Correlation Measures for Solute Transport Model Identification & Evaluation

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Solute Transport Models

- Advection Dispersion Equations (ADE)
- Aggregated Dead-Zone (ADZ)
- Residence Time Distribution (RTD)

- All take input, manipulate, produce output
- *If the input is recorded data, there is usually recorded output to compare model output to*

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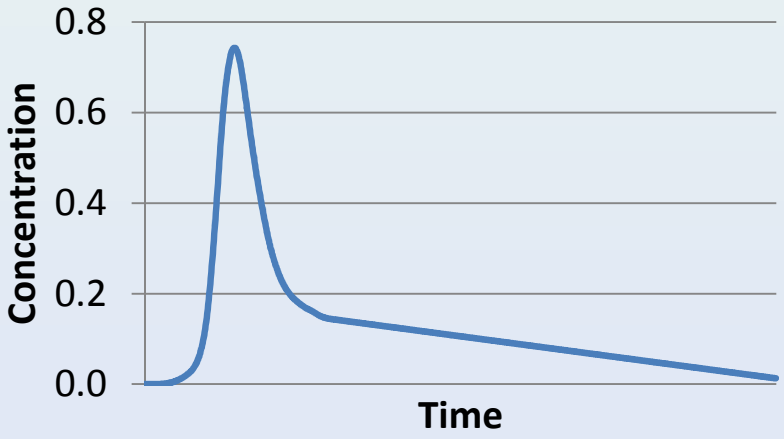
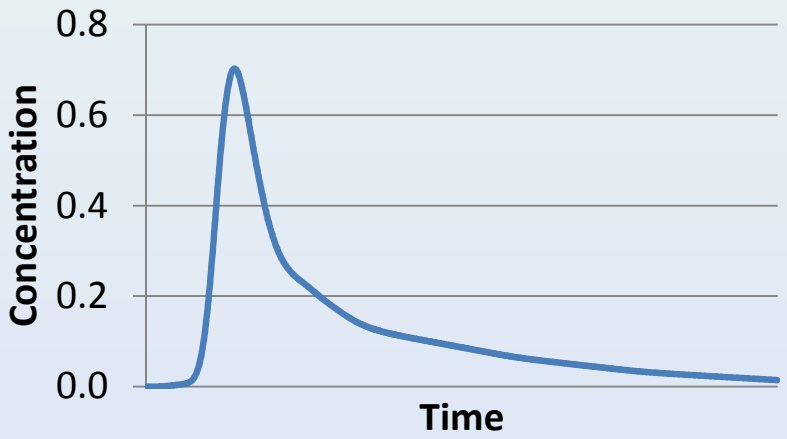
Correlation Measures

- Come in a variety of forms for a variety of purposes
- Describe the similarity between two time-series





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Identification & Evaluation

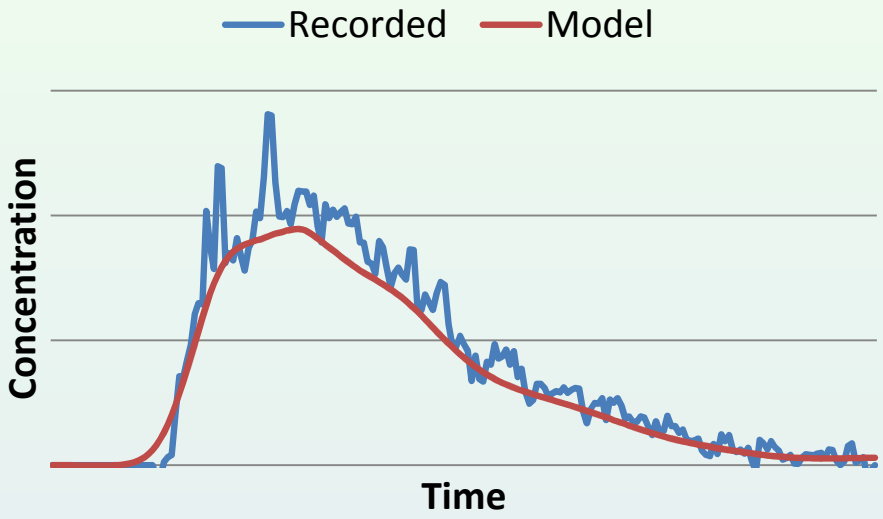
- In context they are two different, but related problems
- **Identification** is getting the model output to match the recorded data through adjustment of model parameters
- **Evaluation** is judging how well one model's output fits compared to another's or how well the model fits the recorded data

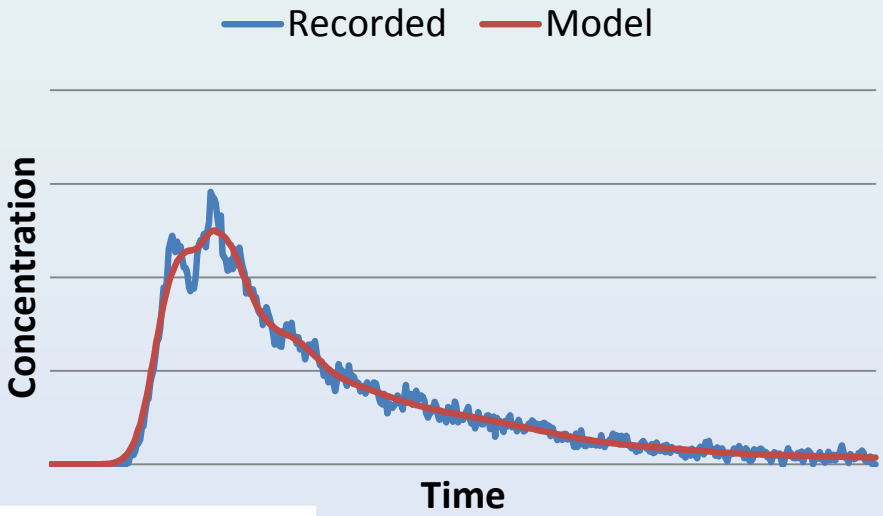
Research Question

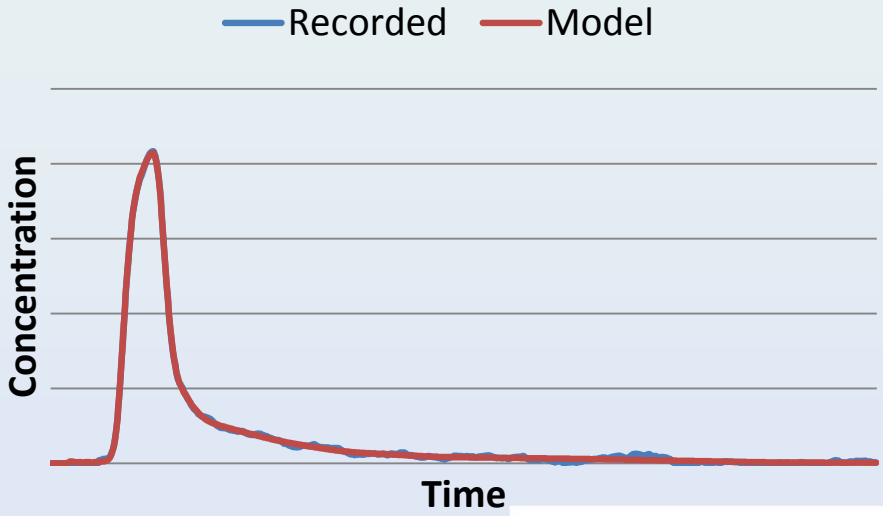
- Deconvolution is an optimisation process for finding the parameters that describe the residence time distribution (Identification)
- Multiple data sets lead to the generation of large numbers of parameterized models to be evaluated (Evaluation)
- Both use correlation measures - how do different correlation measures reflect the difference between measurement and model?

Example (R_t^2)

- 0.96
- 0.99
- 0.999







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Desirable Characteristics of Measures

- Sensitivity to Transformation (change in shape)
- Sensitivity to Transformation Magnitude (scale of change in shape)
- Insensitivity to noise
- Insensitivity to length of time-series (evaluation only)

Methodology

- Identified 12 correlation measures
  - BLC, χ^2, FFCBS, R^2, PMCC, RMSD, R_t^2, SimilB, YIC, CORR2, ISE, APE
- Generated three test scenarios
- Applied transformations at different magnitudes, as well as noise
- Compared modified traces to unmodified traces
- Normalised results and compared

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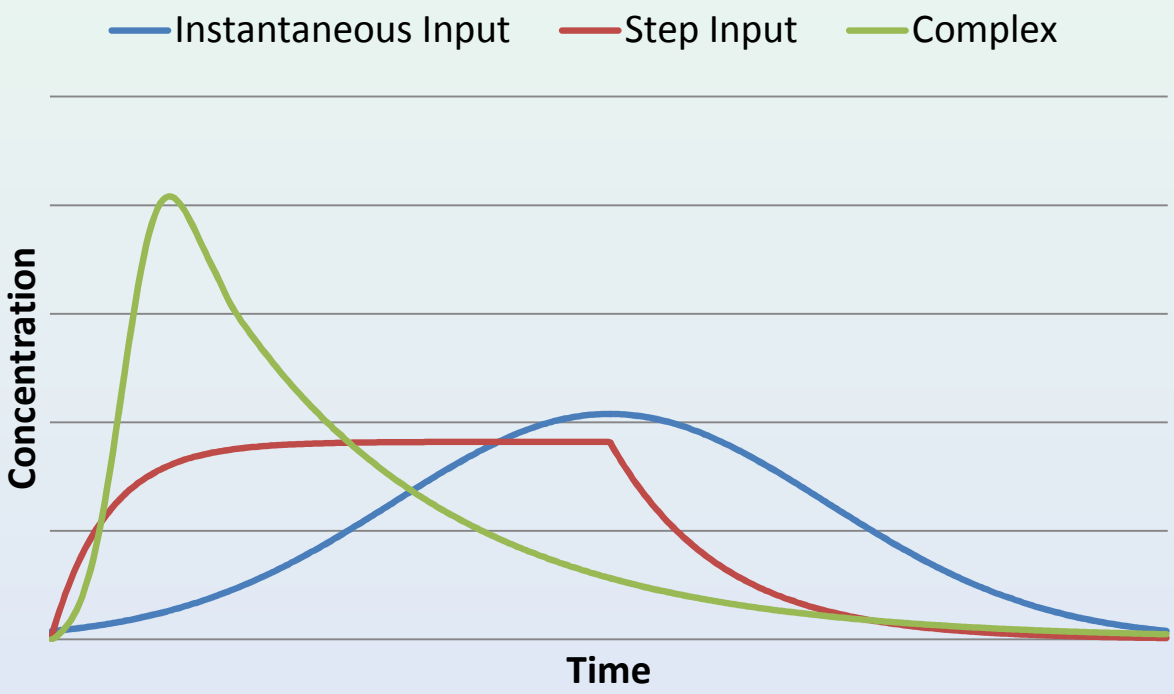
Mixing Scenarios

- Instantaneous Input
- Step Input
- Complex



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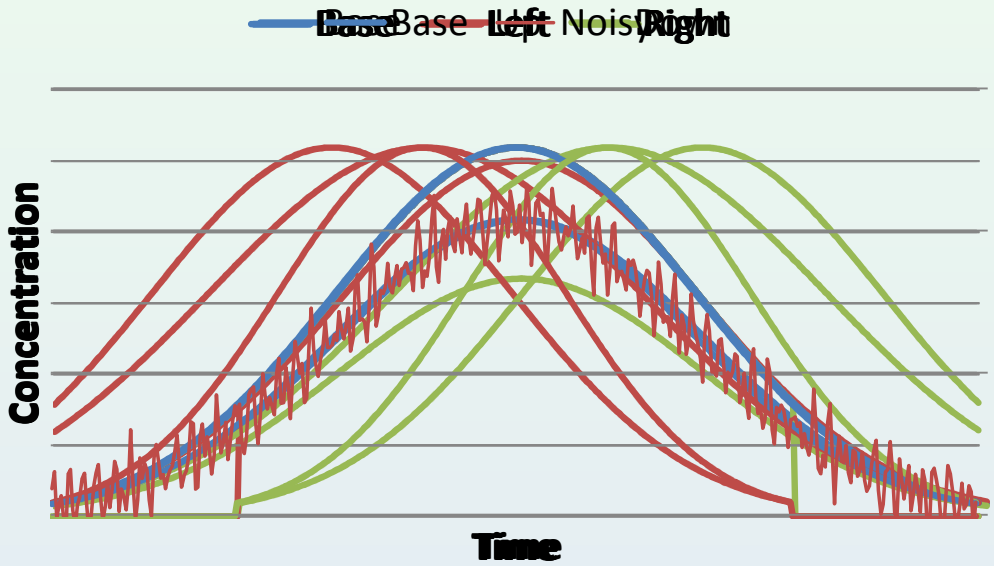
Transformations

- Scaling
- Shifting
- Truncation
- Stretching
- Squeezing



- Noise

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Normalisation and Comparison

- Dimensional and non-dimensional correlation measures
- Possible to compare directly in plots
- *Standard deviation of correlation values with respect to each parameter indicates sensitivity to that parameter*

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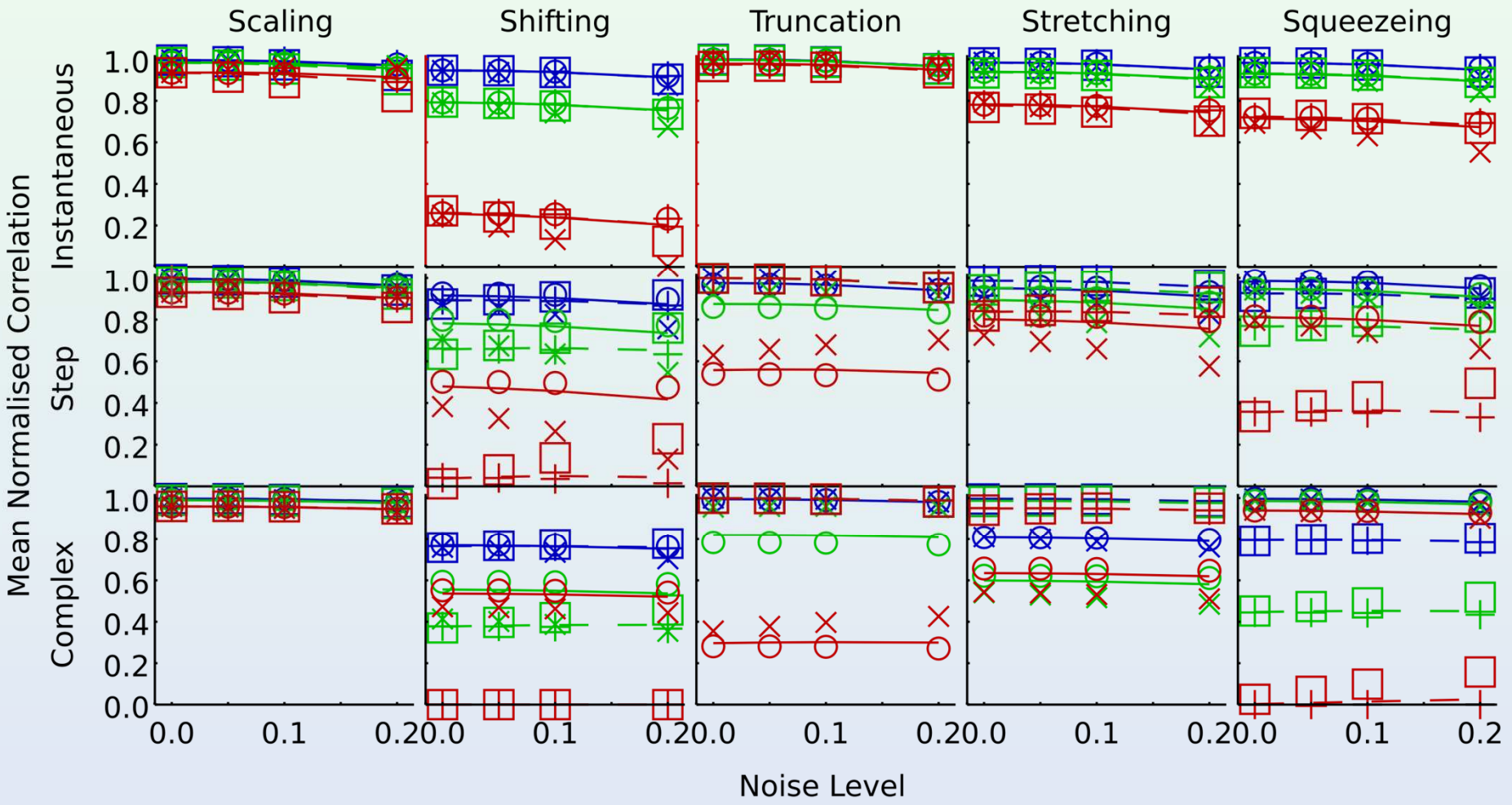
Complete Plots



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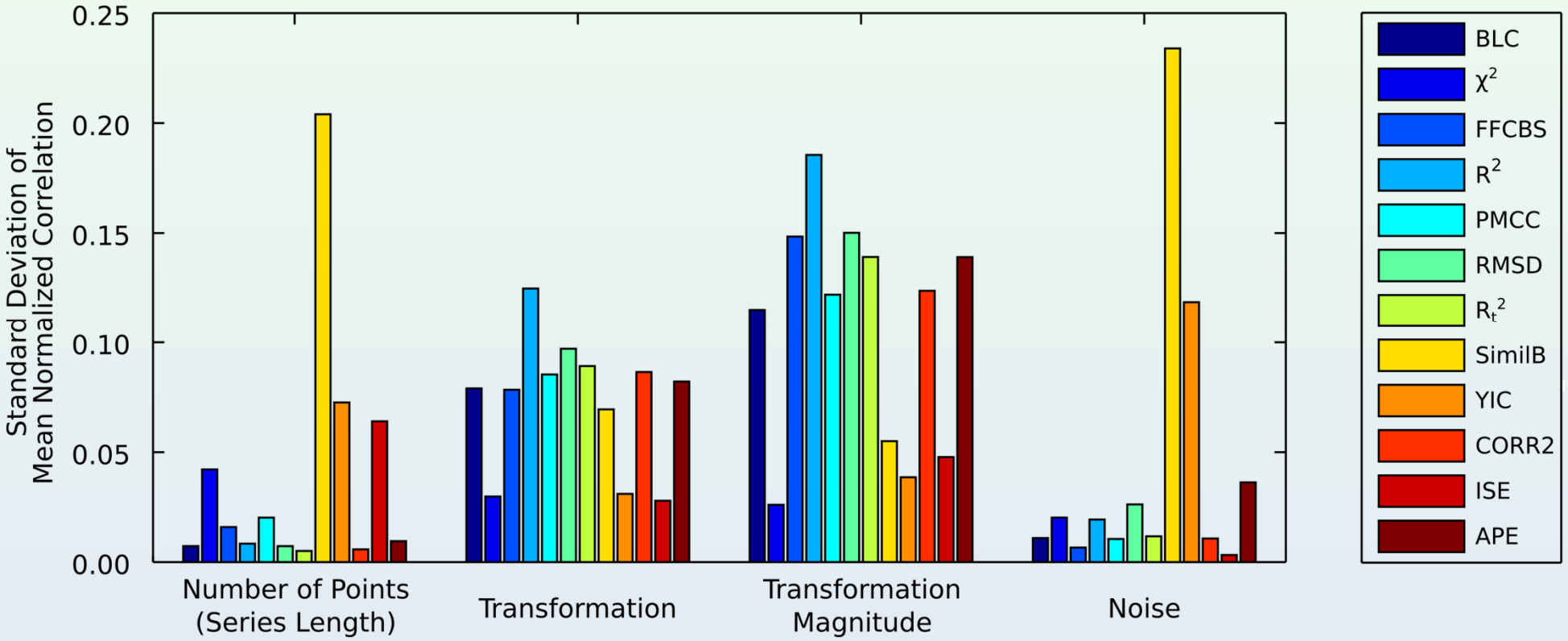
Standard Deviation Plot



- BLC, χ^2, FFCBS, R^2, RMSD, R_t^2, ISE, APE

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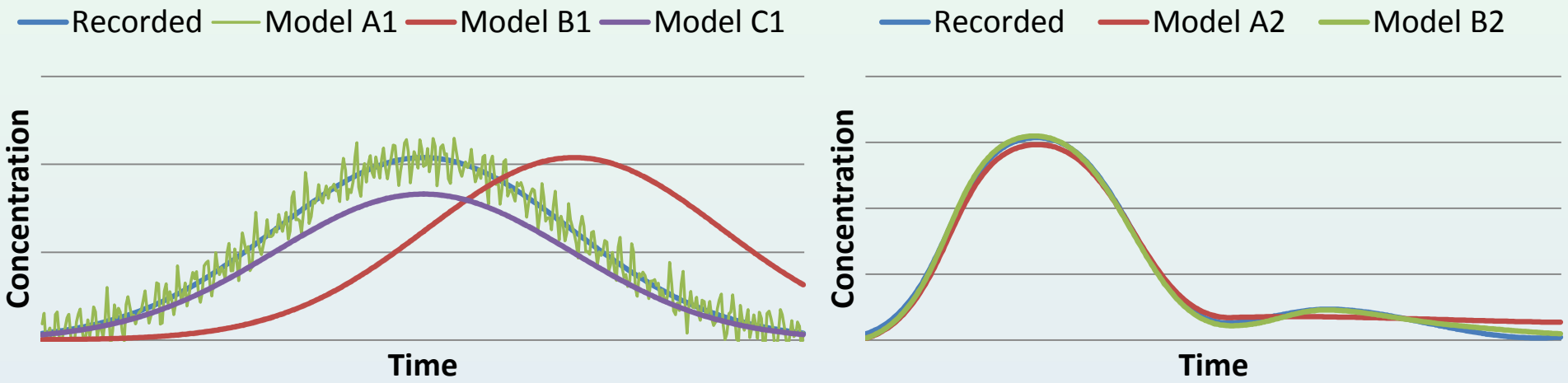
Application to Model Evaluation

- Non-dimensional measures (R^2, R_t^2, APE)



- R_t^2 very elastic about indicating model fit
- R^2 very specific about defining overall shape
- APE reflects small differences extremely well

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Conclusion

- 8/12 measures found suitable for identification
  - BLC, χ^2, FFCBS, R^2, RMSD, R_t^2, ISE, APE
- 3/8 measures found suitable for evaluation
  - R^2, R_t^2, APE
- *Different measures can be more suitable in different scenarios*

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Thank you for listening

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