Efficient Moving Horizon Estimation of DAE Systems

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Outline

- Introduction: Moving Horizon Estimation (MHE)
- Explicit Solution to the MHE Problem
- Observability of Index-1 DAE Systems
- Flash Column Example
- Conclusions and Future Work

Introduction

- Explicit MHE of nonlinear systems (Ramamurthi, Sistu, and Bequette, 1993)
- MHE definitively shown to outperform EKF (Haseltine and Rawlings, 2004). Price of improvement is greater computational expense of MHE.
- This presentation incorporates the recent MHE advances in an explicit solution form
- Motivation: State estimation of large-scale, nonlinear DAE systems
- Strategy: Combine elements of existing technologies in new ways to solve large-scale problems
- *Everything has been thought of before, but the problem is to think of it again.* – Goethe (via Jim Rawlings/via Tom Badgwell)

Moving Horizon Estimation

Nonlinear DAE model (implicit form)

$$0 = f(\dot{x}, x, u) \quad \text{DAE model - implicit form}$$

$$y = g(x) \quad \text{System measurements}$$

Discretized linear time-varying form

$$x_{k+1} = A_k x_k + B_k u_k$$
$$y_k = C_k x_k + D_k u_k$$

$$Y_{model} = \begin{bmatrix} y_{model,0} \\ \vdots \\ y_{model,n} \end{bmatrix}, \quad Y_{meas} = \begin{bmatrix} y_{meas,0} \\ \vdots \\ y_{meas,n} \end{bmatrix}, \quad n = \text{horizon length}$$

MHE optimization (least squares approach)

$$\text{minimize} \left(Y_{meas} - Y_{model}\right)^T Q \left(Y_{meas} - Y_{model}\right)$$

subject to the model equations

Explicit MHE (Previous Work)

Explicit solution to the least squares MHE problem (Ramamurthi, Sistu, and Bequette, 1993 – (Bequette UT PhD grad 1988, now at RPI)

$$\omega_k = C_k \prod_{j=0}^{k-1} A_j \quad \psi_k = C_k \sum_{j=1}^{k} \left[\prod_{i=1}^{j-1} A_{i-k-j} \right] B_{k-j} u_{k-j} + D_k u_k$$

$$Y_{model} = \omega x_0 + \psi$$

$$\hat{x}_0 = \left[\omega^T Q_y \omega \right]^{-1} \omega^T Q_y \left[Y_{meas} - \psi \right]$$

Forgetting factor (α) adds infinite horizon approximation by incorporating previous state estimates (Haseltine and Rawlings, 2004)

$$X_{model} = \begin{bmatrix} x_{model,0} \\ \vdots \\ x_{model,n} \end{bmatrix}, \quad \hat{X}_{prev} = \begin{bmatrix} \hat{x}_{prev,0} \\ \vdots \\ \hat{x}_{prev,n} \end{bmatrix}, \quad n = \text{horizon length}$$

$$\text{minimize} \left(Y_{meas} - Y_{model} \right)^T Q \left(Y_{meas} - Y_{model} \right) + \alpha \left(\hat{X}_{prev} - X_{model} \right)^T \left(\hat{X}_{prev} - X_{model} \right)$$

subject to the model equations

Example 1: Explicit MHE Solution (Unconstrained, Linear)

$$G(s) = \frac{1}{s^2 + 2s + 1}$$

Discrete/State Space Form

$$x_{k+1} = \begin{bmatrix} .8144 & -0.0905 \\ 0.0905 & 0.9953 \end{bmatrix} x_k + \begin{bmatrix} 0.0905 \\ 0.0047 \end{bmatrix} u_k$$

$$y_k = \begin{bmatrix} 0 & 1 \end{bmatrix} x_k + v_k$$

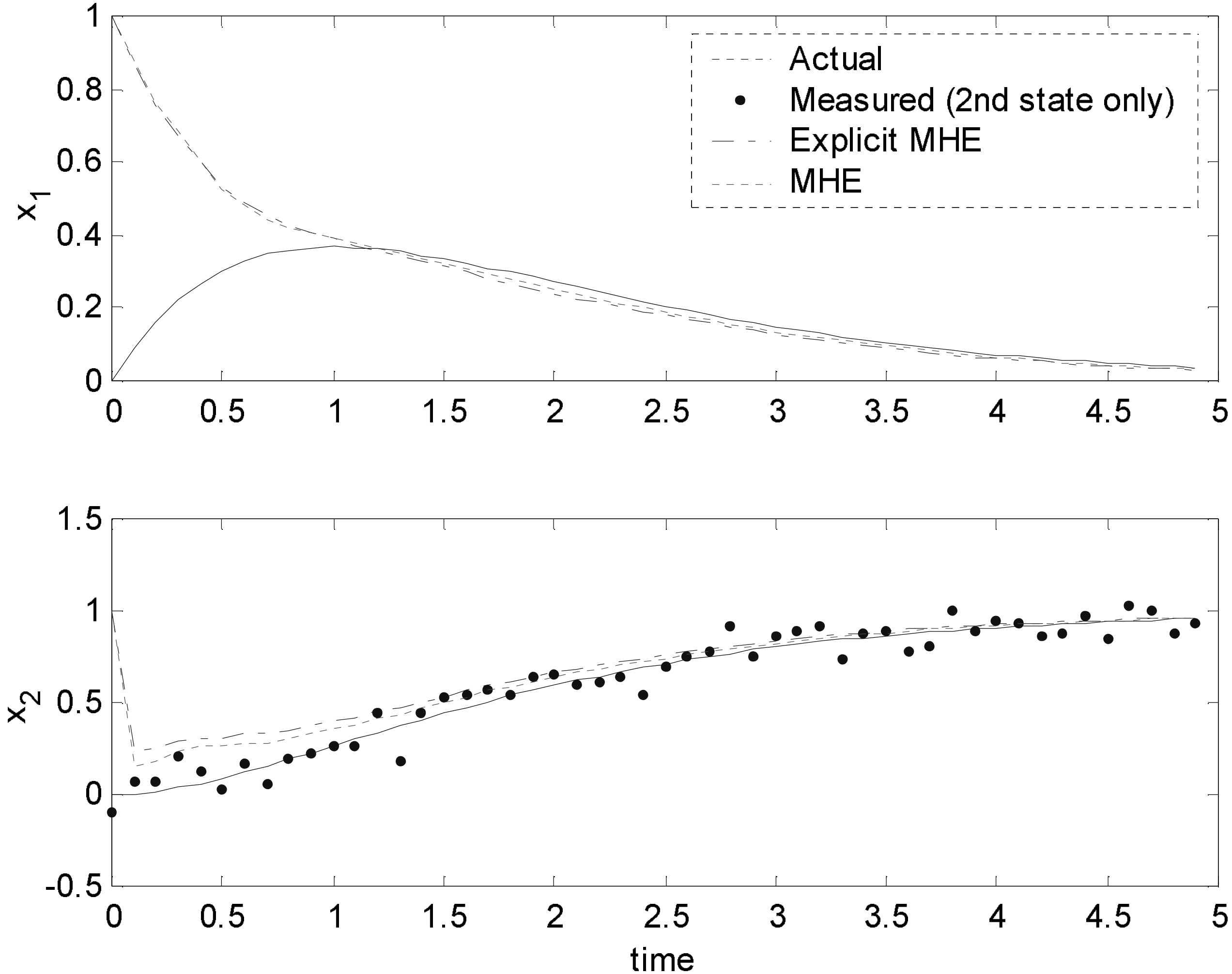
Sampling time: 0.1 sec

ν_k (output noise) is normally distributed with $\mu = 0$ and $\sigma = 0.1$

Initial conditions: Actual = $[0\ 0]^T$ Predicted = $[1\ 1]^T$

MHE values: forgetting factor $\alpha = 0.5$ (weighting on $x_{0,est}$)

Example 1: Results



MHE for Real Systems

- Upper and lower bounds that represent physical limits on state variables (e.g., mole fractions are between 0 and 1)
- Variable measurement frequencies (e.g., temperatures at 1 sample/sec and concentrations at 1 sample/minute)
- Corrupt or missing data
- Large-scale, nonlinear, rigorous DAE models
- Solve MHE subject to real-time constraints

- The new approach in this presentation:
  - Explicitly solves the least squares MHE problem subject to upper and lower bounds on the states
  - Is able to meet real-time constraints for large-scale problems
  - Is flexible to handle variable measurement frequencies and missing data

Incorporate Constraints (Upper and Lower Bounds)

- Iteratively add/remove measurements that add constraint information
- Uses strategies from the active set and penalty methods from nonlinear programming
  - Active set strategy – optimizer only deals with active inequality constraints ($x = a$ or $x = b$) and ignores inactive constraints ($a < x < b$)
  - Penalty method – cost added to the objective function when constraints are violated

$$\text{minimize}\left(Y_{meas} - Y_{model}\right)^T Q\left(Y_{meas} - Y_{model}\right)$$

$$\text{subject to the model equations}$$

$$\text{subject to } a \le x \le b$$

Adding/Removing Constraints

- For active constraints
  - Define the Lagrange multiplier (shadow price) (λ_{lower} = Q (a - Y_{model}) or λ_{upper} = Q (Y_{model} - b))
  - If $\lambda < 0$, remove constraint from the active set
- For inactive constraints
  - If $x > b$ add upper limit constraint with a measurement ($y_{meas} = b$)
  - If $x < a$ add lower limit constraint with a measurement ($y_{meas} = a$)

- Pseudo-code:

  Do
  - Compute Explicit MHE
  - If $\lambda < 0$ remove constraint
  - If $x > b$ add measurement $y_{meas}=b$
  - If $x < a$ add measurement $y_{meas}=a$

  Loop Until No Active Set Change

Constrained Explicit MHE (Other Enhancements)

Forgetting factor (α) adds infinite horizon approximation by incorporating previous state estimates (Haseltine and Rawlings, 2004)

$$X_{model} = \begin{bmatrix} x_{model,0} \\ \vdots \\ x_{model,n} \end{bmatrix}, \quad \hat{X}_{prev} = \begin{bmatrix} \hat{x}_{prev,0} \\ \vdots \\ \hat{x}_{prev,n} \end{bmatrix}, \quad n = \text{horizon length}$$

$$\text{minimize} \left(Y_{meas} - Y_{model}\right)^T Q \left(Y_{meas} - Y_{model}\right) + \alpha \left(\hat{X}_{prev} - X_{model}\right)^T \left(\hat{X}_{prev} - X_{model}\right)$$

subject to the model equations

Explicit solution (new)

$$Q_{x,k} = \left(C_k{}^T Q_{y,k} C_k\right)$$

$$\omega_k = \prod_{j=0}^{k-1} A_j \quad \psi_k = \sum_{j=1}^{k} \left[\prod_{i=1}^{j-1} A_{i-k-j} \right] B_{k-j} u_{k-j} + D_k u_k$$

$$\hat{x}_0 = \left[\omega^T \left(Q_x + \alpha I\right)\omega\right]^{-1} \left(\omega^T Q_x \left[C^T Y_{meas} - \psi\right] + \alpha\omega^T \left[\hat{X}_{prev} - \psi\right]\right)$$

Constrained Explicit MHE (Other Enhancements)

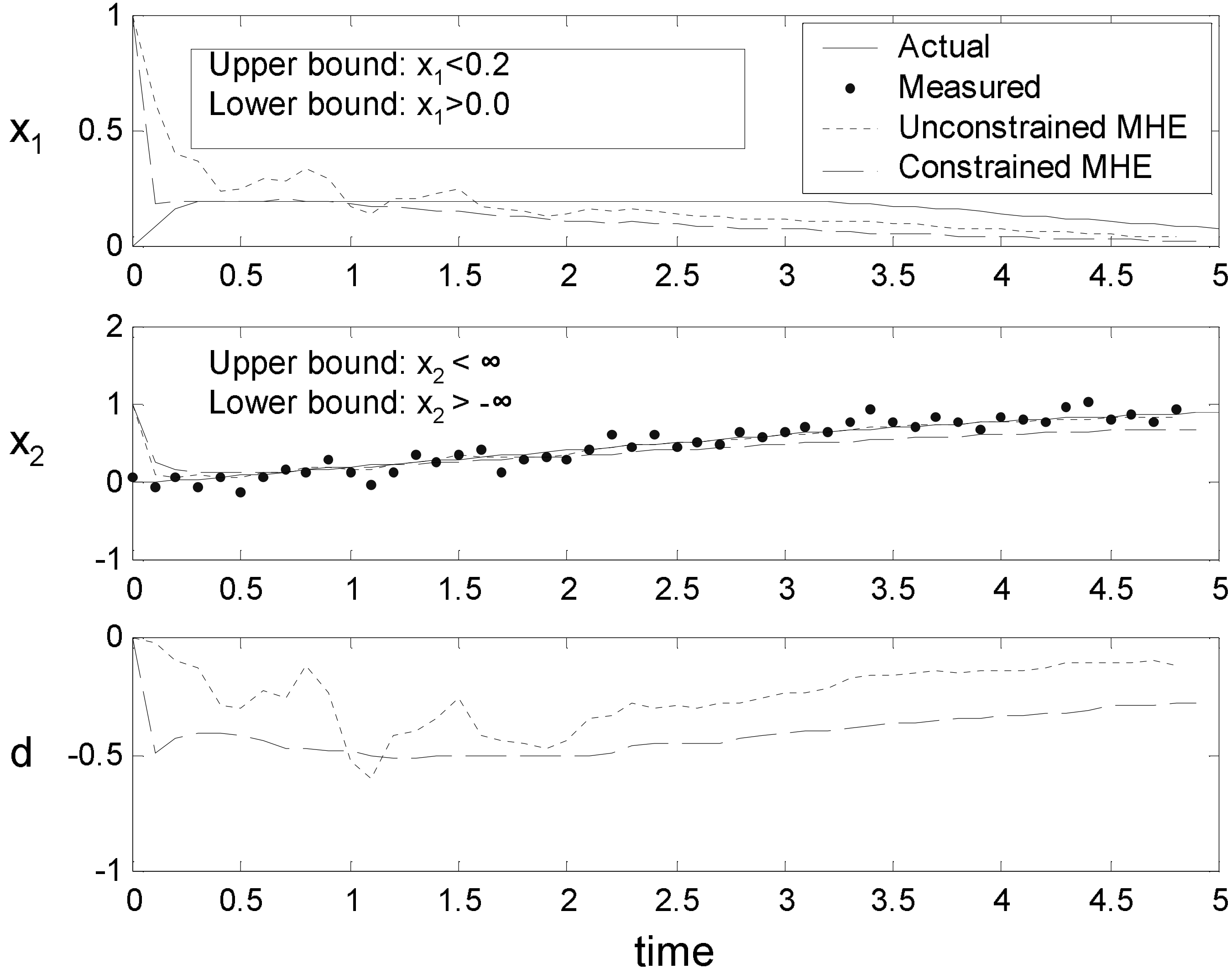
Augment system with input disturbance variables (*d*) (Muske and Badgwell, 2002)

$$\begin{bmatrix} x \\ d \end{bmatrix}_{k+1} = \begin{bmatrix} A & B \\ 0 & 1 \end{bmatrix}_k \begin{bmatrix} x \\ d \end{bmatrix}_k + \begin{bmatrix} B \\ 0 \end{bmatrix}_k u_k$$

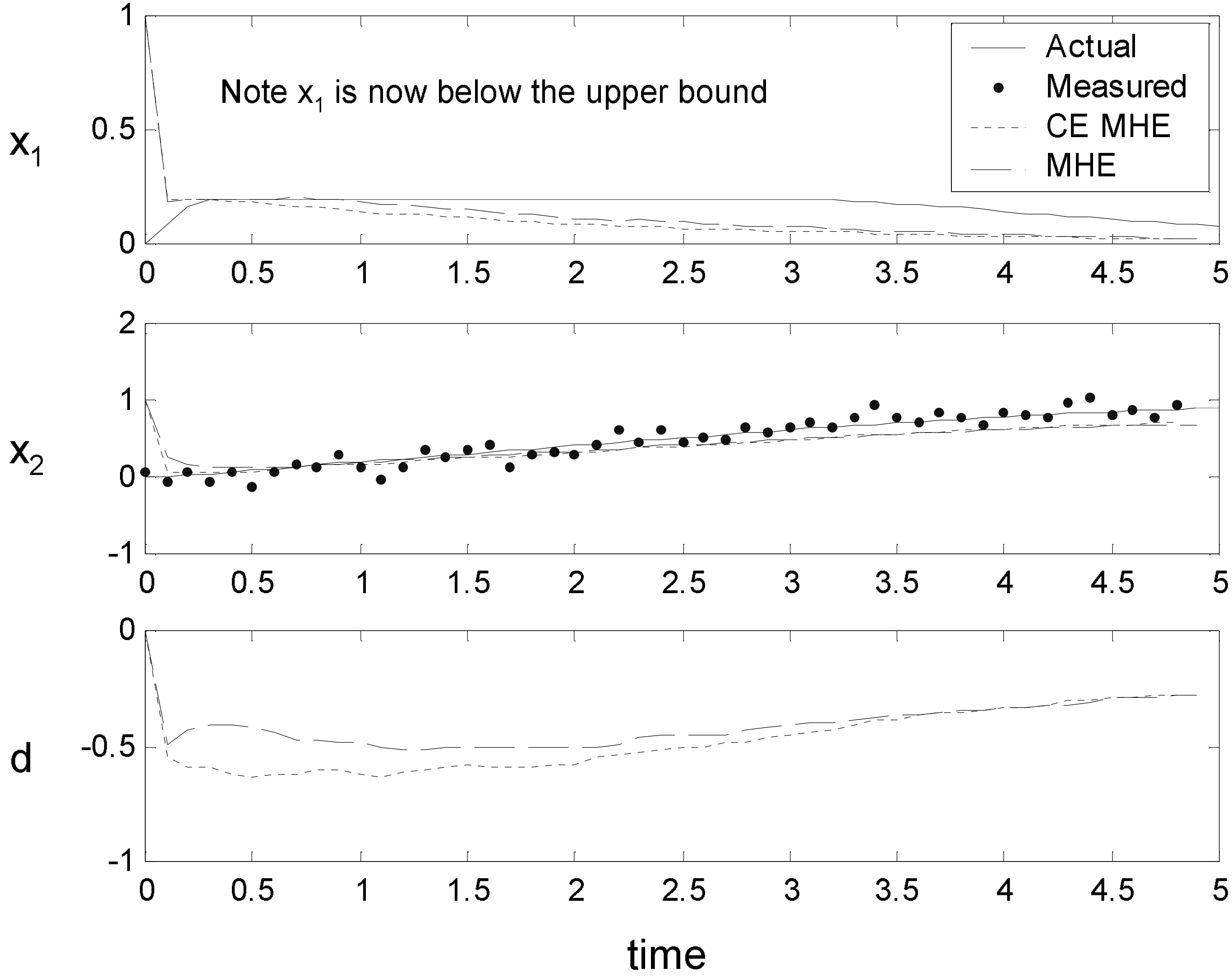
$$y_k = \begin{bmatrix} C & 0 \end{bmatrix}_k \begin{bmatrix} x \\ d \end{bmatrix}_k$$

Estimate input disturbances and states in one explicit step instead of two iterative steps as in Ramamurthi, Sistu, and Bequette (1993)

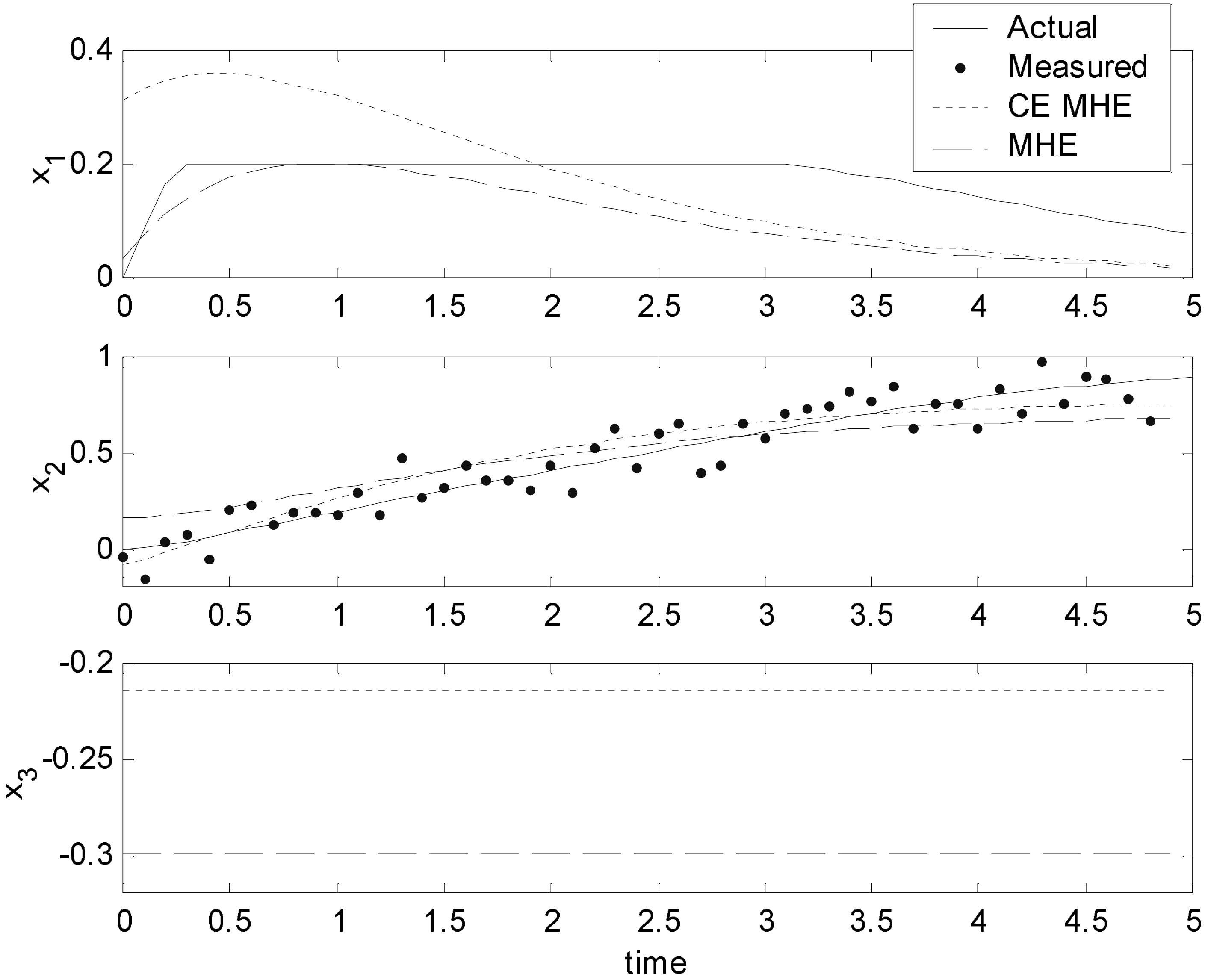
Example 2: (Constrained Version of Example 1)



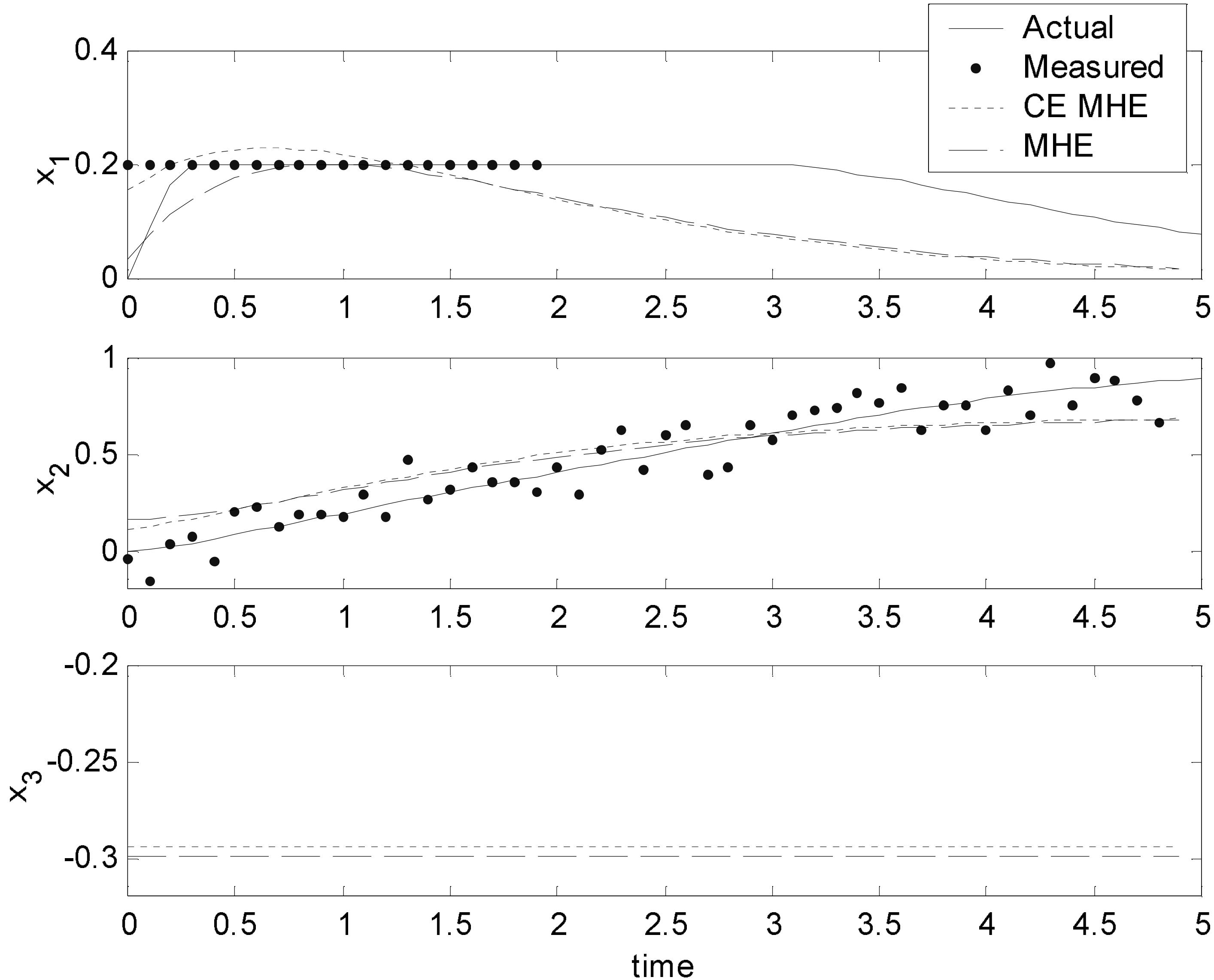
Example 2: Final Solution

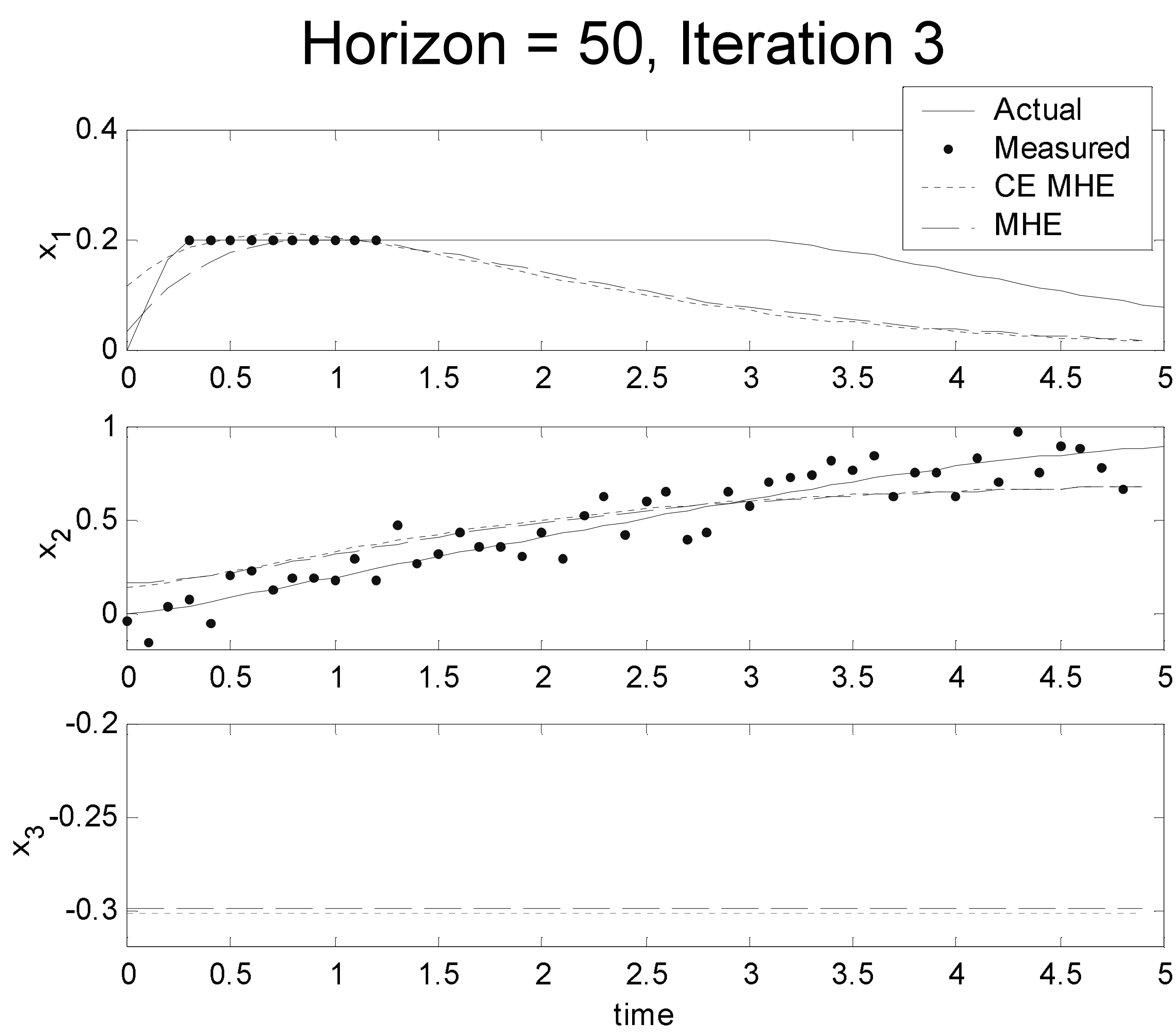


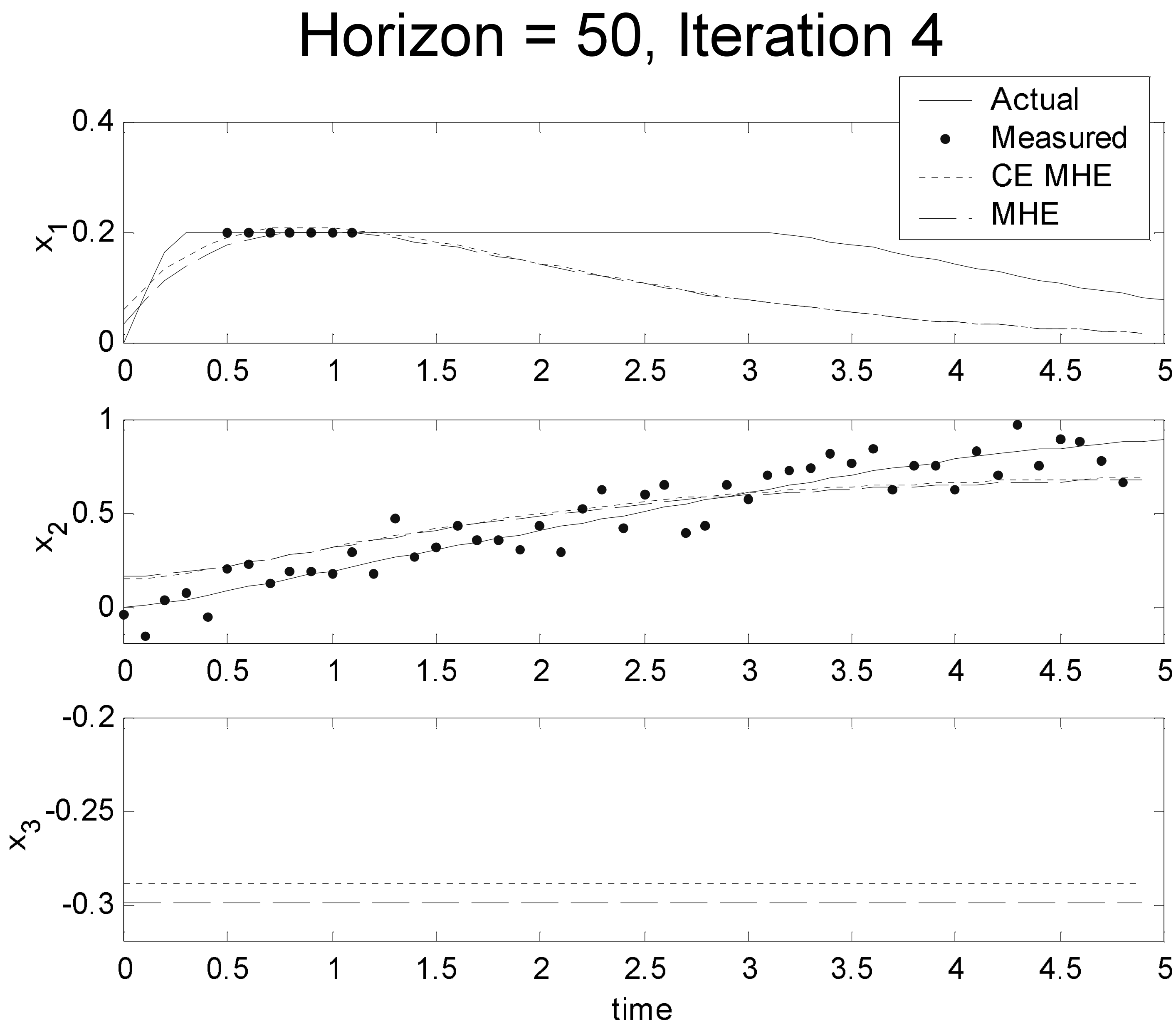
Horizon = 50, Iteration 1



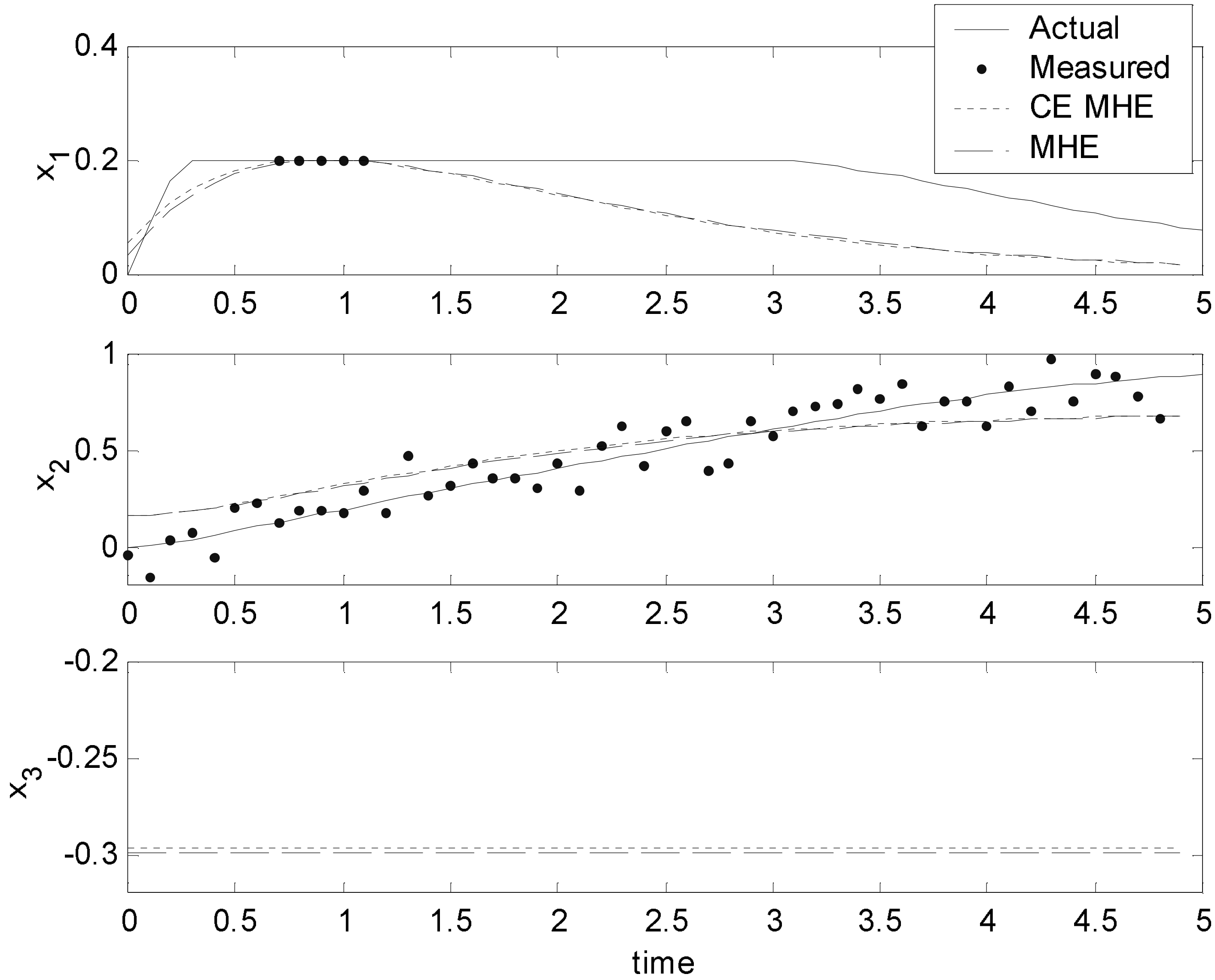
Horizon = 50, Iteration 2




Horizon = 50, Iteration 3
Actual
Measured
CE MHE
MHE
x1
x2
x3
time


Horizon = 50, Iteration 4
Actual
Measured
CE MHE
MHE
x_1
0.4
0.2
0
x_2
1
0.5
0
x_3
-0.2
-0.25
-0.3
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
time

Horizon = 50, Iteration 5



Constrained Explicit MHE Properties

- No optimizers involved
- Explicit solution at each iteration = fast computation, reliable solution
- Incorporate constraints by iteratively adding or removing measurements based on an active set strategy
- Constraints are restricted to upper and lower variable bounds
- Computational costs for the previous example (horizon=50)
  - Constrained Explicit MHE (6,831 flops)
  - MHE (122,048,803 flops)

Local Observability of Index-1 DAE States

- Recall for discrete linear time-invariant (LTI) ODE models:
  - The system is observable iff Γ_o[A,C] (observability matrix) is full rank
- For index-1 DAE models
  - The system is observable if every dynamic mode in A is connected to the output through C

$$\begin{bmatrix} \dot{x}_1 \\ 0 \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} u$$

$$y = \begin{bmatrix} C_1 & C_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + Du$$

Semi-explicit DAE form (linearized)

Local Observability of Index-1 DAE States

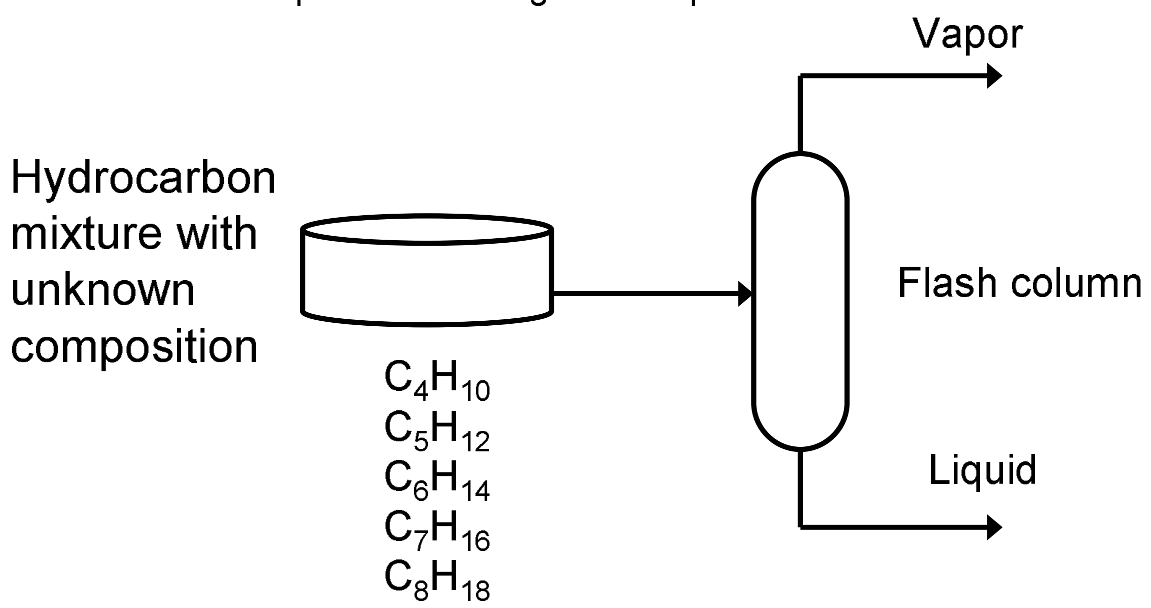
Define how the dynamic modes (differential states) connect to the output (measurements)

$$\tilde{A} = e^{\left(A_{11} - A_{12}A_{22}^{-1}A_{21}\right)\Delta t} \qquad \tilde{C} = C_1 - C_2 A_{22}^{-1} A_{21}$$

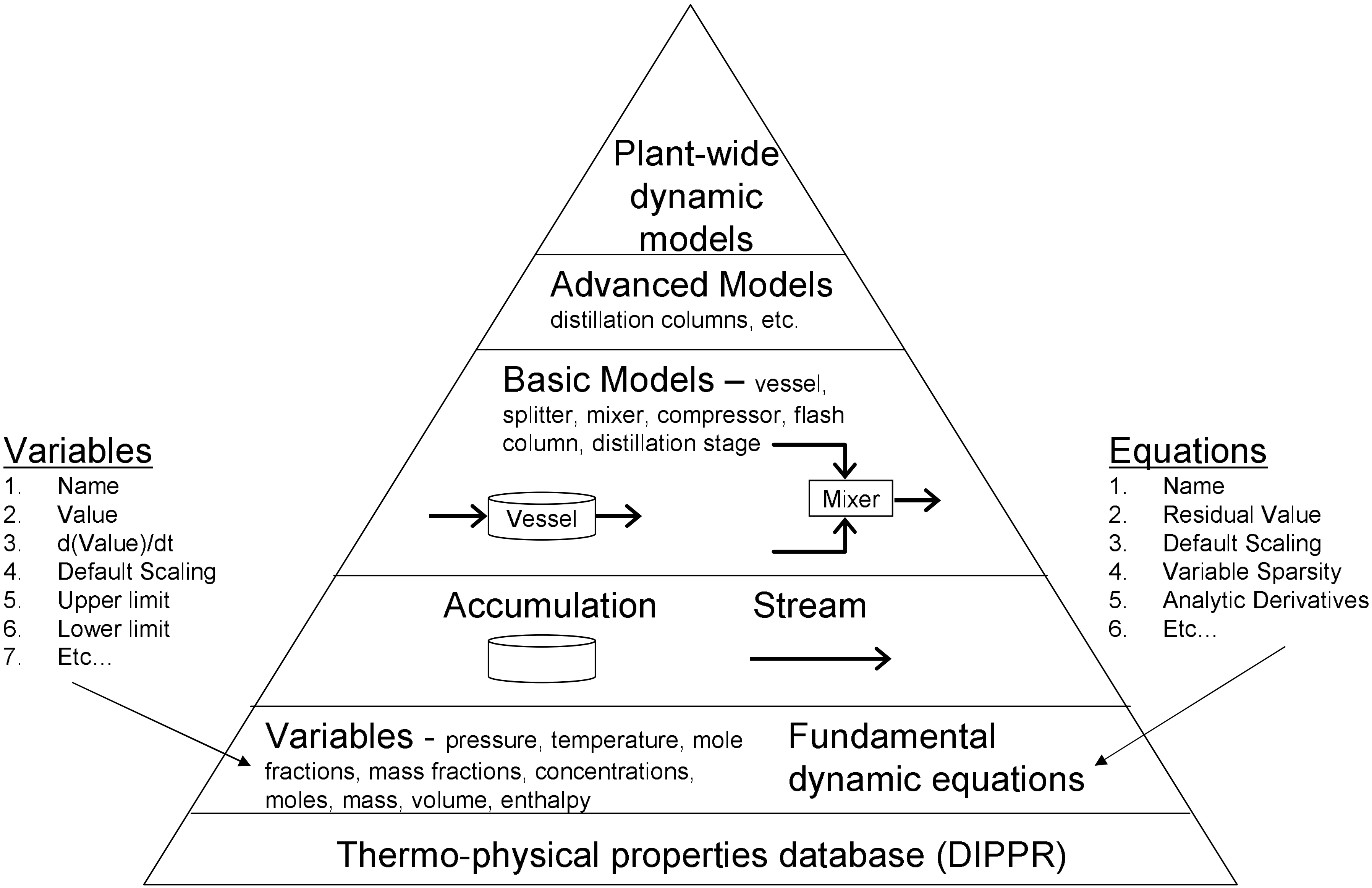
System is observable if and only if $\Gamma_o\left(\tilde{A}, \tilde{C}\right)$ is full rank

Example 3: Composition Estimation Example

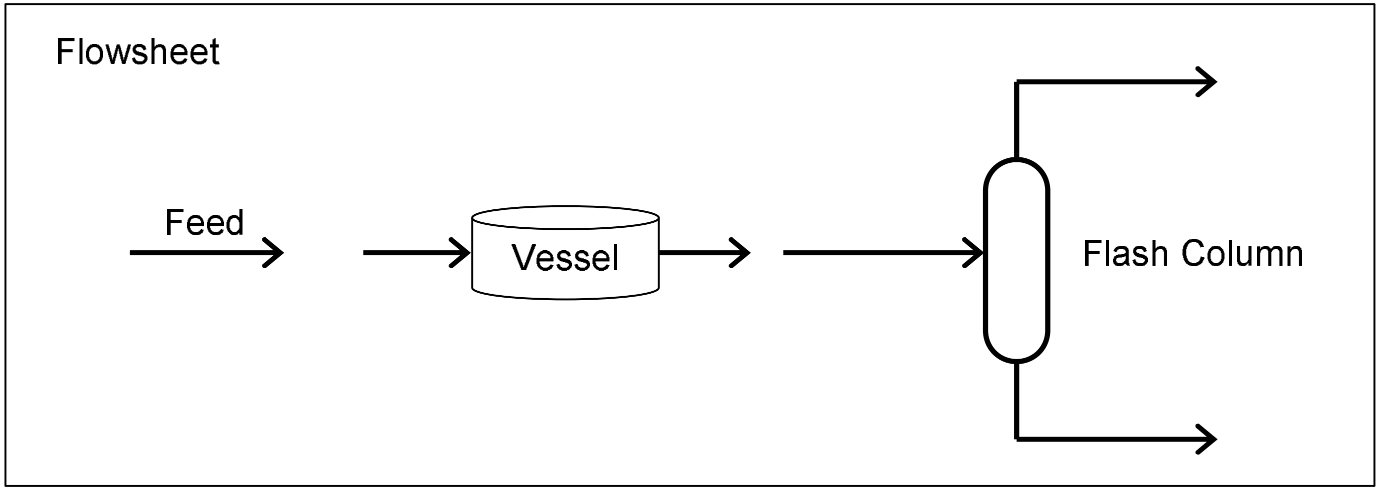
- Can the composition of a hydrocarbon mixture be reconstructed with temperature and flow rate measurements of a flash column?
  - Measure feed and flash temperature
  - Measure vapor and liquid flow rates
  - Rigorous nonlinear flash column model
  - 17 state model (reduced from 157 states)
    - 5 differential equations / 12 algebraic equations



Object Oriented Modeling



Model Reduction: Example 3



Streams (6) – pressure (1), temperature (1), mole fractions (5), mass fractions (5), concentrations (5), molar flow rate (1), mass flow rate (1), volumetric flow rate (1), density (1), enthalpy (1)

Accumulations (1) – pressure (1), temperature (1), mole fractions (5), mass fractions (5), concentrations (5), moles (1), mass (1), molar volume (1), density (1), enthalpy (1)

Additional Vessel Variables – vessel volume (1), heat added (1)

Additional Flash Column Variables – heat added (1)

Total variables/equations: 157

Model Reduction: Example 3

- Lower triangular block diagonalization of the sparsity pattern reveals variables that can be removed from the implicit set – explicit transformation of equations (reduction of 119 variables)
- Merge stream objects instead of defining connection equations (reduction of 12 variables)
- Specify feed stream, vessel volume, heat addition to the vessel, and heat addition to the flash column (specify 9 variables)

- Resulting model size: 17 variables (5 differential/12 algebraic)

Composition Estimation Example

- Measurements every 1 sec

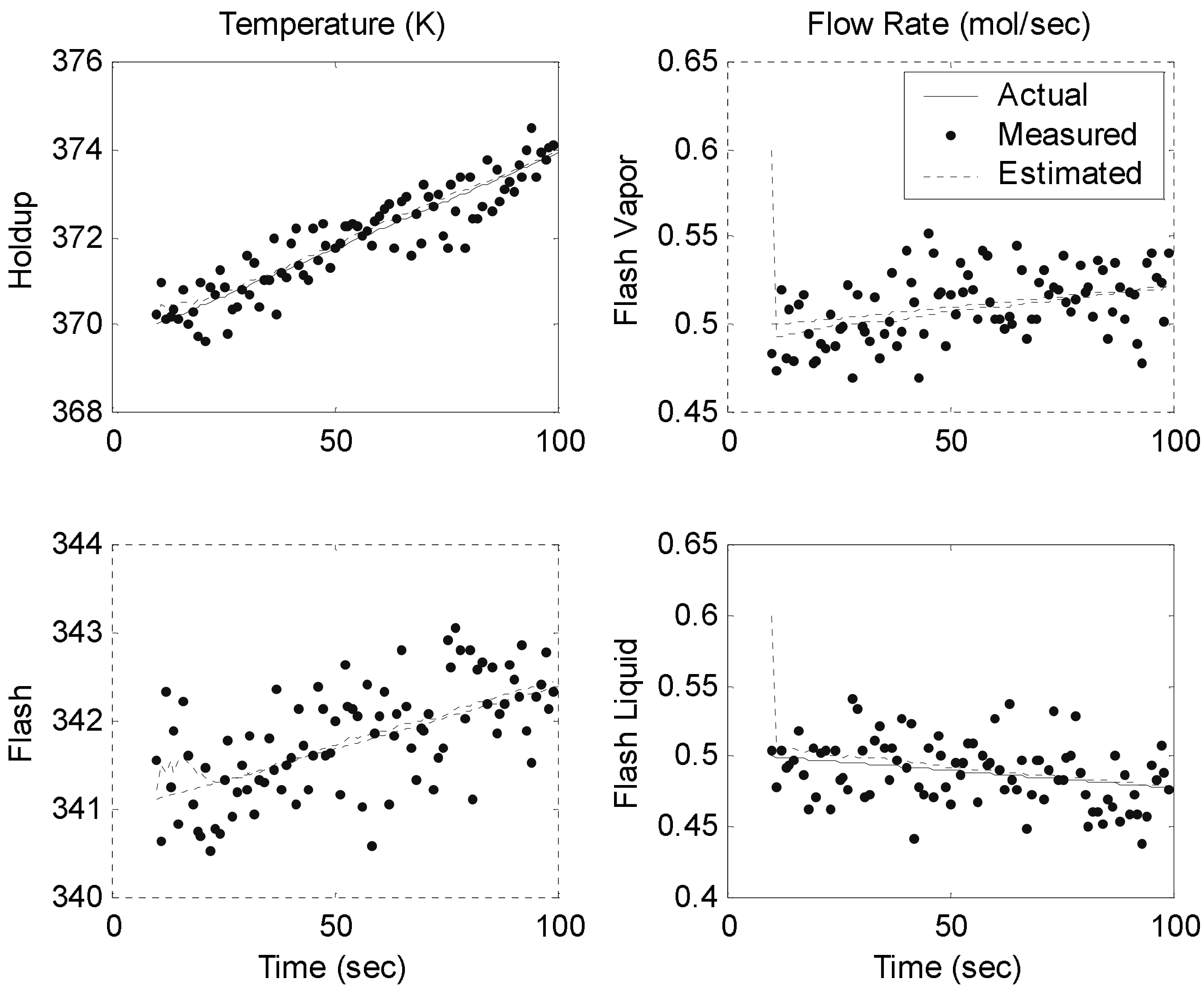
  T_{tank} σ_{noise}=0.5
  dn/dt_{vapor} σ_{noise}=0.02
  T_{flash} σ_{noise}=0.5
  dn/dt_{liquid} σ_{noise}=0.02

- Estimation parameters

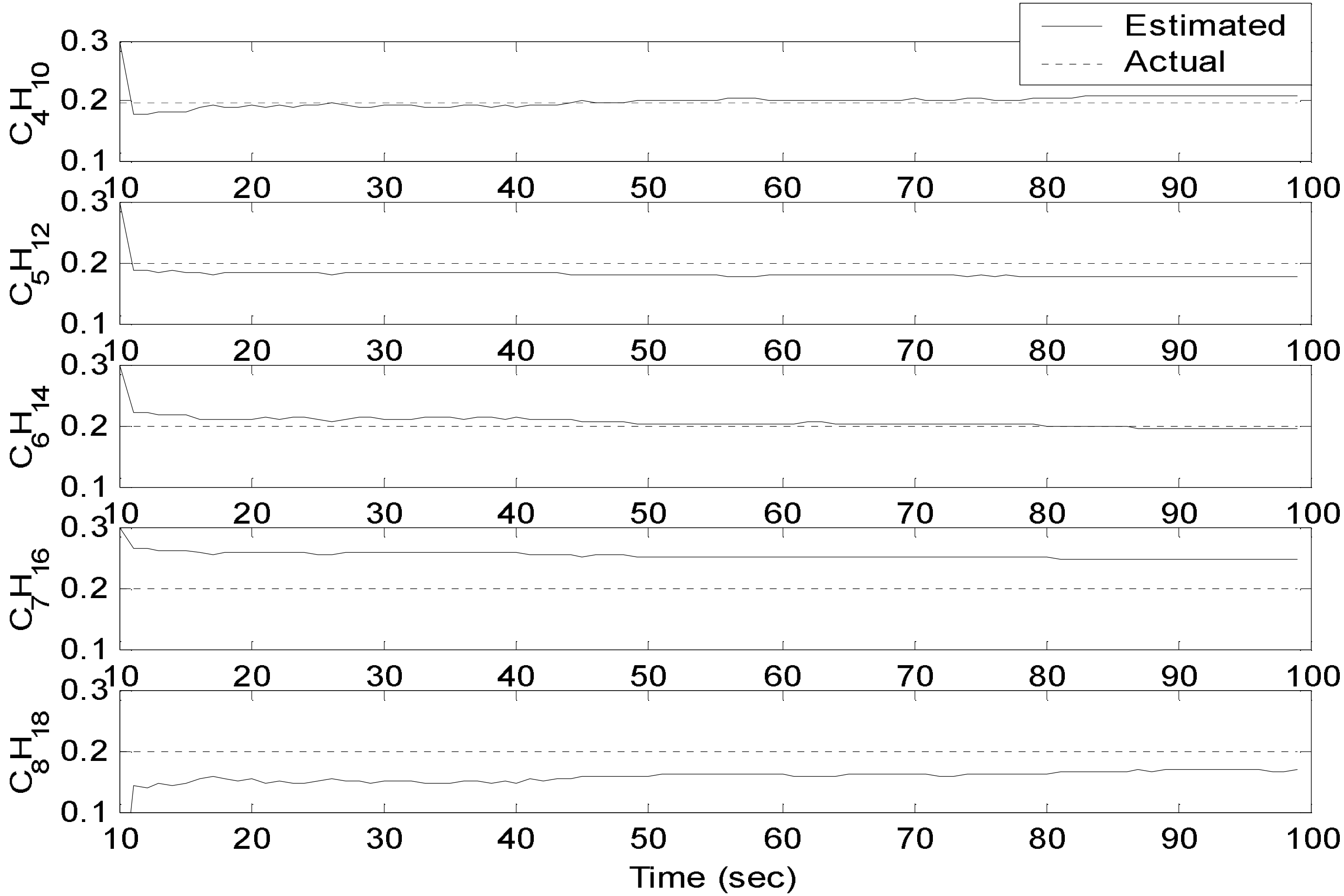
  α=0.5 (forgetting factor – weight only on x_0)
  Expanding horizon (up to 90 as new measurements are available)
  Initial state estimates all have a +0.1 absolute error
  Relative initial state errors vary (50% for mole fractions) (0.03% for temperatures)

- Observability criteria
  - Dynamic modes (5)
    - States: Temperature (1), Mole Fractions (4)
  - Observability matrix rank (3)
  - Conclusion: Not fully observable, but some information may be reconstructed to give estimates that are better than the initial guesses

Composition Estimation Measurements



Partially Observable Compositions

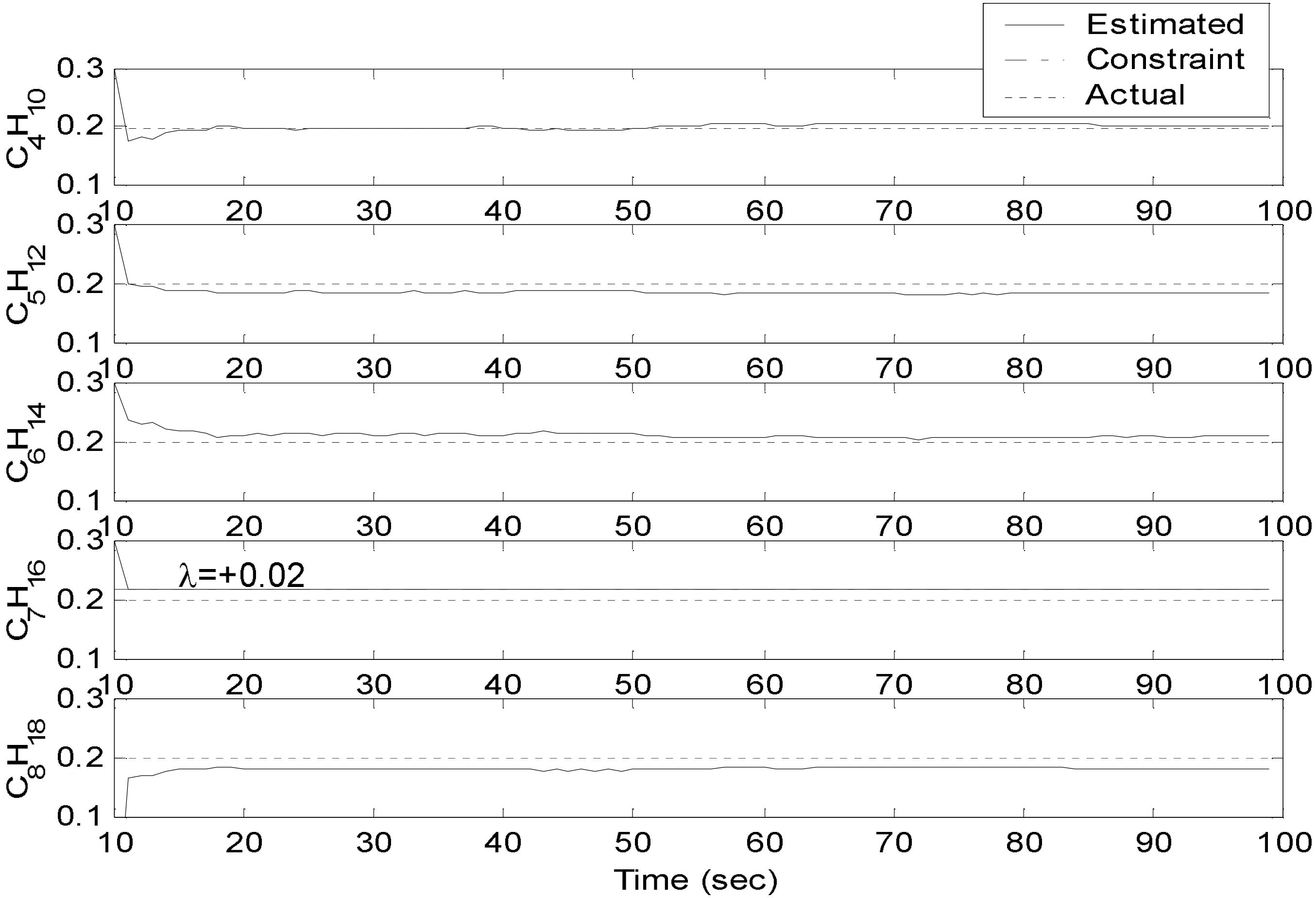


The results are better than the initial estimates but, as indicated by the rank deficiency of the observability matrix (3/5), the system is not fully observable – all states deviate from correct values, some more than others

Constraints and Observability

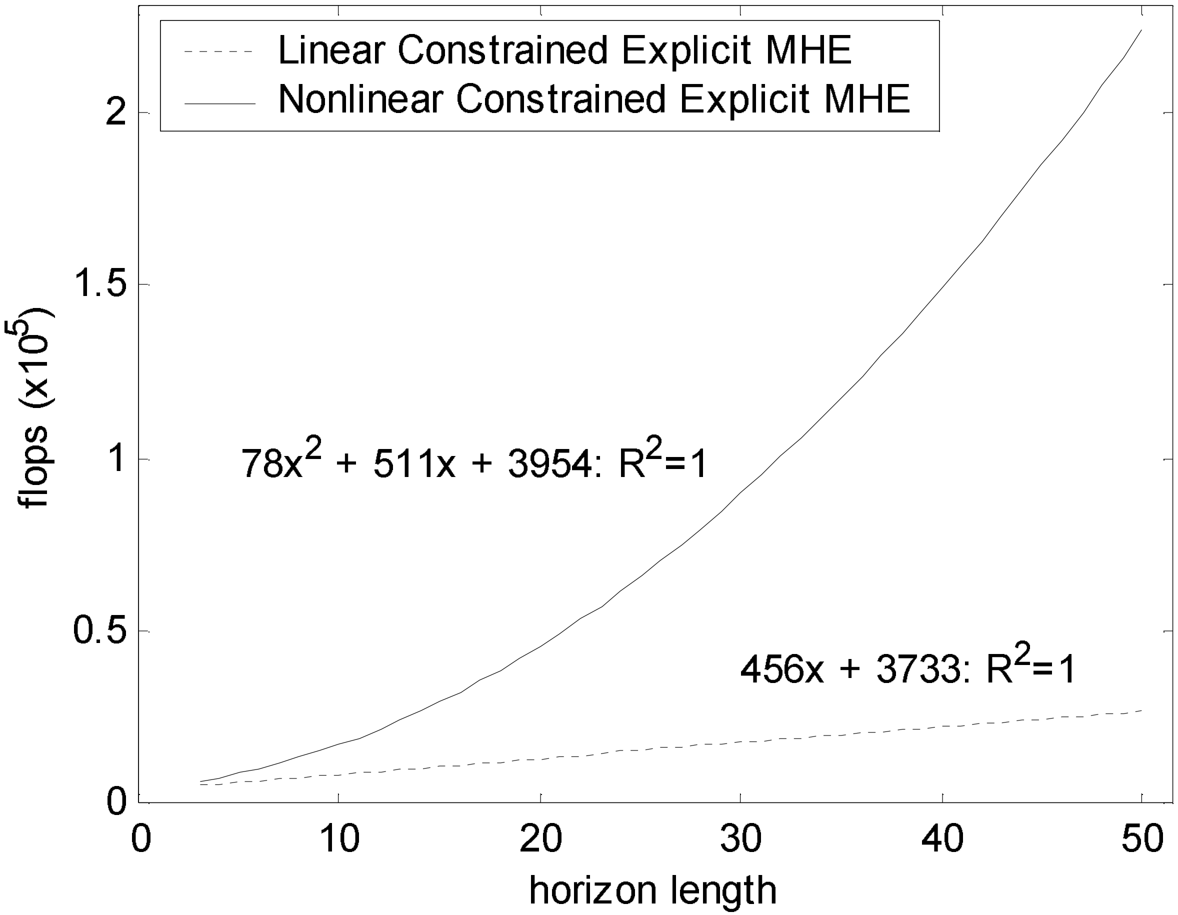
- Suppose you know that the mole fraction of C_7H_{16} should not be above 0.22
- Incorporate this knowledge into the state estimation by adding a constraint to the least squares problem
- Because the constraint is active, the system observability (detectability) is improved

Constraint Improves System Observability

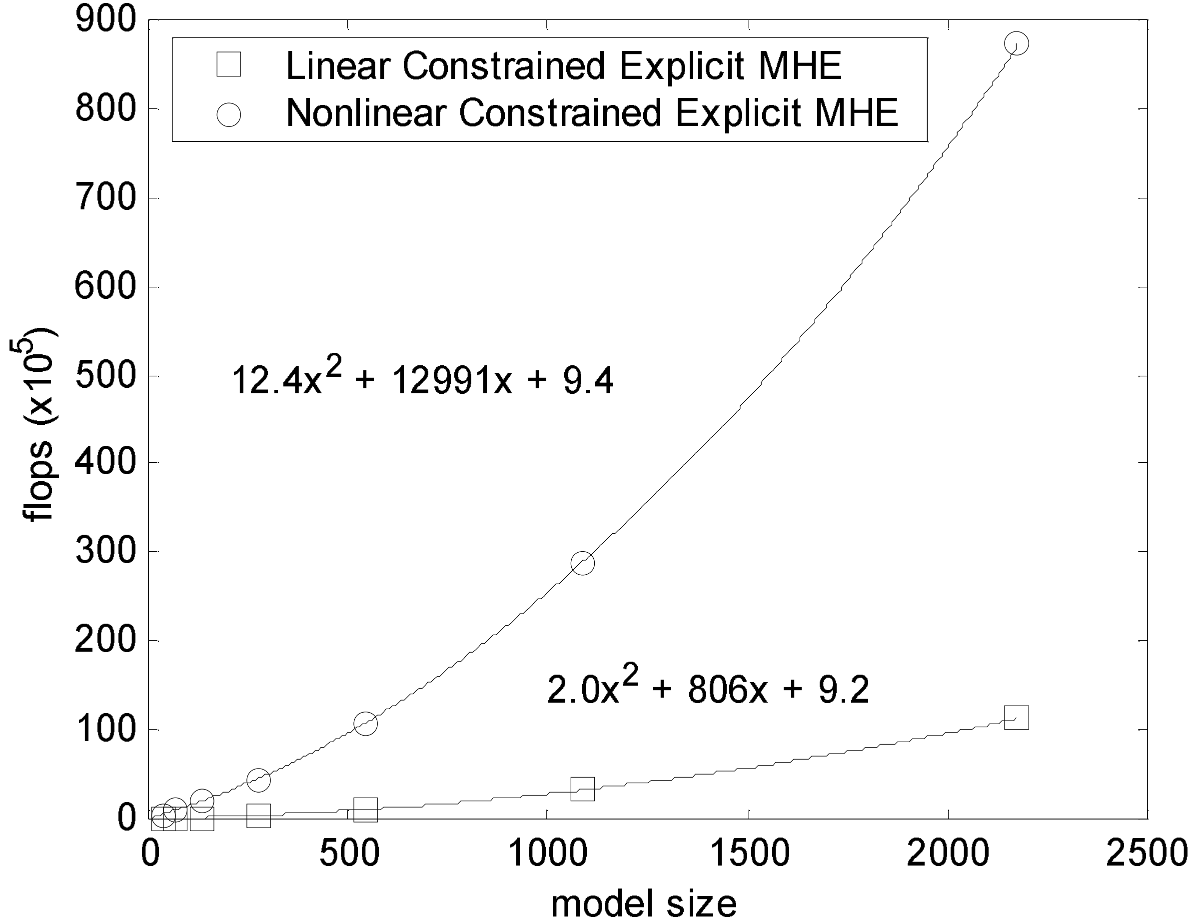


The state estimates are improved, but there is still some deviation from the correct values because the observability matrix is still not full rank (4/5)

Horizon Length Scaling (17 State Model)



Model Size Scaling (Horizon=50)



Conclusions

- New solution approach for MHE problems with upper and lower bounds on the variables
- Applicable for state estimation of any process described by an ODE or index-1 DAE
- Constrained Explicit MHE scaling to large scale problems
  - Nonlinear model
    - $O(n_H^2)$ with increasing horizon length
    - $O(n_v^2)$ with number of variables
  - Linear model
    - $O(n_H)$ with increasing horizon length
    - $O(n_v^2)$ with number of variables
  - Example demonstrates >10,000*x* speed up over MHE solved with optimization software
- Future work
  - Simultaneous state and parameter estimation