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A Comparison of Markov Models and the Ensemble Kalman Filter for Estimation of Sorption Rates

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Outline

- Set Up
- Particle Tracking Model
- Prediction of de/sorption rates
- Application of the EnKF
- Results

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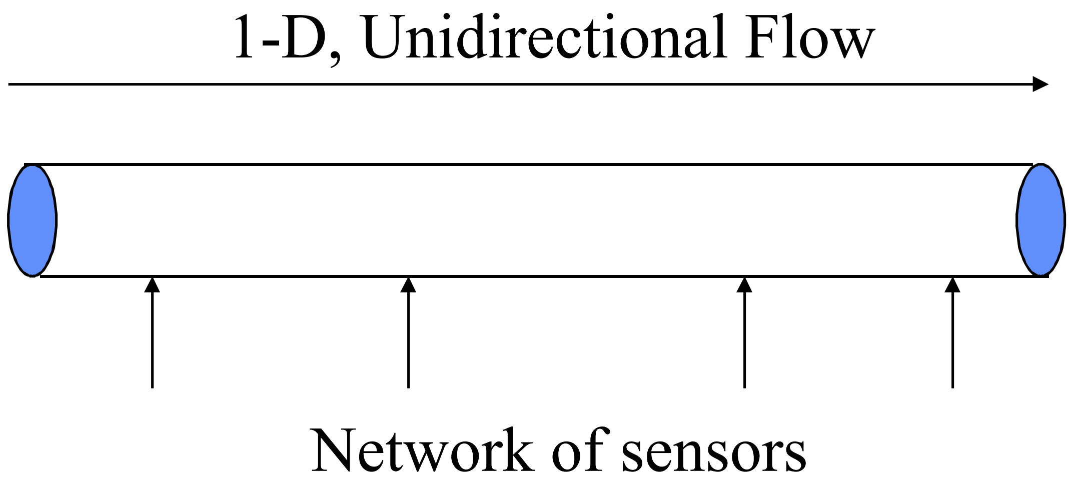
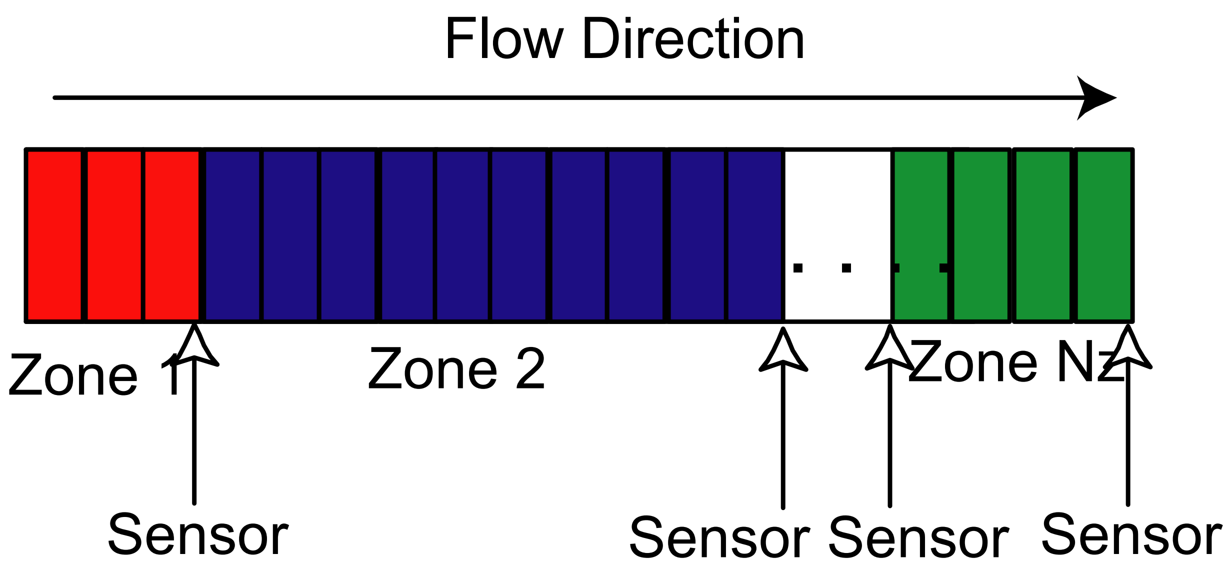
Physical Setup



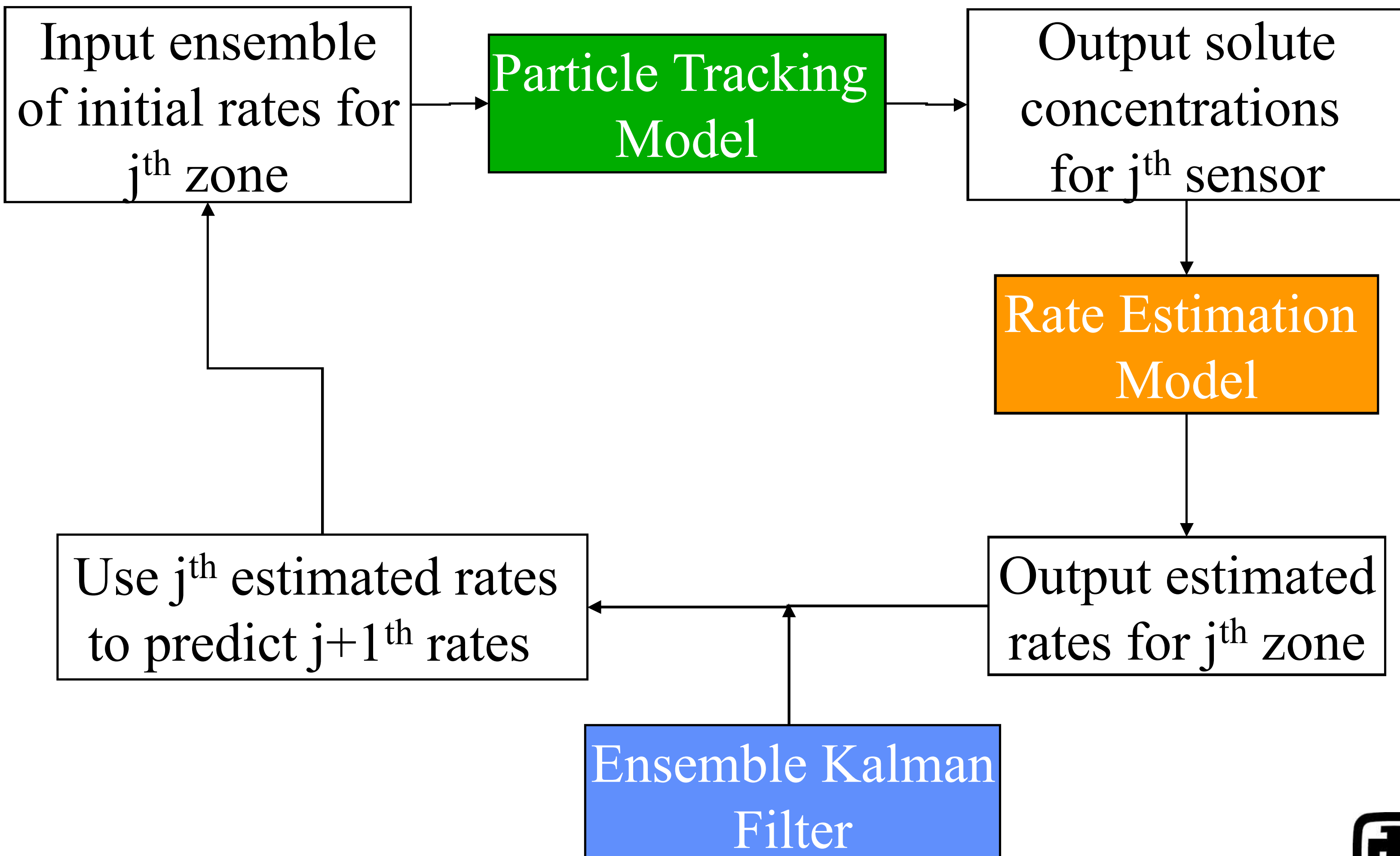
- Setup
  - Streamline with spatially varying de/sorption rates
  - Network of sensors to measure concentration
- Goal: using measured concentration data from sensors for an injected tracer, identify the de/sorption rates in real time

Modeling Set Up

- The streamline is divided into N_z zones
- Each zone is divided into subintervals of uniform length $\Delta x = v \Delta t$
- There is a sensor at the end of each zone
- De/sorption rates are constant in each zone and with respect to time
- At t=0, all particles are injected into the inlet of Zone 1



Rate Estimation Process



Particle Tracking Model: Probabilities

- Mishra et al. developed a Markov model that used constant de/sorption rates to define probabilities that particles transition between sorbed and aqueous phases
- Some key probabilities:
  - Particle in aqueous phase stays in aqueous phase for 1 time step:

$$\hat{p} = 1 - k_f \Delta t$$

  - Sorbed particle transfers to aqueous phase for 1 time step:

$$\tilde{p} = k_r \Delta t$$

- These probabilities form foundation of the particle tracking model

Particle Tracking Model: De/sorption Process

- Phase (aqueous or sorbed) determined at the beginning of each time step
- Particle in solution travels a distance of $\Delta x = v \, \Delta t$ in one time step
- Assume a well-mixed solution so that dispersivity is not an issue
- Implementation in code is a Monte Carlo simulation:
  - A “large” number of particles are tracked
  - Randomly sampled numbers are compared with probabilities to determine phase (and location) of each particle

Rate Estimation Model

- Normalized concentrations are "inverted" to estimate rates
- Example: Assume Zone 1 has 3 subintervals
  - Probability that a particle reaches 1st sensor in 3 time steps is

$$\left[\hat{p}(1)\right]^3 = \left[1 - k_f(1)\Delta t\right]^3$$

  - Particle must always remain in aqueous phase
  - Therefore,

$$C_1(3\Delta t) \approx \left[\hat{p}(1)\right]^3 = \left[1 - k_f(1)\Delta t\right]^3$$

$$\Rightarrow k_f(1) \approx \Delta t^{-1}\left(1 - \sqrt[3]{C_1(4\Delta t)}\right)$$

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Ensemble Kalman Filter (EnKF) Application

- Kalman Filter (KF) is predictor-corrector technique
  - "State" is predicted by linear model, and KF uses observation data and system statistics to "correct" state estimation
- EnKF is popular technique for non-linear applications
- For our application,
  - State = rates + concentrations
  - Predictor= Particle tracking model + rate prediction model
  - Observations = concentrations calculated with particle tracking code and true rates

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Markov Model+EnKF

- Create ensemble of rates by perturbing "true rates"
- For each ensemble member
  1. Run particle tracking model based upon previously defined probabilities to get concentrations at j^{th} sensor
  2. Use rate prediction model to estimate j^{th} rates
  3. Kalman Filter Update
  4. Re-run particle tracking code with new estimates of j^{th} rates to get concentrations at $(j+1)^{th}$ zone
  5. Repeat steps 2-4 until all rates have been estimated

Final rate estimates for each zone are calculated by averaging rates over all ensemble members

Test Case: True Rates

Zone	Boundary (m)	True k_f (1/day)	True k_r (1/day)	True k_d
1	0.0-10	0.005	0.005	1
2	10-15	0.005	0.000005	10^3
3	15-30	0.001	0.009	0.11
4	30-45	0.009	0.001	9.0
5	45-50	0.001	0.0001	10

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Creating the Ensemble

- Ensemble rate = true rate x (1+p) where p is randomly sample from U[min,max]
- Two ensembles created
  - U[min,max] = U[-0.4,0.4]
    - Average perturbation is zero
  - U[min,max] = U[0,0.8]
    - Average perturbation is not 0 so there is a “bias”

Results

- Without bias,
  - With large enough ensembles, both approaches estimated sorption rates fairly well (< 5% error)
  - Desorption rates were not as accurately estimated as well since they generally had less impact on concentrations and they rely on accurate estimation of sorption rates
  - LSEs were comparable for both methods
  - Addition of EnKF does not result in better rate estimates that justify additional computational cost

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Results

- With bias,
  - Markov estimates of sorption rates resulted in REs that converged to mean perturbation
  - Markov estimates of desorption rates resulted in much scatter
  - Addition of EnKF resulted in rejection of “bias” and more accurate estimates of forward rates
  - Addition of EnKF decreased LSE by two orders of magnitude

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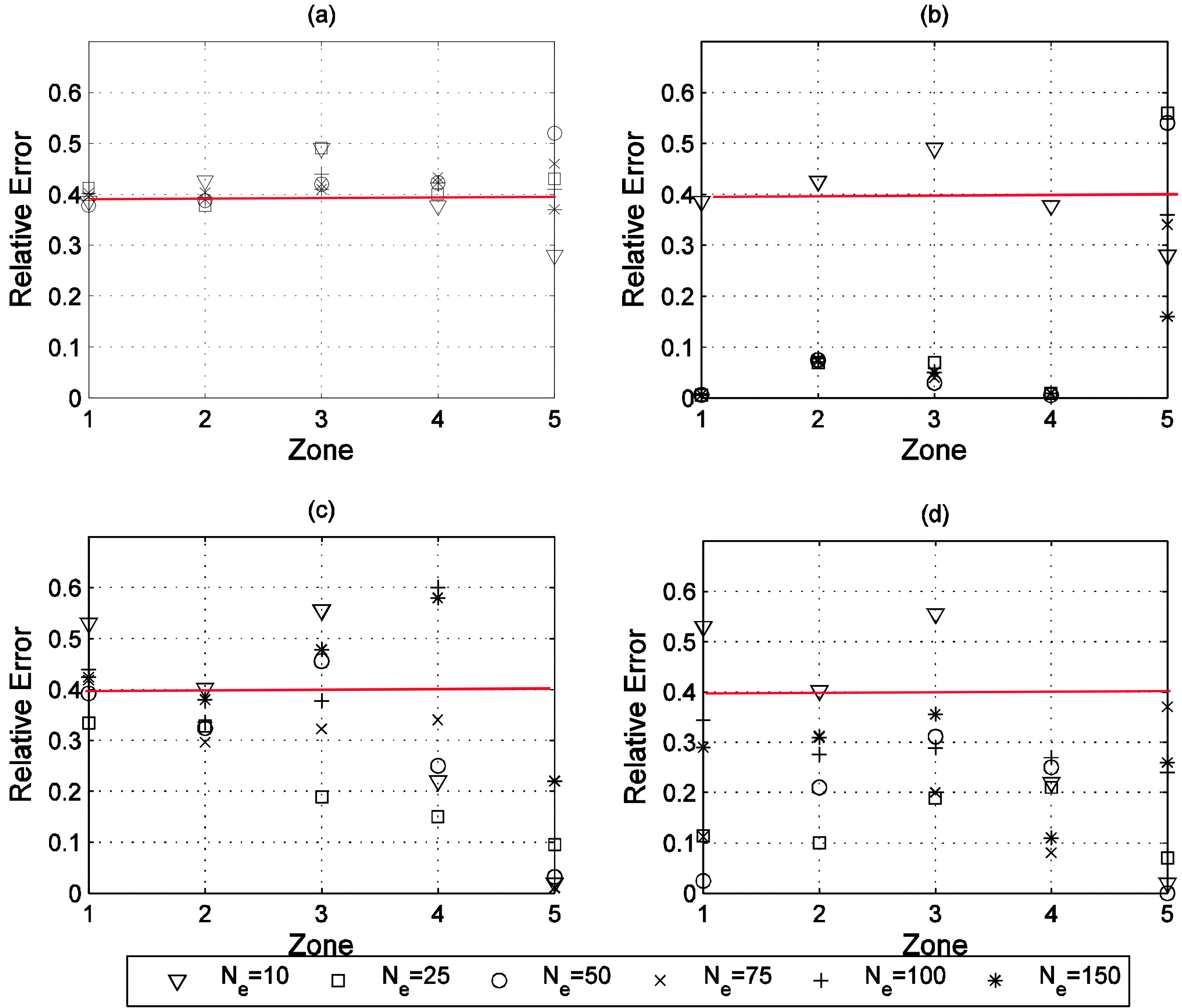
Results with Bias

W/O EnKF | W/EnKF

Sorption

De-sorption



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Results: LSE's with Bias

Ensemble Size	Markov	Markov+EKF
10	5.12e-2	2.96e-4
25	5.20e-2	2.06e-4
50	4.79e-2	1.57e-4
75	5.11e-2	2.05e-4
100	4.97e-2	2.71e-4
150	5.07e-2	2.39e-4

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Questions?