Dynamic and Steady-State Process Investigations Using Functional Data Analysis

P. James McLellan
Department of Chemical Engineering
Queen's University
Kingston, ON
Canada
mclellnj@chee.queensu.ca

Outline

- Brief Exercise
- Motivation
- Functional data analysis

3 Stories –

- Predicting molecular weight distributions using functional regression
- Kinetic model reduction using functional principal components analysis
- Investigating dynamic structure using principal differential analysis

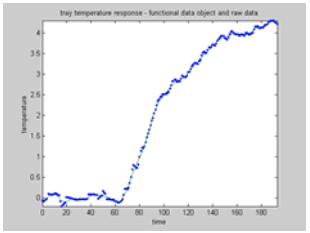
Wrap-up

- Perspective
- Summary and conclusions

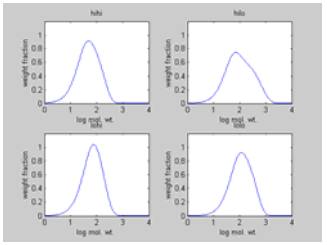
Motivation

When modeling and controlling chemical processes, we frequently encounter responses that are functional – functions of an independent variable such as time or molecular weight

- time traces (time series) – most frequently encountered in process monitoring and control



- species distributions – e.g., polymer molecular weight distributions, particle size distributions

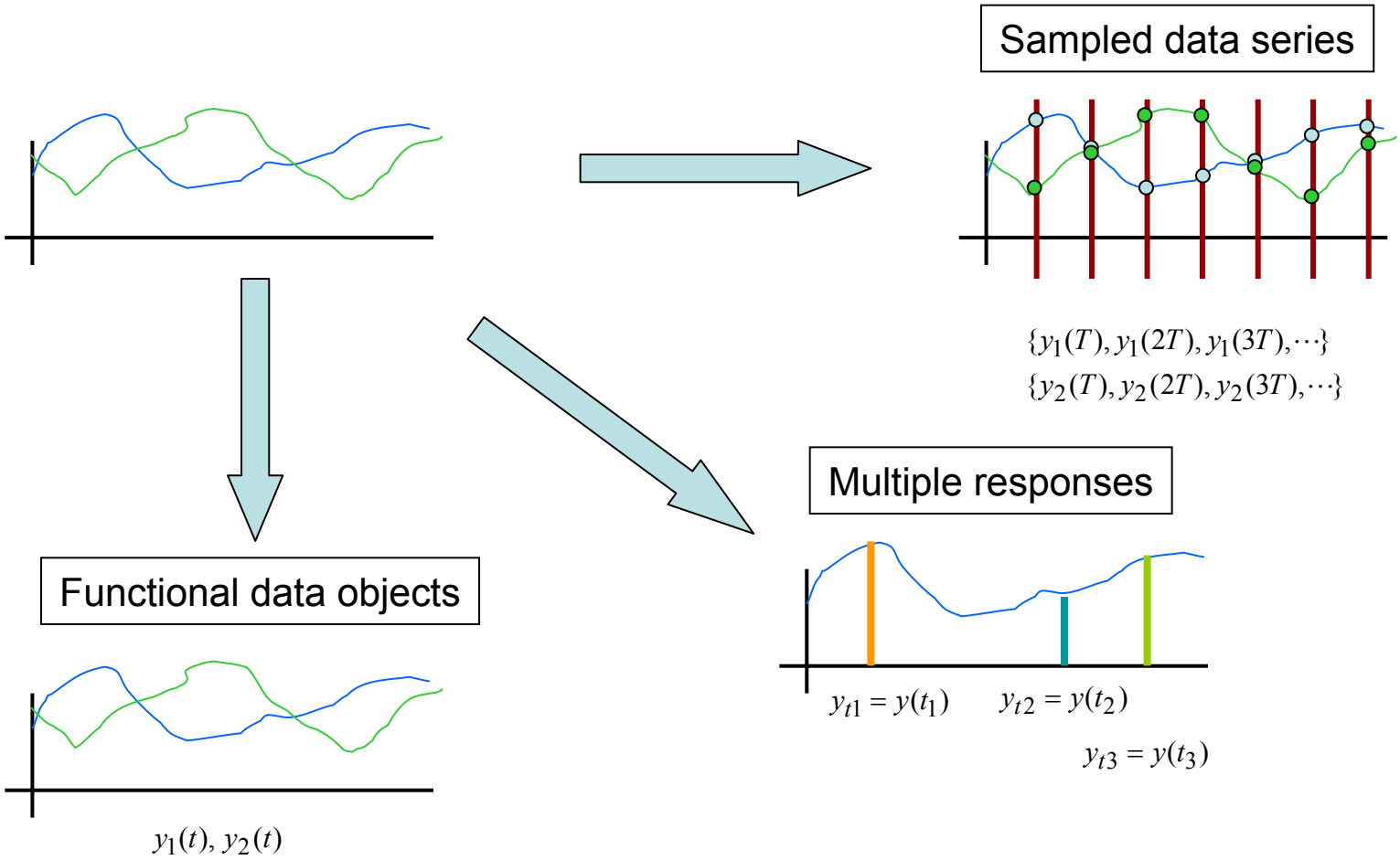


- spectra

In these instances, the elementary data object is a function of one or more independent variables.

How do we work with these responses?

Ways of viewing functional data



Ways of viewing functional data

Sampled data series

- standard approach for dealing with time traces – time series – predominant approach in control modeling and analysis
- typically assume uniform sampling – measurements are available at regular intervals
- models are typically discrete-time – difference or recursion equations e.g., $y_{k+1} = a_1 y_k + b_1 u_{k-1} + e_k$

Multiple responses

- typical approach in chemical reaction analysis – e.g., predicting polymer molecular weight distributions, chemical kinetic modeling
- approach inherent in multivariate statistical approaches (e.g., PCA)

Functional data objects

- the functional data analysis (FDA) perspective
- the data object is an entire curve

Goals of this talk

1. Demonstrate how FDA techniques can be used to analyze dynamic and steady-state process behaviour

2. Provide an overview of relevant FDA techniques

    - Functional regression
    - Functional principal components analysis
    - Principal differential analysis

3. Investigate the relationship between FDA approaches and existing approaches

Three Stories

Story #1 – Modeling the effect of reactor operating conditions on polymer molecular weight distributions

- steady-state process investigation in which the functional response is a molecular weight distribution
- Functional Regression Analysis of a 2-level factorial design

Story #2 – Kinetic model reduction

- Reducing the complexity of chemical kinetic models by identifying intermediate reactions and reactants that have limited effects on predictions of species concentrations
- Functional Principal Components Analysis (fPCA)

Story #3 – Investigating and modeling dynamic process behaviour

- estimating dynamic models from data
- Principal Differential Analysis (PDA)

Functional Data Analysis (FDA)

… is a statistical framework in which the elementary data object is a function of one or more independent variables

- Primary reference – Ramsay and Silverman (1997) – text
- Jim Ramsay presentation at the 1997 GRC
- FDA toolbox for Matlab available free from Jim Ramsay web site (www.psych.mcgill.ca/faculty/ramsay.html)
- Techniques have been developed and used for analyzing handwriting, lip motion, horse gait data, analyzing weather data, eye-hand response times, …

Datasets consist of collections of functional observations

- Multiple observations (realizations) of same response function – e.g., temperature profiles for different runs in a batch reactor – $\{y_1(t), y_2(t),\ldots, y_N(t)\}$

- Observations of multiple functional responses – e.g., time traces for valve input and temperature – {u(t), y(t)}

Functional Data Analysis (FDA)

- FDA is a statistical framework for functional data
  - Standard summary measures defined
    - Sample average

$$\bar{y}(t) = \frac{1}{N}\sum_{i=1}^{N} y_i(t)$$

    - Sample variance

$$s^2(t) = \frac{1}{N-1}\sum_{i=1}^{N}\left(y_i(t) - \bar{y}(t)\right)^2$$

Note that the result is a function of the independent variable – average function, variance function.

Functional Data Analysis (FDA)

- FDA is a statistical framework for functional data
  - Summary measures continued…
    - Sample covariance

$$s_{yy}(t,s) = \frac{1}{N-1}\sum_{i=1}^{N} y_i(t)y_i(s)$$

    - Sample cross-covariance

$$s_{yu}(t,s) = \frac{1}{N-1}\sum_{i=1}^{N} y_i(t)u_i(s)$$

    - Sample variance-covariance matrix

$$\mathbf{S}_{yy}(t,s) = \frac{1}{N-1}\sum_{i=1}^{N} \mathbf{y}_i(t)\mathbf{y}_i^T(s)$$

These functions define surfaces describing covariance across the independent argument, and between variables.

Functional Data Analysis

How do the FDA covariance measures relate to *standard* covariance measures in time series?

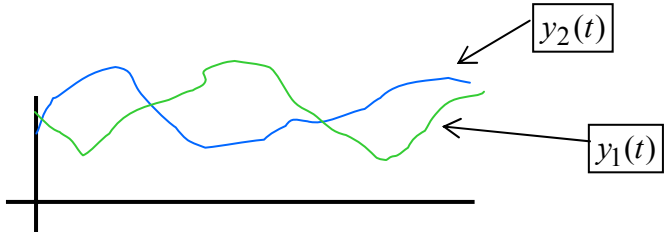
1) No assumption of stationarity or ergodicity
   - defined in terms of ensemble averages rather than time averages
   - philosophical shift from assuming stationarity in functional responses
     (we could similarly work with time series covariances computed using ensemble averages)

2) FDA covariance measures provide information into observed AND interpolated behaviour
   - interpolated – in most instances, the functional data objects are created from measurements at discrete points using smoothing – e.g., splines
   - covariances reflect both the influence of the observed points and the assumptions made when smoothing
   - smoothing should reflect additional insight into the behaviour of measured quantities
     - e.g., temperature time traces, NMR spectra, molecular weight distributions – do we expect underlying behaviour to be smooth, spiky or jumpy?

Functional Data Analysis

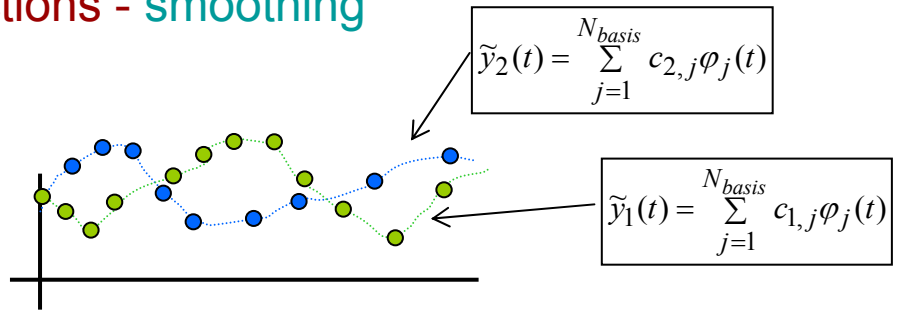
Concept

- data objects are continuous functions of an independent variable



Practice

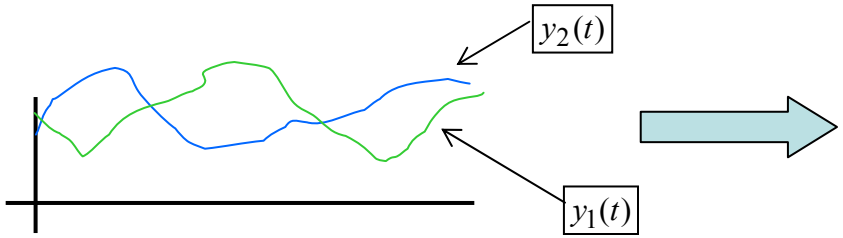
- observations are typically taken at discrete intervals – not necessarily uniform – and functional observations are constructed using appropriate basis functions - smoothing



$\varphi_j(t)$ are basis functions
e.g., splines,
polynomials,
sinusoids

Functional Data Analysis

With the basis function representation, the functional data objects can be considered as lists of coefficients



$$y_1 : \{c_{11}, c_{12}, \ldots, c_{1N_{basis}}\}_{\varphi}$$
$$y_2 : \{c_{21}, c_{22}, \ldots, c_{2N_{basis}}\}_{\varphi}$$

- basis function representations of data have previously been used to assist the application of conventional statistical techniques. For example, fault detection can be enhanced by introducing time-scale separation in operating data by first representing data using wavelets and then applying standard PCA

HOWEVER

FDA computations are frequently cast in terms of the smooth functions and not only in terms of the coefficients in the functional basis

FDA and the statistical cultures

- Classical
  - Models/distribution formalism
- Modern
  - Non-parametric
  - Directly data driven

In FDA, the data objects (smoothed curves) used in the analysis come from the “modern” culture, with classical techniques (e.g., models) expressed in terms of these objects.

- PLSR
  - relationship?

Three Stories

1. Predicting molecular weight distributions using functional regression

2. Kinetic model reduction using functional principal components analysis

3. Investigating dynamic structure using principal differential analysis

Functional Regression Modeling for Predicting Polymer Molecular Weight Distributions

Motivation

- polymer molecular weight distributions (MWDs) are important because they influence end-use and processing properties of polymer products
- MWDs are presented as functional observations, in which weight fraction is a function of molecular weight (or log(MW))
- conventional approaches for modeling and predicting MWDs include
  - discretization and treatment as multi-response estimation problems
  - characterization using moments
  - detailed mechanistic modeling to predict fractions for each chain length
- Issues
  - loss of information vs. complexity
  - problem conditioning
- alternative is to treat the MWDs as functional observations, and use techniques from Functional Data Analysis (FDA)
- objective - develop and apply empirical modeling techniques for investigating the impact of operating parameters on molecular weight distributions

Functional Regression

- Functional regression refers to regression modeling in which factors and/or responses are functional
- Example – functional response *y(r)* as a function of non-functional factors x_1 and x_2

$$y(r) = \beta_0(r) + \beta_1(r)x_1 + \beta_2(r)x_2 + \varepsilon$$

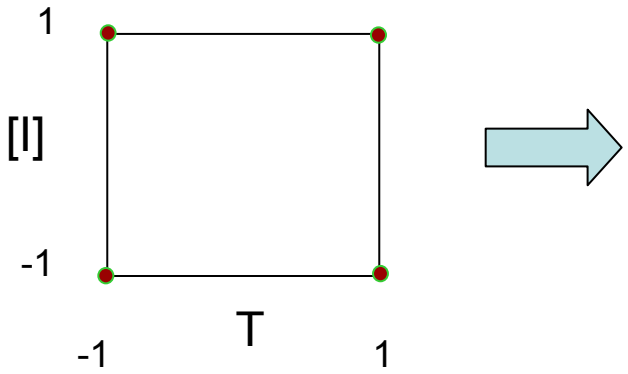
  - In the MWD modeling example, the response is functional, the factors are non-functional, so the parameters in the model are functions of the independent variable r, which is log(MW)
- Least squares estimation criterion – minimize integral squared error between predicted and observed response functions

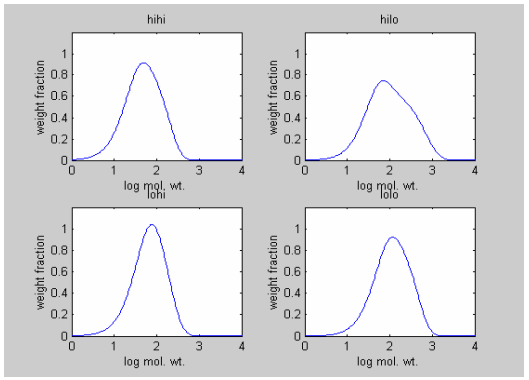
$$\min_{\beta_0(r),\beta_1(r),\beta_2(r)} \int_{r_{\min}}^{r_{\max}} \left(y(r) - \hat{y}(r)\right)^2 dr$$

- Solution – can be determined by expressing parameter functions using basis functions

Functional Regression for MWD Analysis

- Functional regression is used to estimate an empirical model predicting the effect of isothermal reactor temperature (T) and initial initiator concentration [I] on the resulting MWD in a bulk polymerization of styrene
- Response (weight fraction, *y*) is functional, while factors T and [I] are non-functional
- Synthetic data have been generated using Predici™ polymer modeling software for a 2^2 factorial design in T and [I]





Functional Regression for MWD Analysis

Functional regression analysis for estimating MWDs follows the following sequence –

- smooth raw data using basis functions
- transform MWD response to ensure that resulting model can't give negative predictions
- fit linear plus two-factor interaction model, estimating parameter functions using basis functions
- transform back to original coordinates

Smoothing and Response Transformation

- B-spline bases were chosen for all smoothing and parameter representation because their non-periodic and polynomial structure is suitable for MWDs
- Functional MWD responses were transformed to give dln(y(r))/dr
  - MWDs are inherently positive, and from fundamental models, we know that MWDs can be treated as members of an exponential family of distributions with kernel W(r)
  - In particular, the distribution can be expressed as the solution of the following differential equation

$$Dg(r) = w(r)g(r)$$

  - Since g(r) is positive for all *r*,

$$\frac{dg(r)}{g(r)} = w(r)$$

and

$$w(r) = d(\ln(g(r))/dr$$

$$g(r) = C\exp\left(\int_{r_0}^{r} w(u)du\right)$$

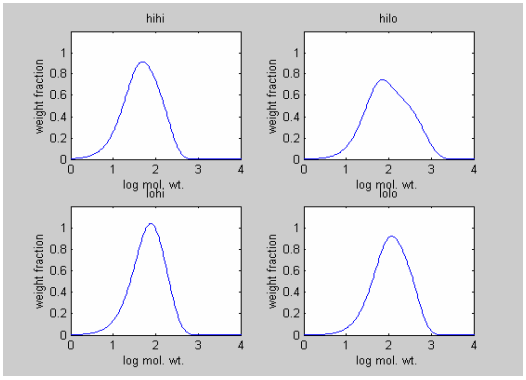
  - advantage – working with exponential distributions ensures non-negative weight fraction predictions from MWD model

Note – kernel w(r) can be used to provide insight into type of distribution

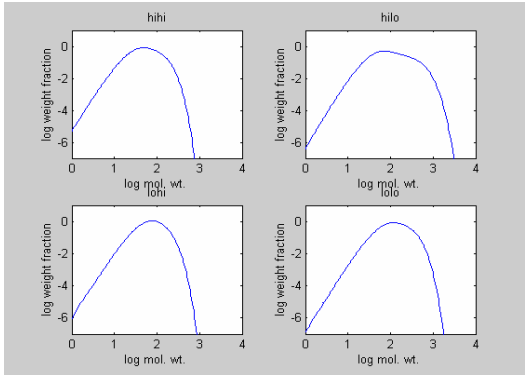
Reference – Ramsay J.O., "Differential equation models for statistical functions", Can. Journal of Statistics **28**, 225-240(2000)

Preliminary data investigation

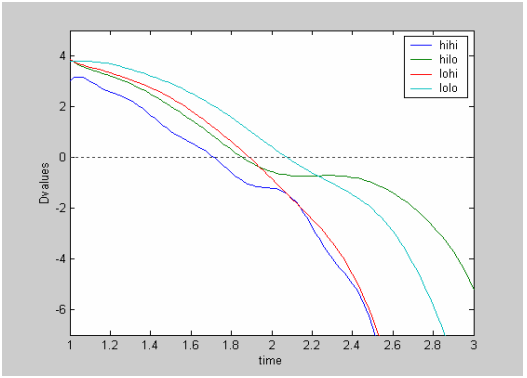
- Simulated MWDs are available at each of 4 combinations of T and [I]
- Splines gave good fits to the original data plots using 14 basis functions
  - 4^{th} order B-splines were used, with knots at points at which MWD values were provided by Predici – non-uniform intervals
- There is a marked change in the degree of symmetry, with a pronounced shoulder at low initiator concentration and high temperature



Original data y(r)



Transformed responses
ln(y(r))

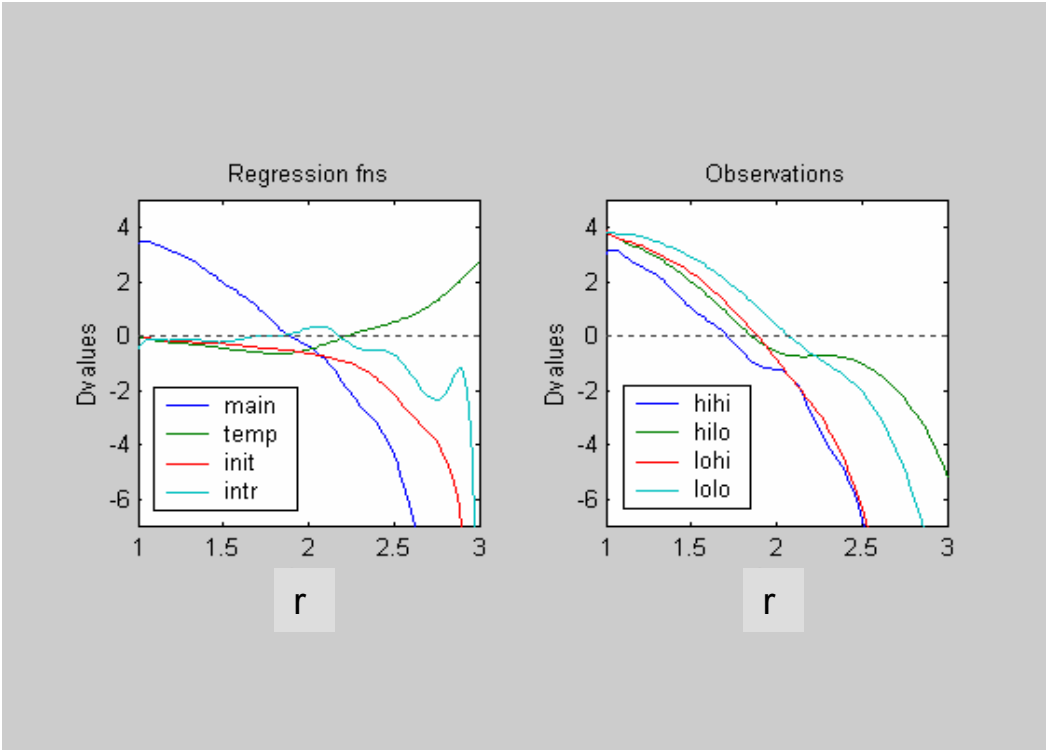


Transformed responses
d(ln(y))/dr
computed from spline fits

Estimated functional parameters

Model

$$\frac{d(\ln(y))}{dr} = \beta_0(r) + \beta_1(r)T + \beta_2(r)[I] + \beta_{12}(r)T[I] + \varepsilon$$



Transforming back to MWD

- to obtain MWD, we must integrate estimated model
  - introduces integration constant to be determined

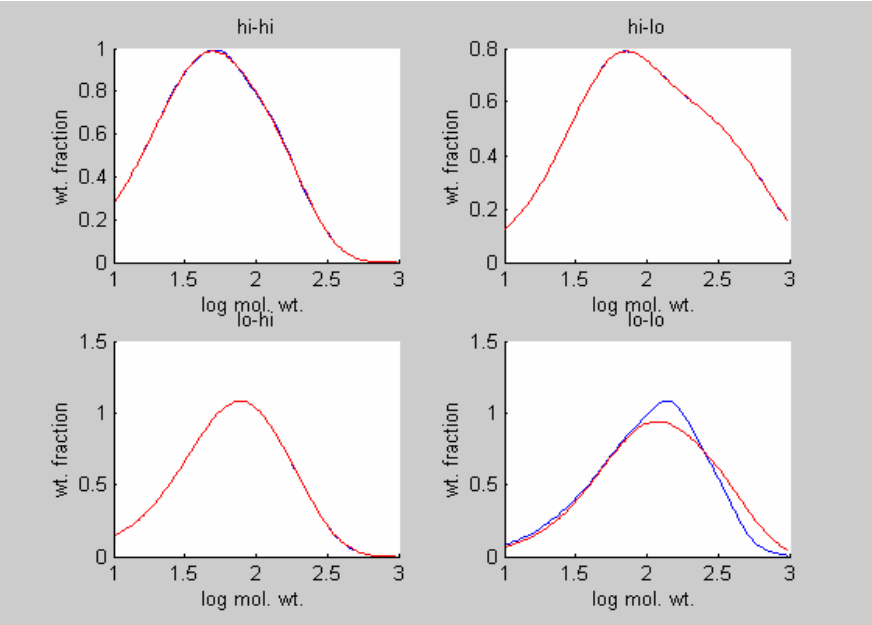
- taking exponential provides final model predicting weight fraction of polymer

$$y(r) = C \exp\left\{\gamma_0(r) + \gamma_1(r)T + \gamma_2(r)[I] + \gamma_{12}(r)T[I]\right\}$$

- the constant C is computed to normalize the area under the estimated MWD

Model Predictions

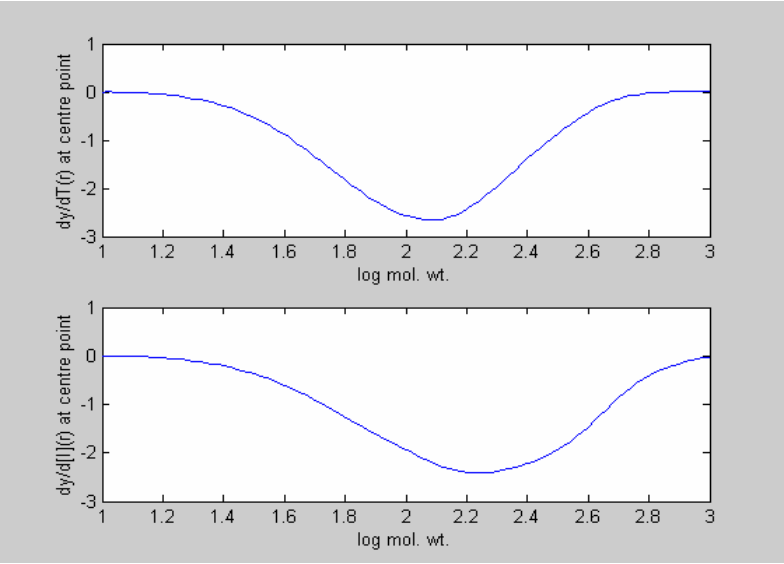
- Functional regression model fits data well
- Poorer fit obtained at low initiator concentration and low temperature
- Considered nonlinear terms in T and [I] and higher-order experimental design to get improved fit



Observed (blue) and predicted (red) MWDs for 2^2 factorial design

Assessing impact of operating factors

Consider parameter estimates in transformed domain (main effects, two-factor interaction), or consider sensitivities of predicted MWD to perturbations in operating factors, i.e., examine plots of $\partial y(r,x)/\partial x$, where x is T or [I]



Impact of temperature perturbation operating at centre point of design

Impact of temperature perturbation operating at centre point of design

Sensitivities of MWD to Temperature and Initiator

What we learned

- Temperature influences the MWD
  - Impact is symmetric
  - Increasing T increases the breadth of the MWD
- Initiator skews the MWD
  - Increasing initial initiator concentration can produce a shoulder on the MWD – asymmetric influence
- Model was useful for selecting operating conditions to produce desired MWDs
  - Tried in blind test simulation study

Potential applications

- Developing empirical models relating reactor operating conditions to MWDs
  - For new product development and reactor scale-up
  - Guiding subsequent experimental work

- Developing empirical models to relate MWD to end-use properties

What other approaches could have been used, and how would the results compare to those obtained using functional regression?

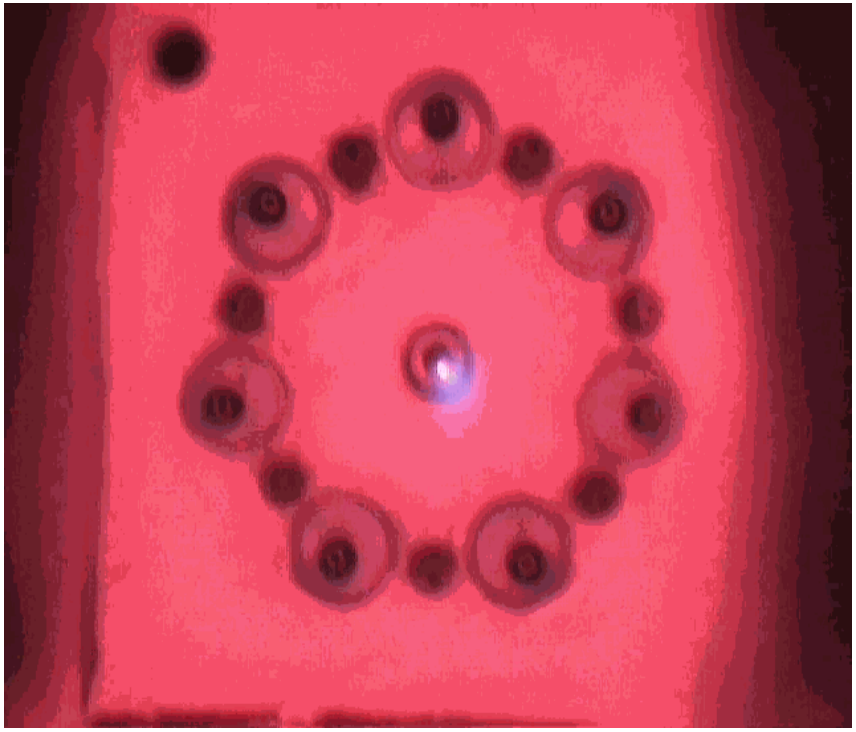
  - Discretization and multivariate statistical approaches (e.g., PLS)
  - Multiresponse estimation using assumed model structure

Second Story

Kinetic Model Reduction Using Functional Principal Component Analysis (fPCA)

Motivation

Develop simplified mechanistic kinetic model to support the development of a Ultra-Low-NOx Burner – complement experimental program.



Why do we need model reduction?

- Reactive flow simulation
  - Combined computational fluid dynamics model with chemical kinetic models
  - Models consist of partial and ordinary differential equations that require long computation times to solve
  - Incentive to reduce the complexity of the kinetic models by eliminating reactions and species that make negligible contributions to predicted behaviour
- Kinetic expressions are developed from experiments in well-mixed reactors giving ordinary differential equations of the form

$$\frac{d\mathbf{C}}{dt} = \mathbf{f}(\mathbf{C};\mathbf{k}), \quad \mathbf{C}(t_o) = \mathbf{C}_o$$

  - k's are the kinetic constants, and C's are the chemical species concentrations

Model Reduction Using Traditional Principal Components Analysis

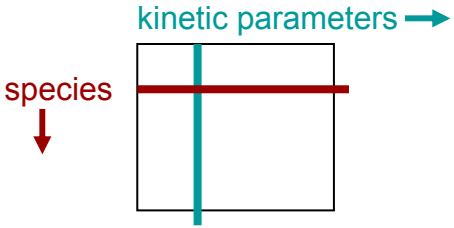
- Approach proposed by Vajda et al. (1985)
  - Use parameter sensitivity information to identify which kinetic parameters have important influence on predicted concentrations

- Scaled instantaneous parametric sensitivities

$$S_{i,j}(t) = \left(\frac{k_j}{C_i(t)}\right)\left(\frac{\partial C_i(t)}{\partial k_j}\right)$$

- Sensitivity matrix defined at each time point of the experimental trajectory

$$\mathbf{S}(t_k) = \begin{bmatrix} S_{1,1}(t_k) & \cdots & S_{1,m}(t_k) \\ \vdots & \ddots & \vdots \\ S_{n,1}(t_k) & \cdots & S_{n,m}(t_k) \end{bmatrix}_{n \times m}$$

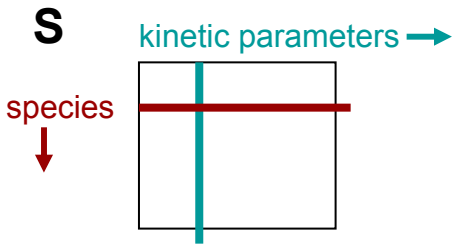


- Decomposition applied to the overall sensitivity matrix over the entire trajectory – stacking of sensitivities
- In order to do this, fundamental model equations and parameter guesses are required

$$\mathbf{S} = \begin{bmatrix} [\mathbf{S}(t_1)]_{n \times m} \\ [\mathbf{S}(t_2)]_{n \times m} \\ \vdots \\ \vdots \\ [\mathbf{S}(t_p)]_{n \times m} \end{bmatrix}_{(n \times p) \times m}$$

Model Reduction Using Principal Components Analysis (PCA)

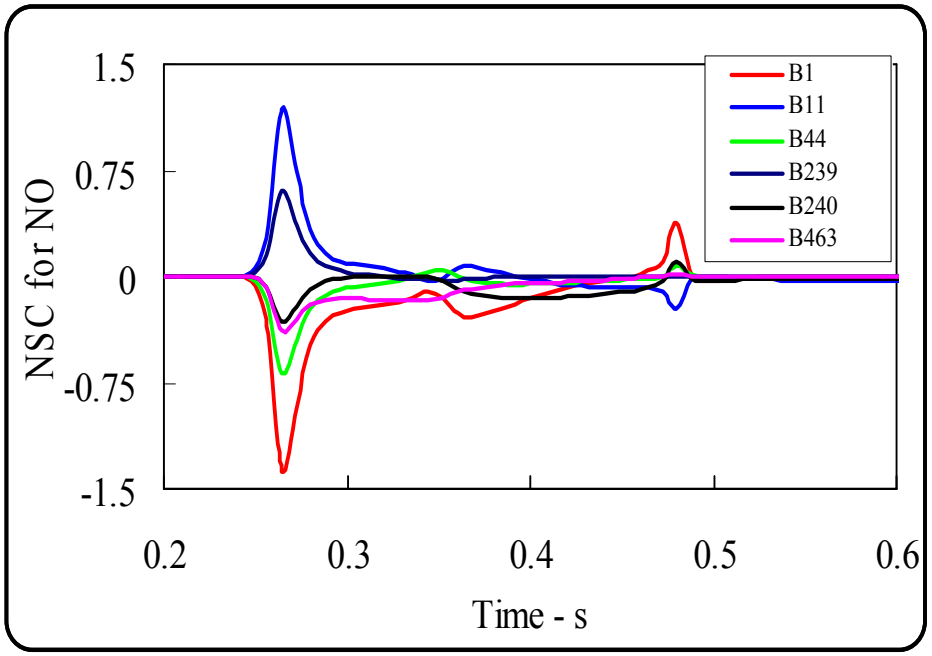
- Perform PCA on sensitivity matrix **S**



- Model reduction approach
  - principal components consist of combinations of reactions
    - kinetic rate constant sensitivities
  - retain those reactions with large loadings in the significant principal components
  - retain those chemical species appearing in the retained chemical reactions
  - provides a time-averaged model reduction since constant loadings are used over entire time horizon

Functional Data Analysis Approach

- View the sensitivity trajectories as functions of time – objects are no longer sensitivities at discrete time points, but instead are sensitivity trajectories
- Use functional PCA (fPCA) to perform time-varying decomposition, yielding loading trajectories
- Set of dominant reactions can change depending on time



Normalized Sensitivity Coefficient Time Profiles

Normalized Sensitivity Coefficients (NSC)

$$S_{i,j}(t) = \left(\frac{k_j}{C_i(t)}\right)\left(\frac{\partial C_i(t)}{\partial k_j}\right)$$

Definition of Functional PCA

- fPCA is defined using the covariance operator representing ensemble averaging at each time

- Covariance between values of variables i and j at times τ and t over N runs are two-dimensional surfaces

$$v_{ij}(\tau,t) = \frac{1}{N}\sum_{k=1}^{N} S_{ik}(\tau)S_{jk}(t), \quad \tau,t \in [0,T]$$

- Functional principal components analysis is defined as an eigenvalue-eigenvector decomposition on covariance operator V(τ,t) defined in terms of v_{ij} (τ,t)
  - Conceptually, the approach is analogous to conventional PCA, except that eigenvector decomposition is expressed in terms of an integral with respect to time

$$V\mathbf{p}(t) = \lambda\mathbf{p}(\tau) = \int_0^T V(\tau,t)\mathbf{p}(t)dt$$

  - fPCA produces set of orthogonal eigenfunctions $\mathbf{p}_k(t)$ representing time-varying loadings

Functional PCA Computations

- Solution Approaches
  - Discretization
  - Basis Function Expansion
    - Software available from Jim Ramsay (free!)
    - Computational burden is higher than for discretization approach

$$S_{i,j}(t) = \left(\frac{k_j}{C_i(t)}\right)\left(\frac{\partial C_i(t)}{\partial k_j}\right)$$

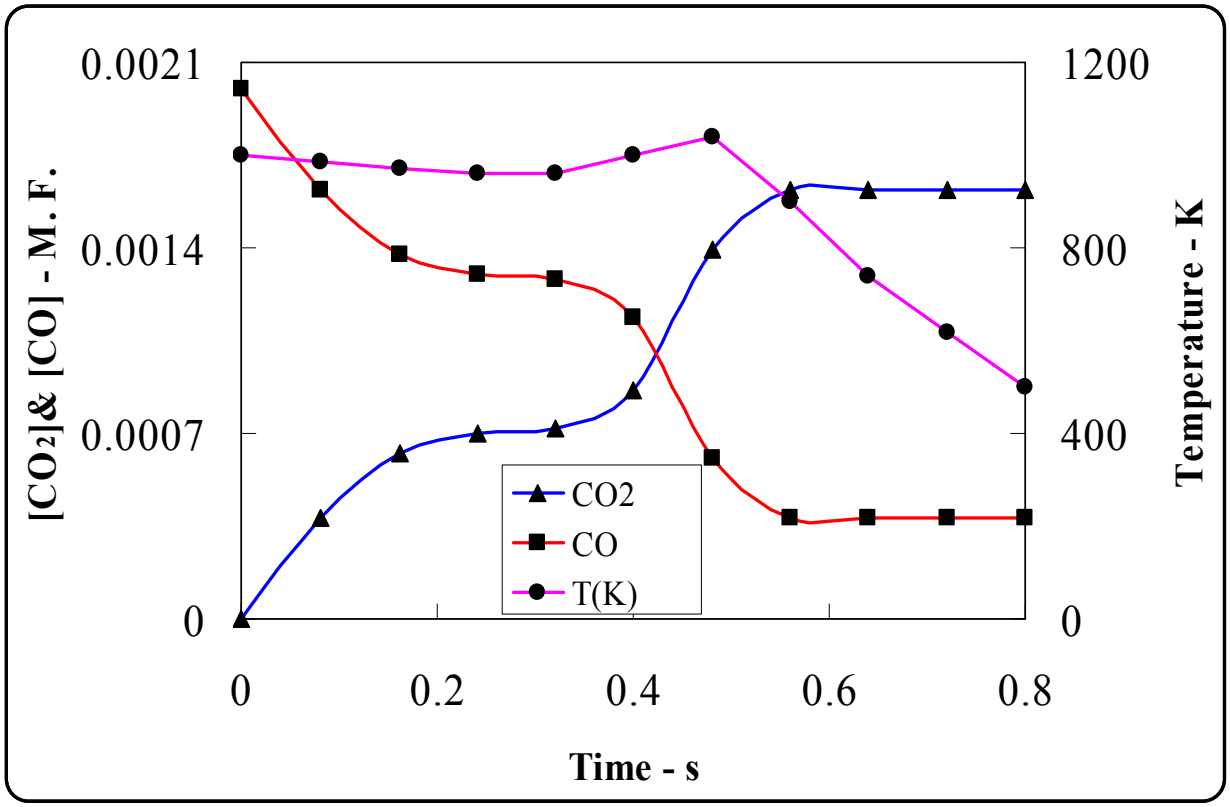
- Discretization Approach
  - Generate sensitivity trajectories values at discrete points using the mechanistic model – not necessarily uniformly spaced
  - Earliest approach to functional PCA – Rao (1958, 1987), Tucker (1958)
  - Sensitivity matrices $\mathbf{S}(t_k)$ at discrete points in the time horizon: $t_1, \ldots, t_p$
  - Data matrix formed by stacking sensitivity matrices sideways
    - » rows correspond to different chemical species and runs
    - » columns correspond to reactions at different sampling times

$$\breve{\mathbf{S}} = \left[\left[\mathbf{S}(t_1)\right]_{n\times m} \quad \left[\mathbf{S}(t_2)\right]_{n\times m} \quad \cdots \quad \left[\mathbf{S}(t_p)\right]_{n\times m}\right]_{n\times(m\times p)}$$

  - Compute loading vector elements using PCA (SVD). Loading vector elements represent values of the loading functions (eigenfunctions) at sampling points along the time horizon.
  - Looks like one form of unfolding for multi-way PCA

Functional PCA Results for CO Oxidation Model (Simple Test Model)

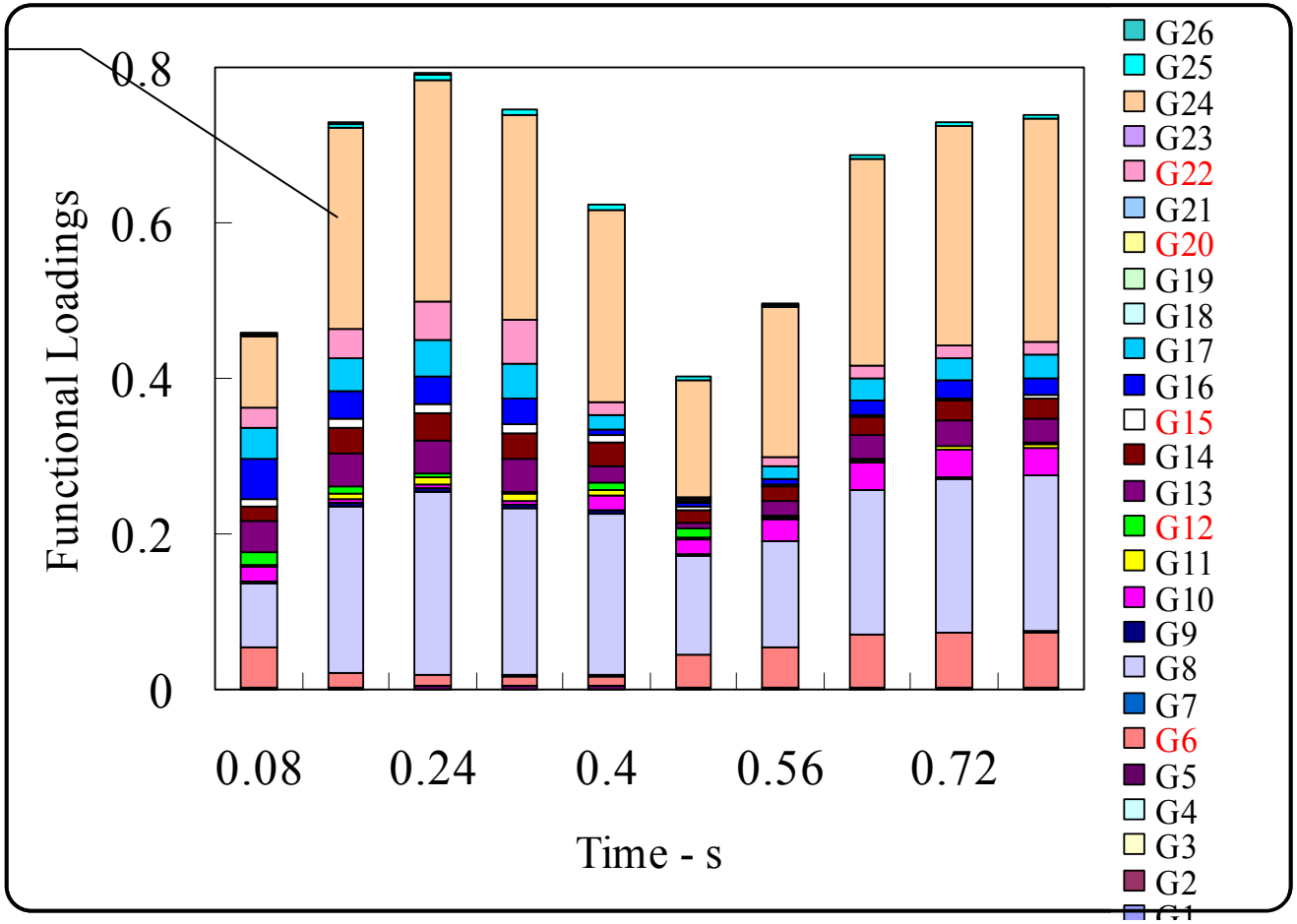
Concentration time profiles for major species in carbon monoxide oxidation – note gradual change in profiles



Functional PCA Results for CO Oxidation Model

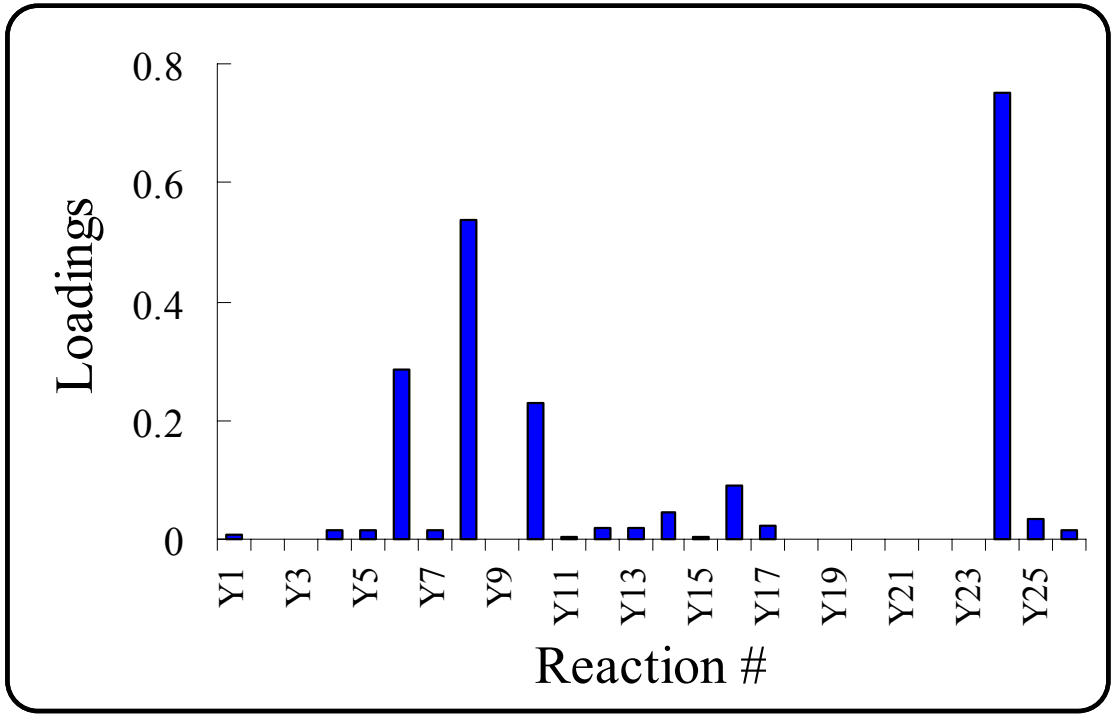
Significant loadings indicate reaction G24 should be retained over time horizon

Significant reactions:
24, 8, 22, 10, 6, 16
- loadings (importance?) change over time



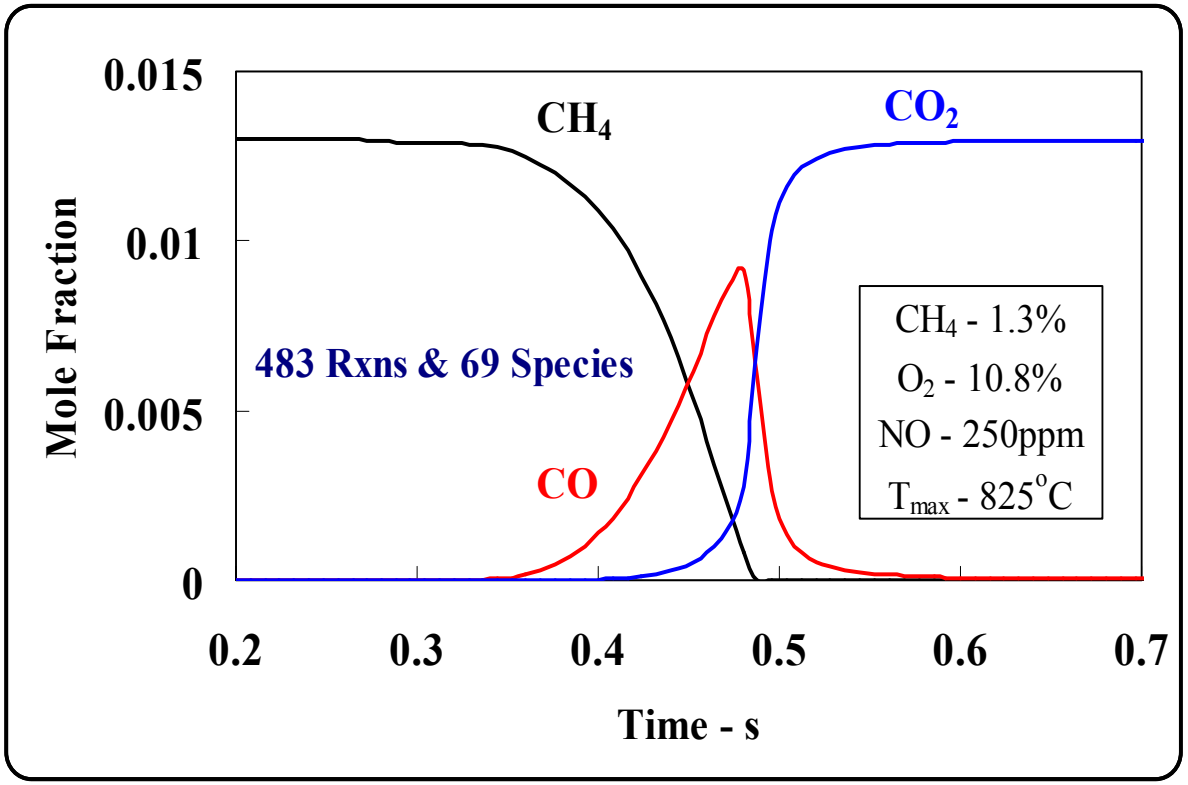
Conventional PCA Results for CO Oxidation Model

Significant reactions:
24, 8, 6, 10, 16

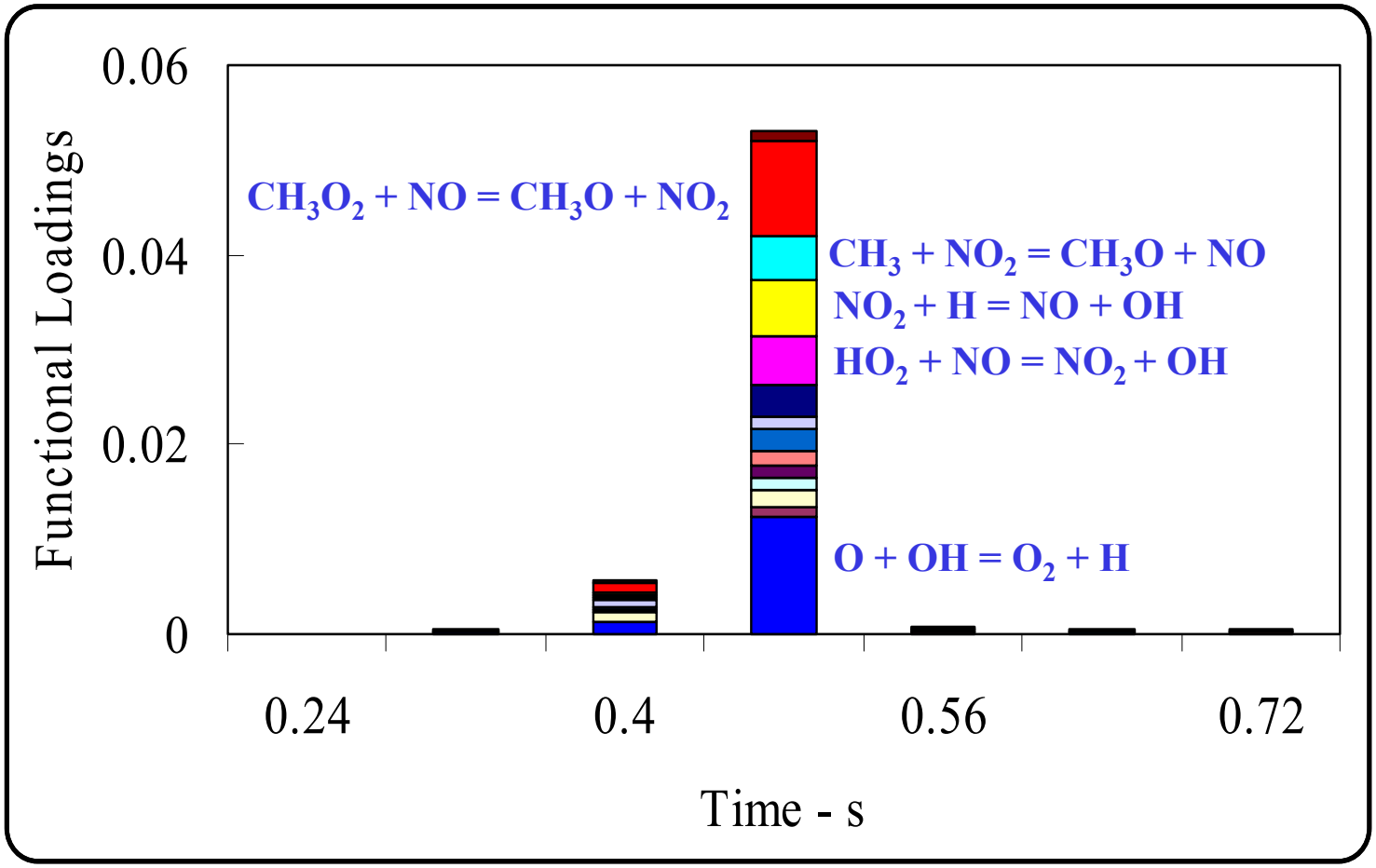


Functional PCA Results for NO-Sensitized Oxidation (Complicated Model)

Concentration time profiles for major species in NO-sensitized oxidation
- note sharp transition in profiles at 0.45 s



Functional PCA Results for NO-Sensitized Oxidation



Conclusions

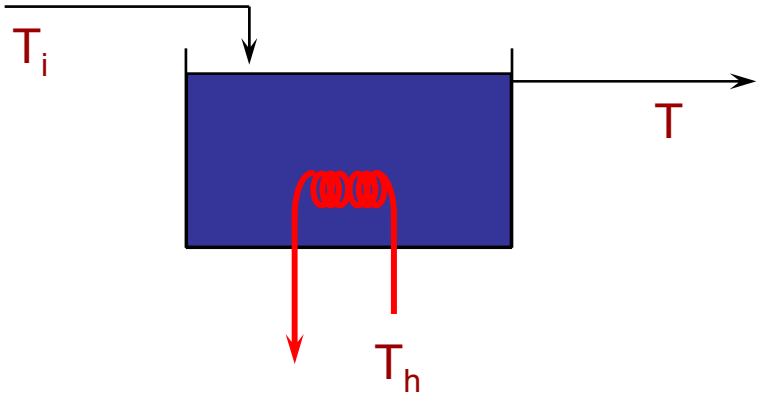
- Functional PCA can be used to perform kinetic model reduction using sensitivity information
- Time-varying loadings allow progression of significant reactions to be identified as combustion progresses
- Discretization approach - looks like one unfolding for multi-way PCA
  - Alternatives – basis function approach, numerical quadrature
- Computational load is a problem with the basis function approach
  - We have encountered this problem, but we haven't given up
- Extensions – regularized fPCA
  - imposing smoothness on the loading functions

Third Story

Investigating Process Dynamic Structure Using Principal Differential Analysis (PDA)

Motivation – Process Dynamics and Differential Operators

Example – Heated Tank



Mechanistic Dynamic model:

Accumulation = in – out + generation - consumption

$$\frac{dT}{dt} = \frac{F}{V}T_i - (\frac{F}{V} + \frac{UA}{\rho V C_p})T + \frac{UA}{\rho V_c C_p}T_h$$

Denote x = T, u = T_h , d = T_i

$$\frac{dx}{dt} = -(\frac{F}{V} + \frac{UA}{\rho V C_p})x + \frac{UA}{\rho V_c C_p}u + \frac{F}{V}d$$

Notation for Differential Operators

View system dynamics as differential operator acting on [x(t),u(t),d(t)]

$$\frac{dx}{dt} = -\left(\frac{F}{V} + \frac{UA}{\rho V C_p}\right)x + \frac{UA}{\rho V_c C_p}u + \frac{F}{V}d$$

$$D^1 x + w_{x0} D^0 x + w_{u0} D^0 u + w_{d0} D^0 d = 0$$

$$D^n \equiv \frac{d^n}{dt^n}$$

$$with \quad w_{x0} = \left(\frac{F}{V} + \frac{UA}{\rho V C_p}\right), \quad w_{u0} = \frac{-UA}{\rho V_c C_p}, \quad w_{d0} = \frac{-F}{V}$$

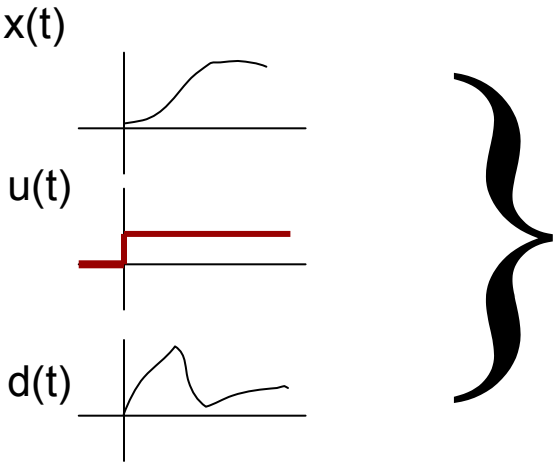
The tank dynamics are described by $L[x(t), u(t), d(t)] = 0$

where $L \equiv D^1 + w_{x0} D^0 + w_{u0} D^0 + w_{d0} D^0$

Differential Operators

Differential operators appear in mechanistic and empirical models for process dynamics

Mechanistic modeling ⇒ Differential operators ⇐ Empirical Modeling (PDA & traditional approaches)



$$D^1 x + w_{x0} D^0 x + w_{u0} D^0 u + w_{d0} D^0 d = 0$$

Dynamic model for controller design

Empirical Modeling Approaches

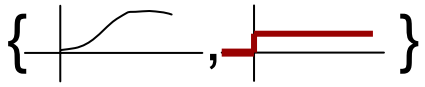
- Discrete-time models
  - Predominant method for estimating dynamic process models from data
  - Transfer function or recursion equation models
- Continuous-time models
  - Identification of discrete time model, conversion to continuous time
  - Estimation of parameters in differential equation model using nonlinear regression
- Principal differential analysis – technique in FDA
  - Directly estimate linear differential operators describing process dynamics
  - Look for linear combinations (with weights that can change with time) of measured functions and their derivatives that sum close to zero
  - Why?
    - Non-uniform sampling
    - Models can easily include time-varying coefficients
    - Can handle data from multiple dynamic experiments

Principal Differential Analysis – Estimation

Data

- e.g., observations of temperature, heating medium temperature

$$\{[x_i(t), u_i(t)]\}, \; i = 1, \ldots, N_{\text{expts}}$$



Estimation

- Least squares criterion

$$\min_{w_{x,j}(t), w_{u,j}(t)} \sum_{i=1}^{N_{\text{expts}}} \int_0^{t_f} e_i(t)^2 \, dt$$

with residuals given by

$$e_i(t) = L[x(t), u(t)] = D^k x_i(t) + \sum_{j=0}^{k-1} w_{x,j}(t) D^j x_i(t) + \sum_{l=0}^{m} w_{u,l}(t) D^l u_i(t)$$

Residual function

General differential equation model that is k-th order in x, m-th order in u

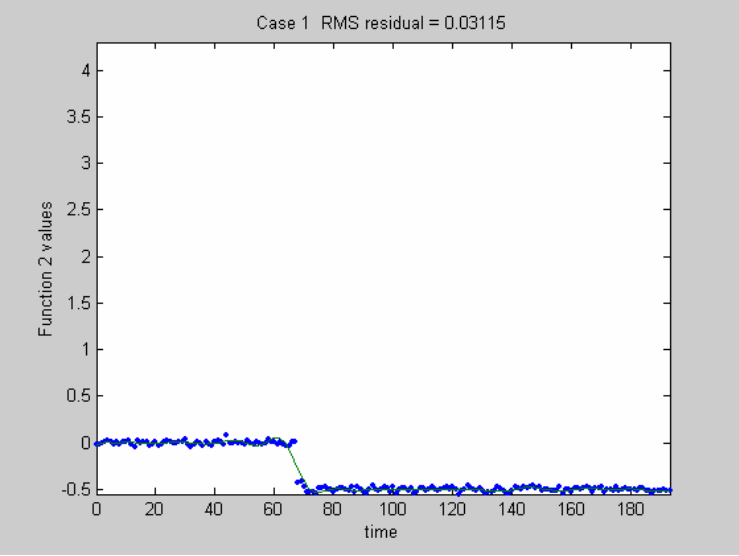
Notice that we are penalizing residuals for the highest-order derivative, rather than residuals for the predicted responses.

PDA Modeling Sequence

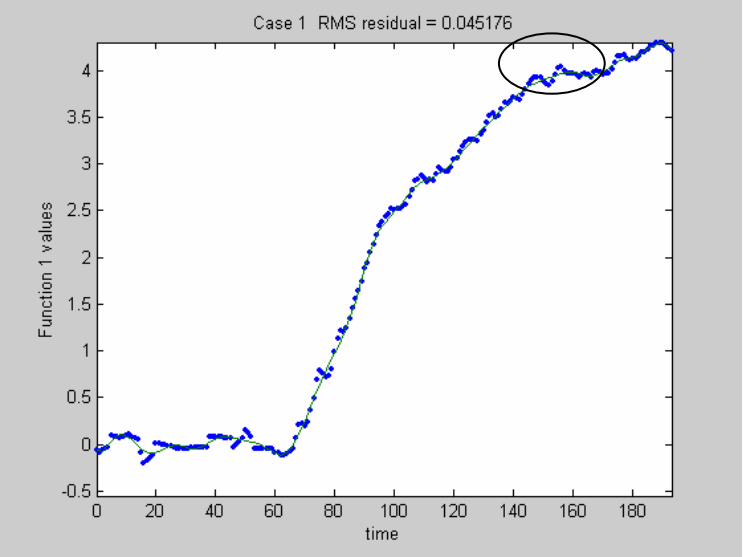
- Smooth functional observations to generate functional data object
  - What basis functions should be used?
    - Characteristics of data – periodic?, smooth?
  - Should roughness penalties be applied?
    - Tradeoff between biasing process trend and impact of noise
    - Disturbances can be picked up as additional forcing functions
  - Estimate linear differential operators to annihilate observed functions
- Computation
  - Basis function representation for weight functions leads to matrix algebra solution
- Diagnostics
  - Examine residual plots
  - Sampling properties of weight functions yet to be developed

Example – Industrial Petroleum Refinery Data

- Single-input single-output estimation
- Debutanizer industrial step test data
- Estimate constant coefficient model – differential operator has constant coefficient functions
- B-spline bases used with no roughness penalties
  - 30 basis functions, 4th order B-splines



Input

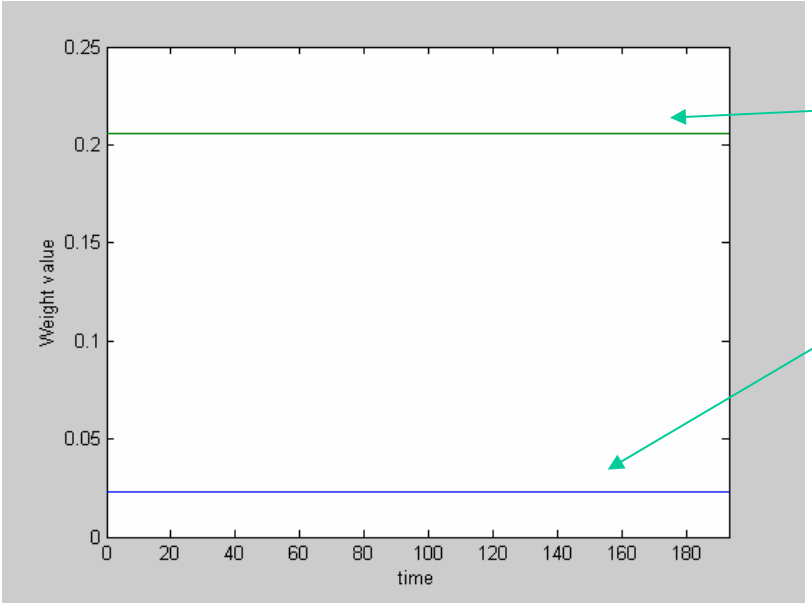


Output

Example – Industrial Petroleum Refinery Data

- Weight functions – time-invariant models

Estimated -
Gain: 9.0
Time constant:
43.6 min

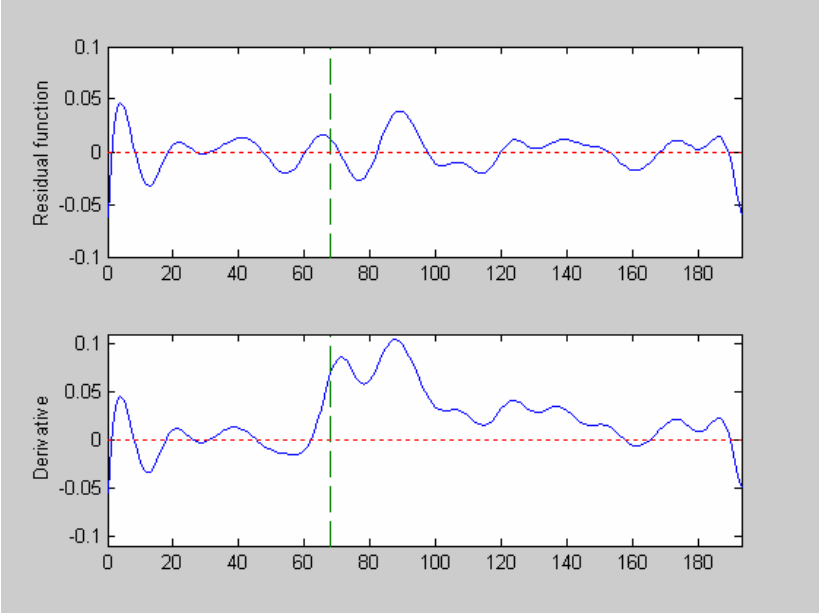


- Estimated model

$$Dx(t) + 0.023x(t) + 0.206u(t) = 0$$

Example – Industrial Petroleum Refinery Data

- Residual function and derivative of output
- Use derivative of output as magnitude benchmark
  - Dx is the "response", by rearrangement: $Dx(t) \approx -0.023x(t) - 0.206u(t)$



Residual Function

Derivative of output function

Magnitudes of residuals fall within 50% of peak magnitude of Dx: is this good?

Extension – Dealing with Processes Exhibiting Time Delays

- Extend PDA to incorporate delay differential operators
  - Differential operator acts on delayed inputs
  - In linear case, delay can be assigned to inputs or responses

- Estimation of delay
  - Via a direct search optimization which minimizes integral squared error of residuals
  - Choose delay that provides the smallest integral squared error of residuals

- Alternative
  - Use registration of functions to align landmarks reflecting time delay

Outstanding PDA questions

- Choice of basis function – relation to input signal type – PRBS, step
- Degree of smoothing
- Time-varying vs. time-invariant modeling – weighting functions
- Objective function penalizes residuals of derivatives rather than residuals of predicted responses
- Extension to multi-input multi-output models
- Identification of partial differential equation models – differential operators on two- or higher-dimensional domains

Currently, we are using simple simulation studies to develop understanding and experience in the application of PDA

  - Simple dynamic systems
  - Types of input signals – PRBS, step
  - Comparison to standard system i.d. techniques

Conclusions

PDA can be used to identify process dynamic structure

- Using irregularly sampled data
- More flexible interpolation between points
- Direct estimation of continuous-time models
- Estimation of delays via delay-differential operators
- Time-varying models
- Parallel framework to discrete-time identification techniques – process + disturbance models

Wrap-up

Functional data analysis provides alternative framework for dealing with functional data

- Recognizes that responses are continuous functions
- Standard statistical tools are extended to account for functional nature of the responses (fPCA, functional regression)
- Additional tools are provided (PDA)

Practical implications

- Sampling representation
  - Conceptually the data are functions, however practically they are represented using basis functions
  - Basis function representation provides higher level of interpolation
    - Potential Benefit – incorporation of additional knowledge about the response, such as the degree of smoothness (knowledge about behaviour of derivatives)
    - Risk – incorporation of spurious behaviour into the analysis because of noise. Is the risk in FDA greater than in conventional approaches (e.g., discrete time-series analysis)?
    - Traditional discrete time series approaches essentially use an impulse basis to represent the data

Practical Implications

- By viewing data as inherently functional and using basis functions to represent data
  - Non-uniform sampling can be handled readily
  - Time-varying dynamic system behaviour can be readily modeled
- Better understanding is required before these techniques will be widely adopted by the chemometrics and chemical engineering community

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