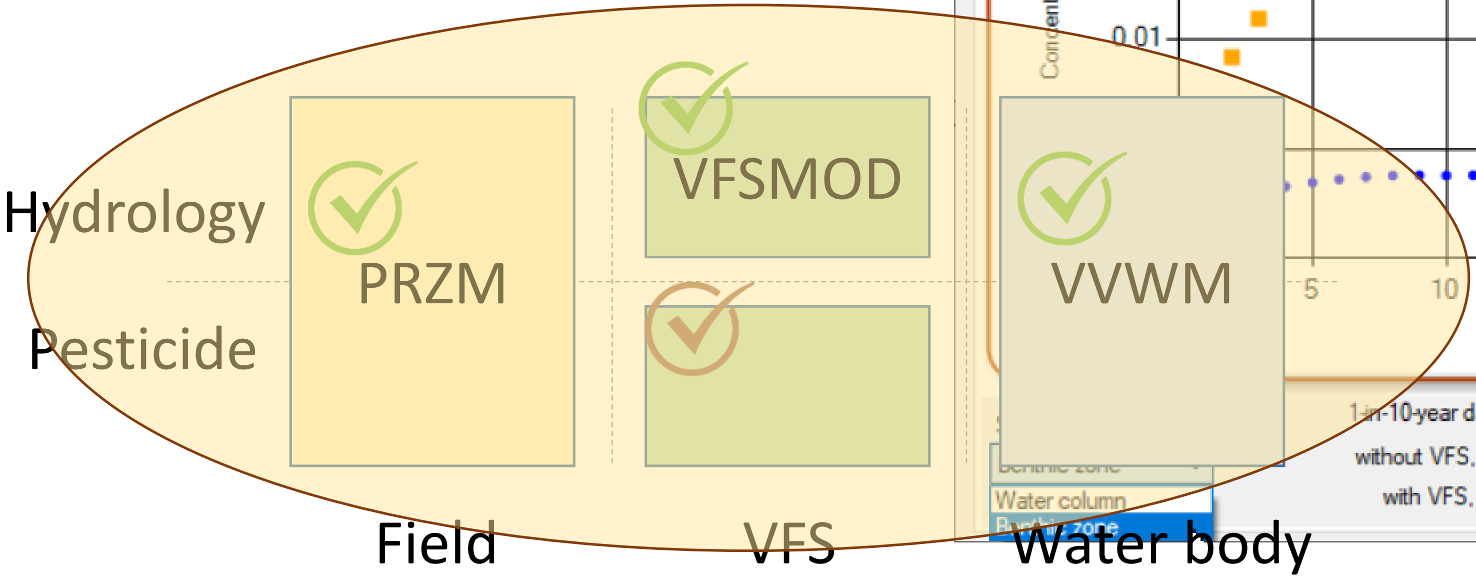
- Very limited field data, only 6 measurements (out of 244)
- All for *permethrin*, with average measured ΔP of 80%
- The regression equation may underestimate ΔP for Kd≥1000

Showing predictions with f_{thr} = 0.4 (40% runoff interacting with soil) and f_{res}=0 (no effective resuspension)

Computer implementation

- Incorporated with CDPR's Pesticide Registration Evaluation Model (PREM)
- Also developed as a stand-alone program for linking with PWC v1.52 (through a .SWI file)





Limitations and next steps

- Spray drift to a VFS is not considered
  - VFS adjacent to treated fields, associated with high drift fraction
- Heterogeneity of the hydrological regime over VFS is not considered
  - ~ half of flow was handled by 10% of the VFS area (White and Arnold, 2009)
  - Plan to model flow zones in a VFS with low-rate vs. high-rate flow
- VFS maintenance and long-term operations
  - Current results actually establish the upper bound of mitigation effectiveness
- More field measurements for pyrethroids

Summary & recommendation

General design — Use VFSMOD for hydrological simulation, and develop pesticide modeling approach separately

Approach — Develop the approach by formulating transport processes in soil-water interaction

Product — Collaborate for one set of standard approaches

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