An Investigation into the Nonlinearity of Polyethylene Reactor Operation

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Outline

- Motivation
- Background: nonlinearity measures
- Scaling
- Introduce the polyethylene model
- Examples - Visual Interpretation of Curvature
- Measuring Curvature of the Polyethylene Model
- Controller Performance
- Summary
- Conclusions and Recommendations

Motivation

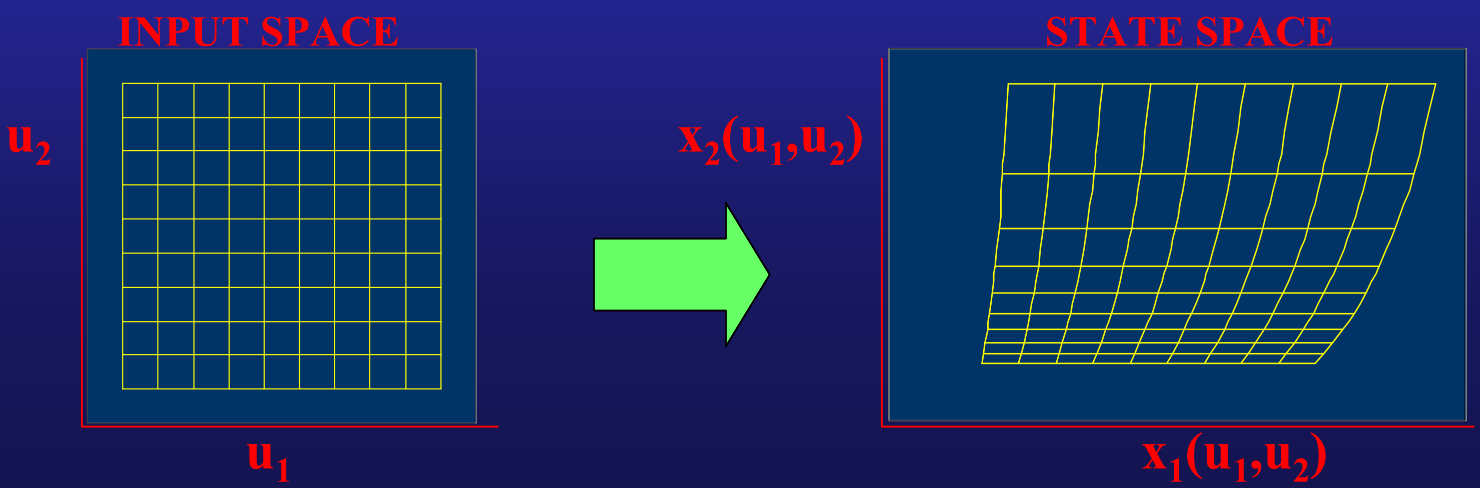
- inherent nonlinearity of chemical processes
  - bilinear -- bulk flow; exponential + ratios -- kinetics with adsorption; power law -- heat transfer ...
- linear control techniques more immediately accessible
  - mathematical framework and knowledge base in control practice
- *are there performance costs associated with relying on linear techniques?*
- **broad goal** - efficient allocation of control engineering resources
- a number of measures of nonlinearity have been proposed
- **specific goal** - examine nonlinearity of industrial process - gas-phase polyethylene reactor - product property control
  - fundamental model available - McAuley (1992)

Measures of Nonlinearity

- linearity properties - scaling - graphical test
- changes in linear approximations
    - Ogunnaike et al.
- deviations of linear approximations from full nonlinear behaviour
  – Allgower, Nikolaou
- curvature assessment using derivative information
  – Guay et al.
- **optimal control structure - closed-loop approach**
  – Stack and Doyle III

Nonlinearity and The Steady-State Locus

- The steady-state locus, $\Xi(\mathbf{u})$, is a hyper-surface that describes steady-state input/state behaviour
- $\Xi(\mathbf{u})$ is parameterized by P inputs and resides in N-dimensional state space
- Nonlinearity assessment is done by examining the local geometry of the steady-state locus - Guay et al. (1995)



Manifestation of Nonlinearity

There are two types of nonlinearity:

1) Parameter effects, or tangential acceleration

2) Intrinsic nonlinearity, or the normal component of nonlinearity

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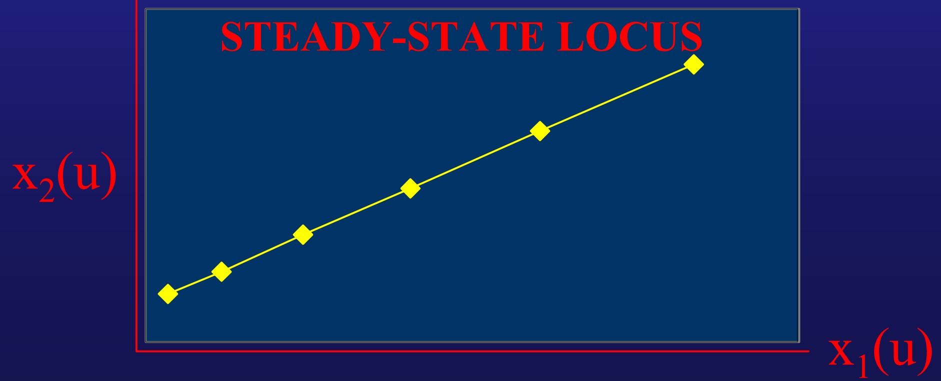
1) Tangential Acceleration

- Due to the change in *magnitude* of the model gains
- Presents itself as non-uniform spacing of points on the steady-state locus



Manifestation of Nonlinearity

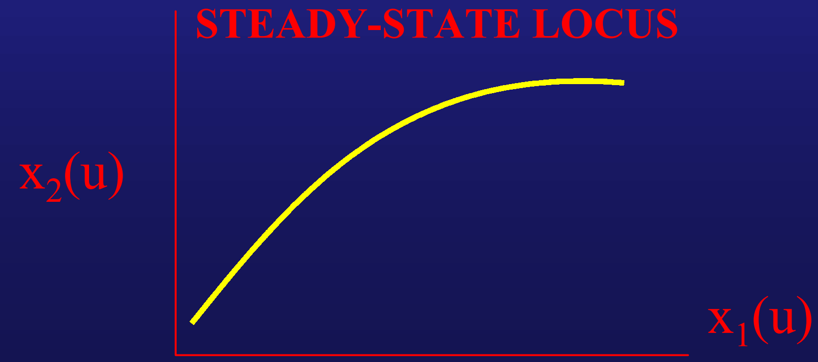
There are two types of nonlinearity:

1) Parameter effects, or tangential acceleration

2) Intrinsic nonlinearity, or normal component of nonlinearity

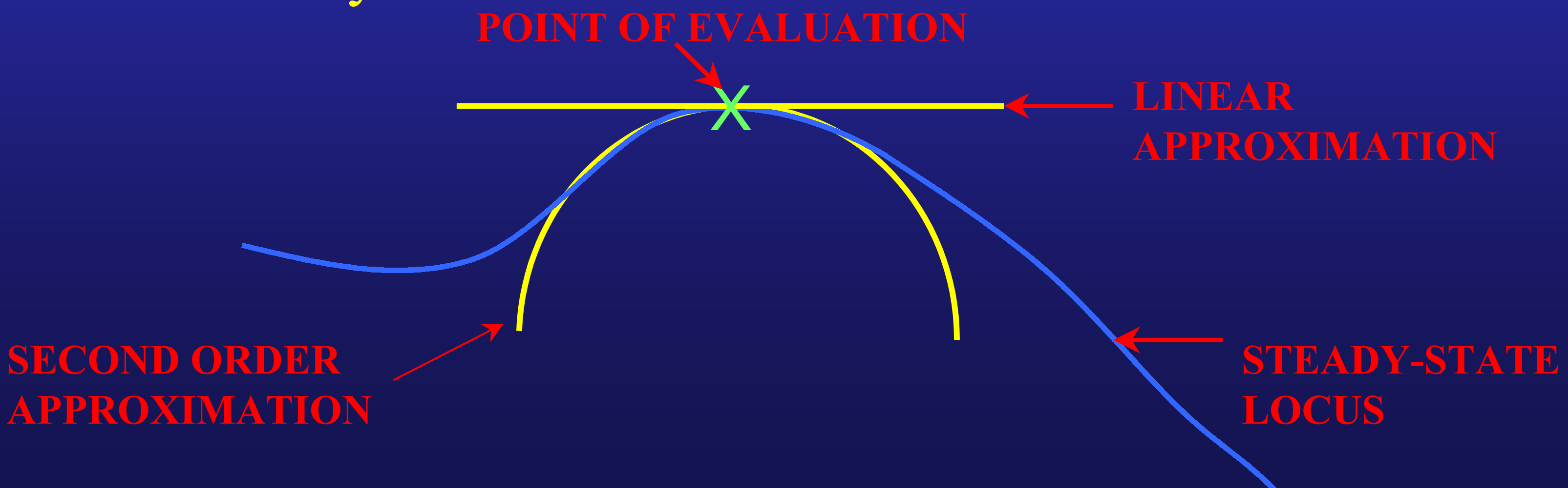
2) Normal Component of Nonlinearity

- Due to the change in *direction* of the model gains
- Presents itself as the curvature of the steady state locus relative to the surrounding state space.
- Present only if P<N



Assessing Nonlinearity

- A model is nonlinear if a nonzero second derivative with respect to inputs exists
- $\Xi(\mathbf{u})$ is locally approximated by first and second order Taylor series expansions
- The degree to which the first order approximation differs from the second order approximation gives an indication of nonlinearity.



Assessing Nonlinearity

- The degree of nonlinearity is evaluated by comparing the magnitude of the second order terms to the magnitude of the first order terms of the Taylor series approximation
- The first order terms (linear terms) are velocities, or gains:

$$\dot{\mathbf{v}}_i = \frac{\partial \Xi(\mathbf{u})}{\partial u_i}, \quad 1 \le i \le P$$

- The second order terms (nonlinear terms) are accelerations:

$$\ddot{\mathbf{v}}_{pq} = \frac{\partial^2 \Xi(\mathbf{u})}{\partial u_p \partial u_q}, \quad 1 \le \{p,q\} \le P$$

- The curvature, c_e, of $\Xi(\mathbf{u})$ in a specific input direction, e is:

$$\mathrm{c_e} = \frac{\left\|\mathrm{acceleration_e}\right\|}{\left\|\mathrm{velocity_e}\right\|^2}$$

A Measure of Average Nonlinearity

- c_e is a measure of curvature along a specific input direction, e

$$c_e = \frac{\left\| \text{acceleration}_e \right\|}{\left\| \text{velocity}_e \right\|^2}$$

- A more useful technique would be to average the curvature over the entire operating region
- Root Mean Square curvature (c_{RMS}) integrates curvature over all input directions.
- Guay, McLellan and Bacon (1995) suggested that significant nonlinearity is indicated by a $c_{RMS} > 0.3$

Scaling

- Scale to reflect intended operating region
- Scaling removes the unit dependence of RMS curvature on state variables
- RMS curvatures are based on a standard scaling which affords a generic measure of nonlinearity
- The intended region of operation is approximated by an ellipsoid

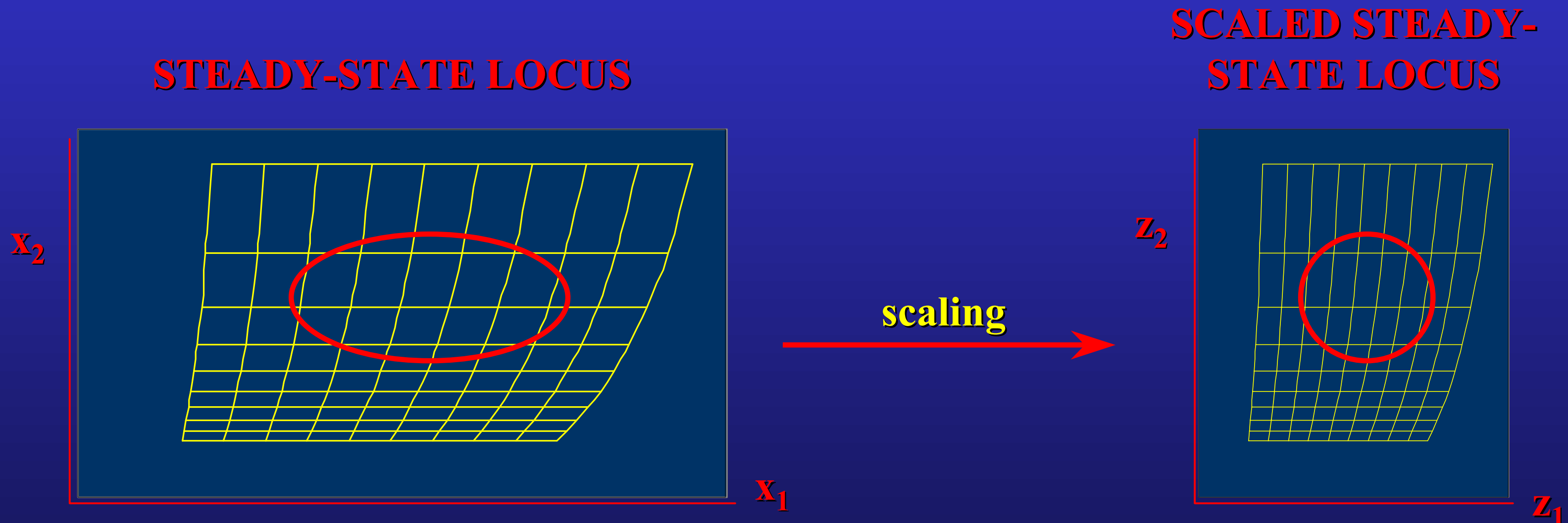
$$\Delta\mathbf{x}'(\mathbf{S}'\mathbf{S})\Delta\mathbf{x} = 1 \quad \text{where} \quad \Delta\mathbf{x} = \mathbf{x} - \mathbf{x}_0, \quad \mathbf{S} = \text{scaling matrix}$$

- Scale ellipsoidal region to unit spheroid (Guay et al., 1995)

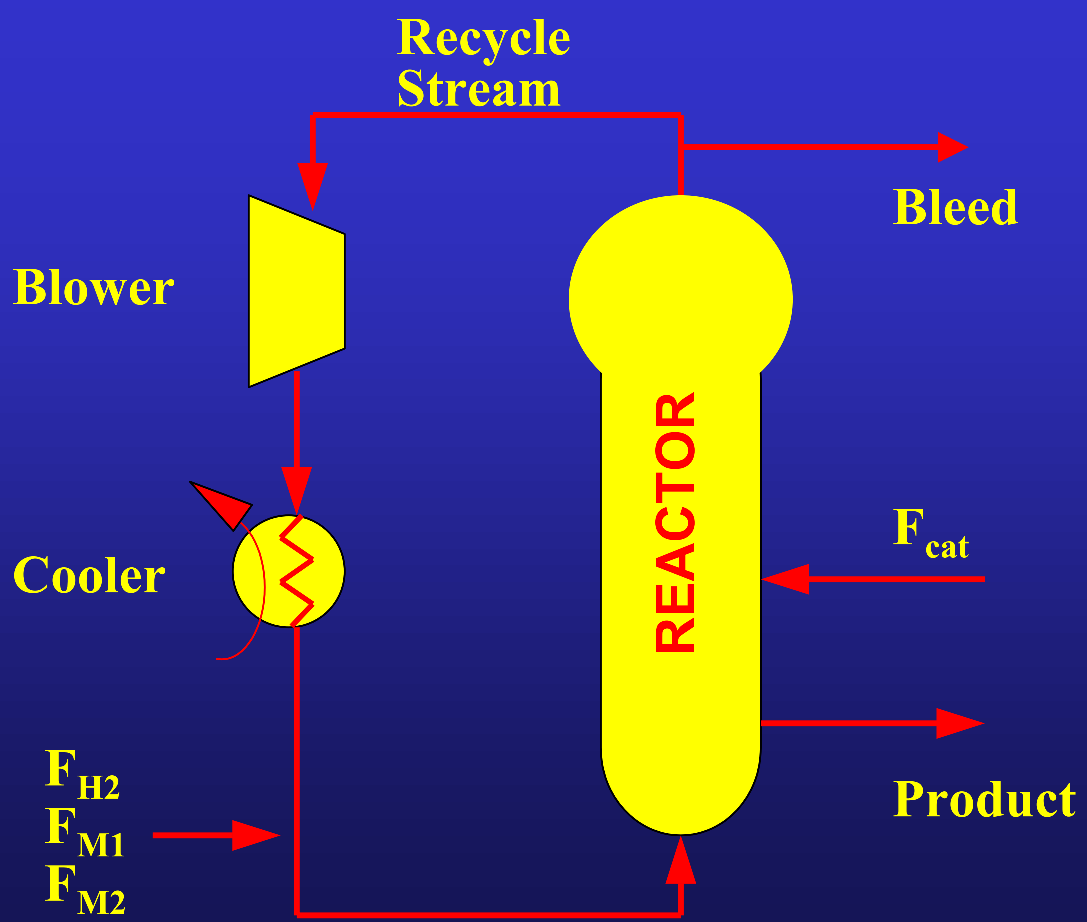
$$\mathbf{z}'\mathbf{z} = 1 \quad \text{where} \quad \mathbf{z} = \mathbf{S}\Delta\mathbf{x}$$

Scaling

- RMS curvatures are calculated based on the unit sphere scaling



Polyethylene Reactor



Polyethylene
Gas Mass Balance Model

$$\frac{d[H_2]}{dt} = 0 = \frac{1}{Vg}\left(F_{H2} - \frac{k_h \cdot F_{cat} \cdot a_{cat} \cdot [H_2]}{\frac{PR}{Bw} + k_d} - \frac{[H_2] \cdot b}{C_t} - gl \cdot [H_2] \right)$$

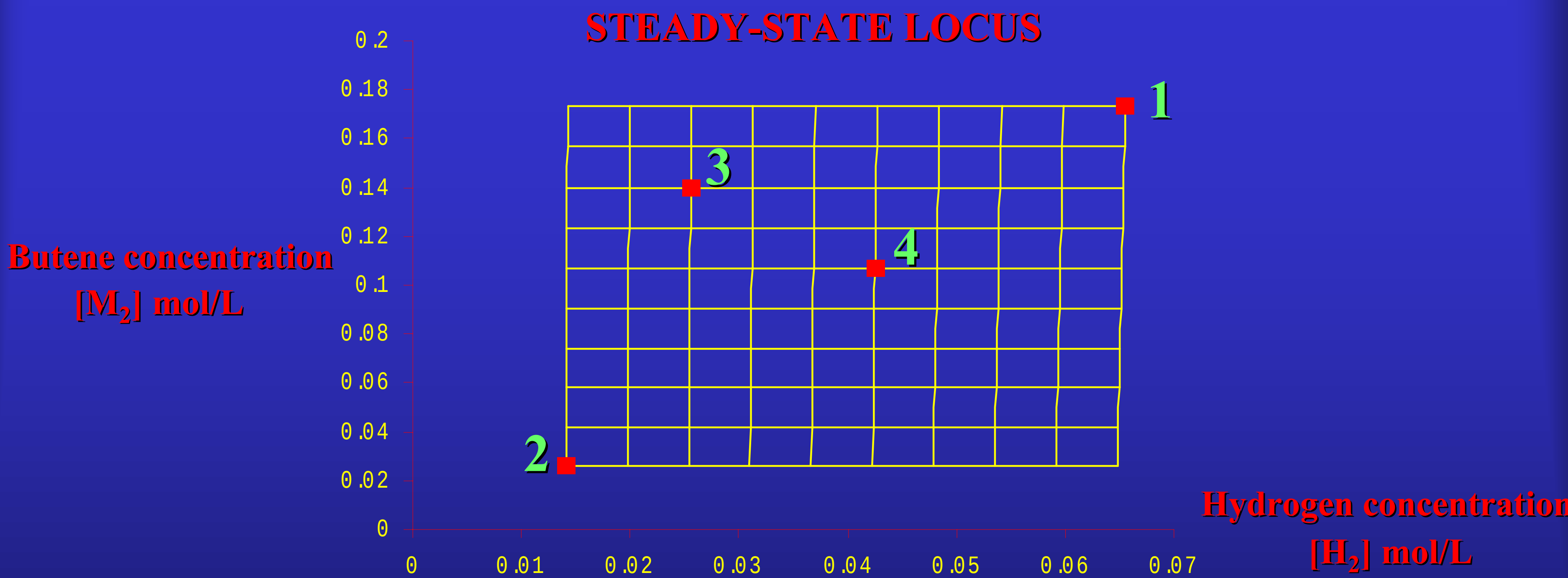
$$\frac{d[M_2]}{dt} = 0 = \frac{1}{Vg + Vs}\left(F_{M2} - \frac{k_{p2} \cdot F_{cat} \cdot a_{cat} \cdot [M_2]}{\frac{PR}{Bw} + k_d} - \frac{[M_2]b}{C_t} - S[M_2]PR \right)$$

$$\frac{dBw}{dt} = 0 = F_{cat} a_{cat} \frac{\left(k_{p1}[M_1]mw_1 + k_{p2}[M_2]mw_2\right)}{\frac{PR}{Bw} + k_d} - PR$$

Assumptions:

- The total concentration C_t, and ethylene concentration $[M_1]$, are held constant by control
- The bleed flow is kept constant by a flow controller
- The reactor is operating under perfect bed weight control
- Temperature effects are negligible

Visualizing Curvature - Example 1



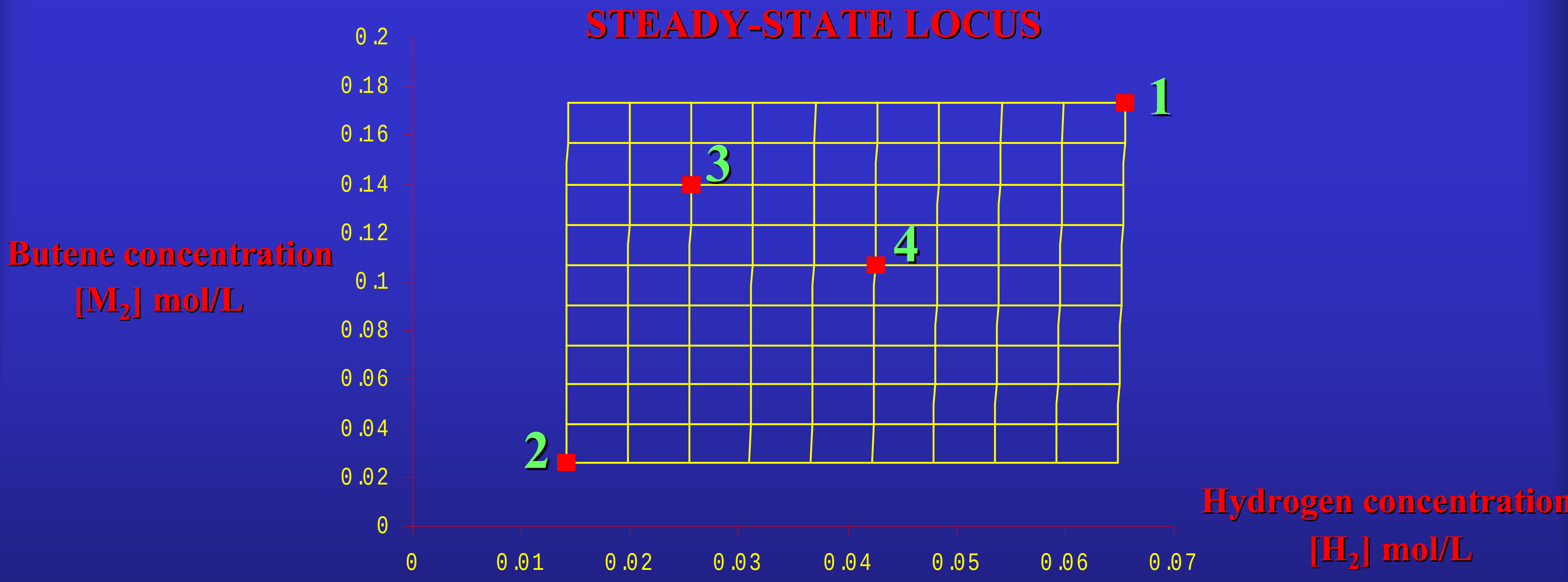
Input conditions:

$F_{cat} = 5.6$ kg/h, Fixed

$500 \le F_{H2} \le 2300$ mol/h, Varying

$10000 \le F_{M2} \le 64000$ mol/h, Varying

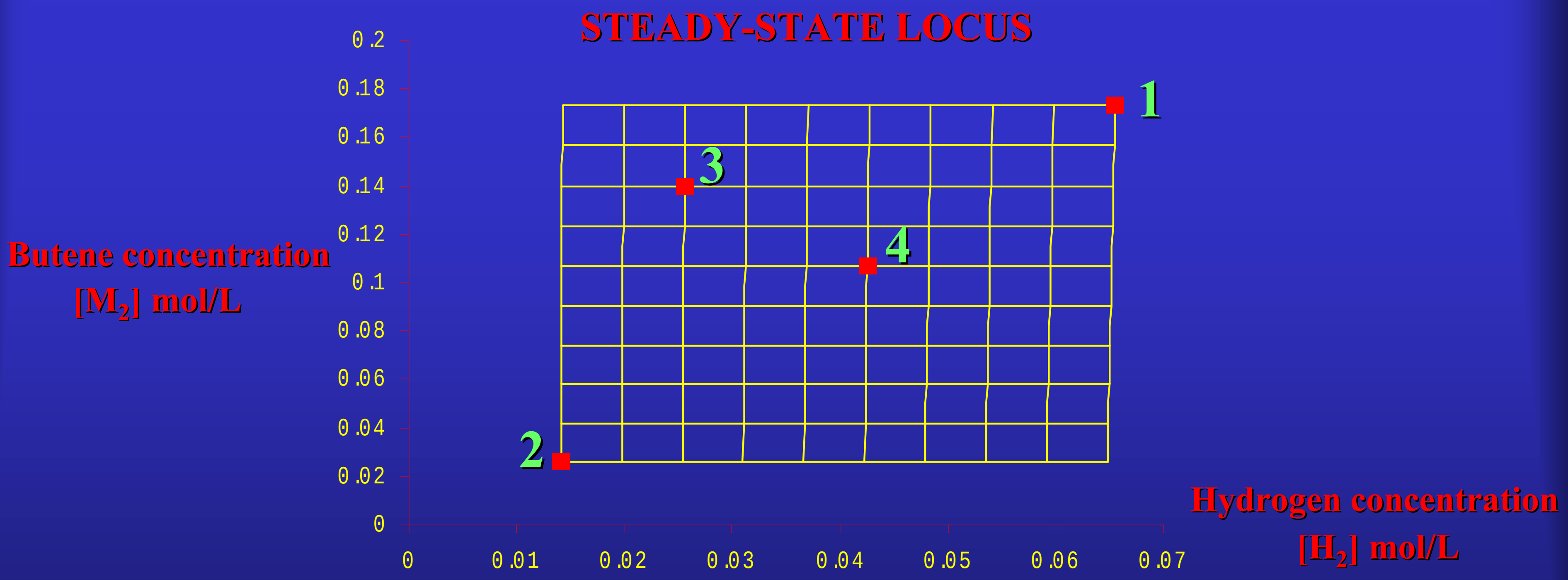
Visualizing Curvature - Example 1



Visual Inspection

- no curve to constant input lines
- equally spaced points
- implies little or no nonlinearity

Visualizing Curvature - Example 1

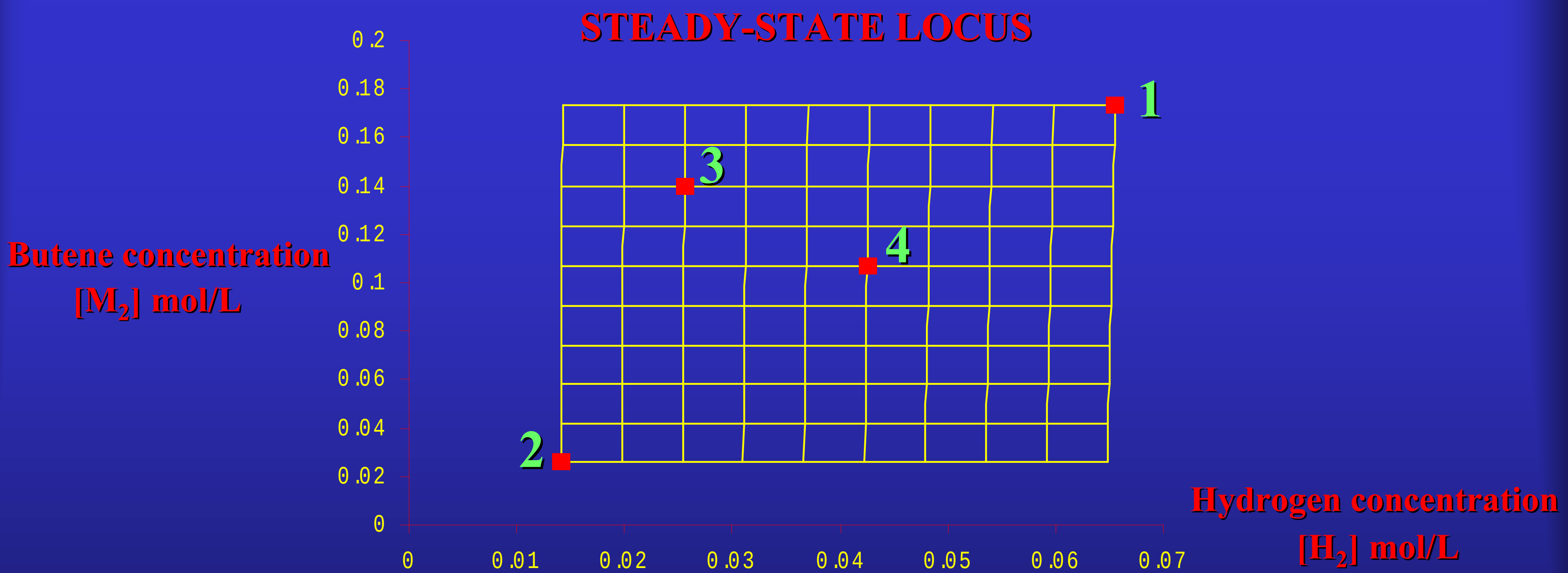


Visual Inspection

- no curve to constant input lines
- equally spaced points
- implies little or no nonlinearity

Point	RMS value
1	0.023
2	0.024
3	0.023
4	0.024

Visualizing Curvature - Example 1

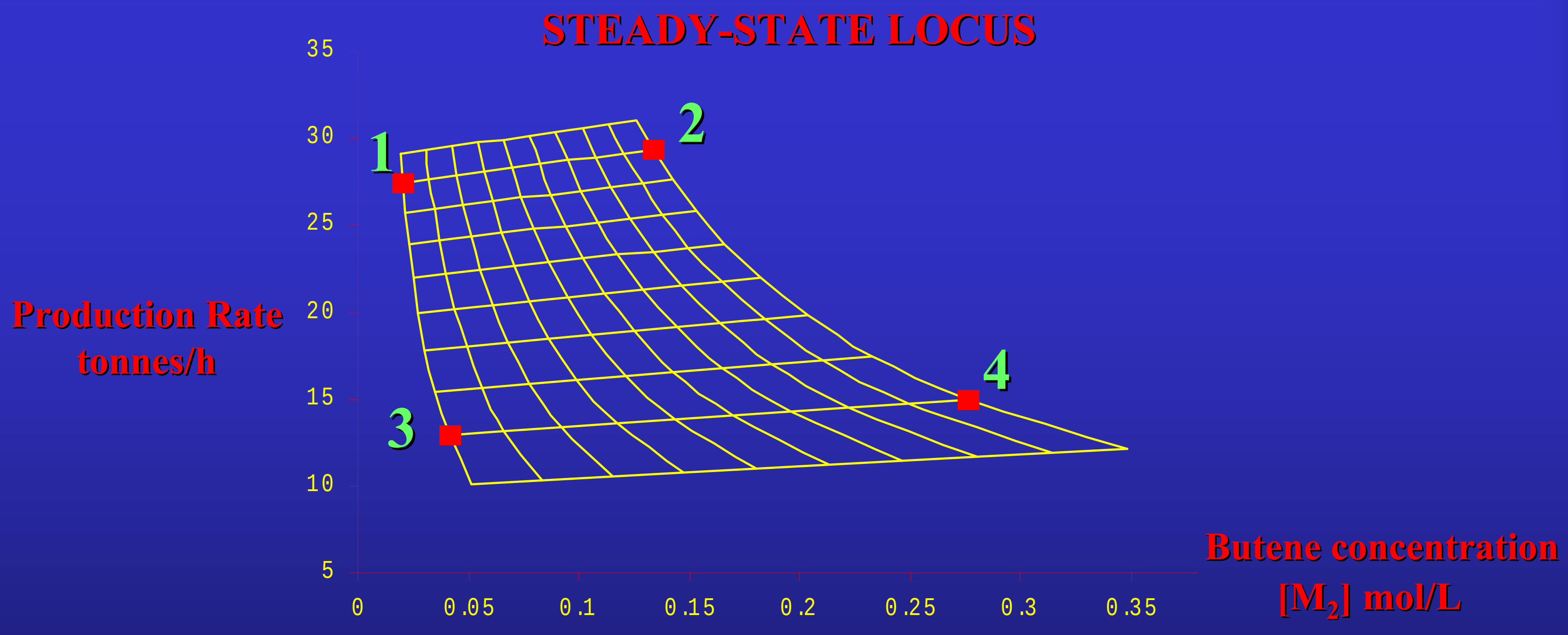


Control Expectation:

Control of this system should be accomplished well with a linear controller

Point	RMS value
1	0.023
2	0.024
3	0.023
4	0.024

Visualizing Curvature - Example 2



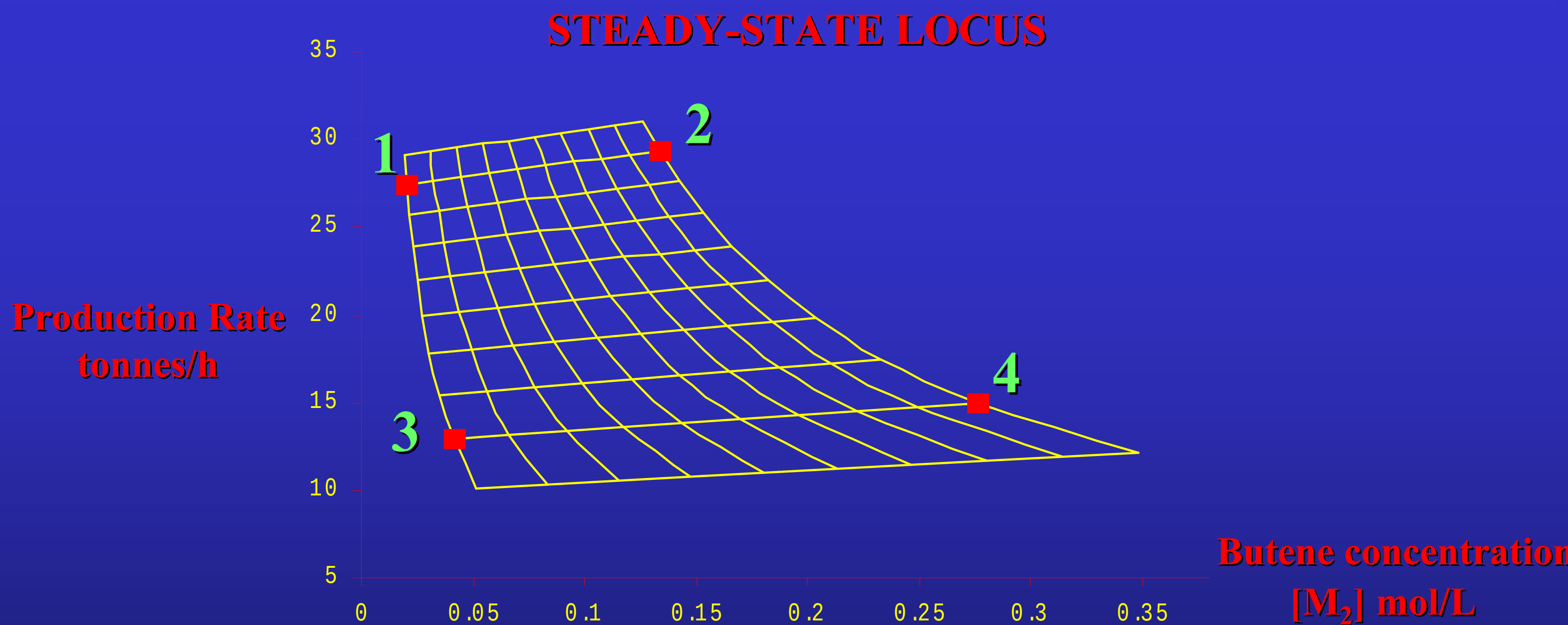
Input conditions:

F_{H2} = 1500 mol/h, Fixed

$2.0 \le F_{cat} \le 9.2$ kg/h, Varying

$10000 \le F_{M2} \le 64000$mol/h, Varying

Visualizing Curvature - Example 2

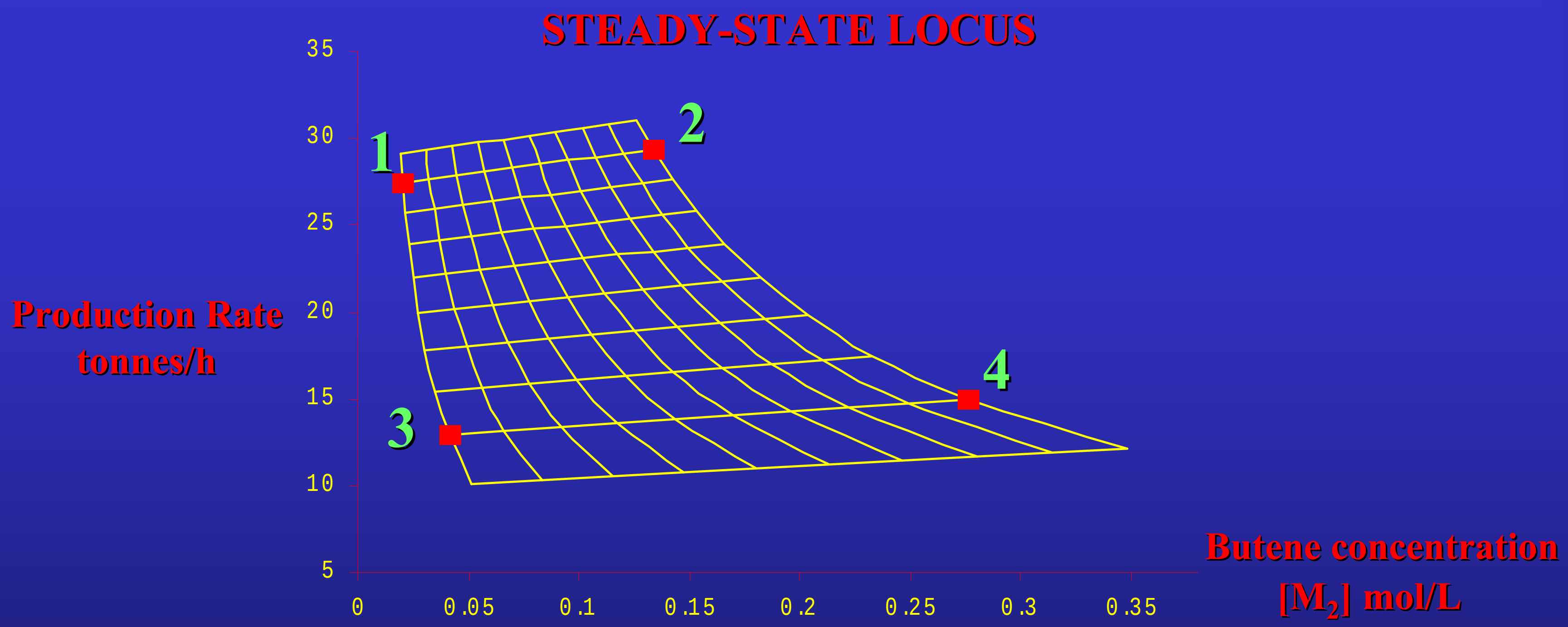


Visual inspection

- Point 1 shows the least curve in the constant input lines. Also most even spacing of lines

Point	RMS value
1	0.23

Visualizing Curvature - Example 2

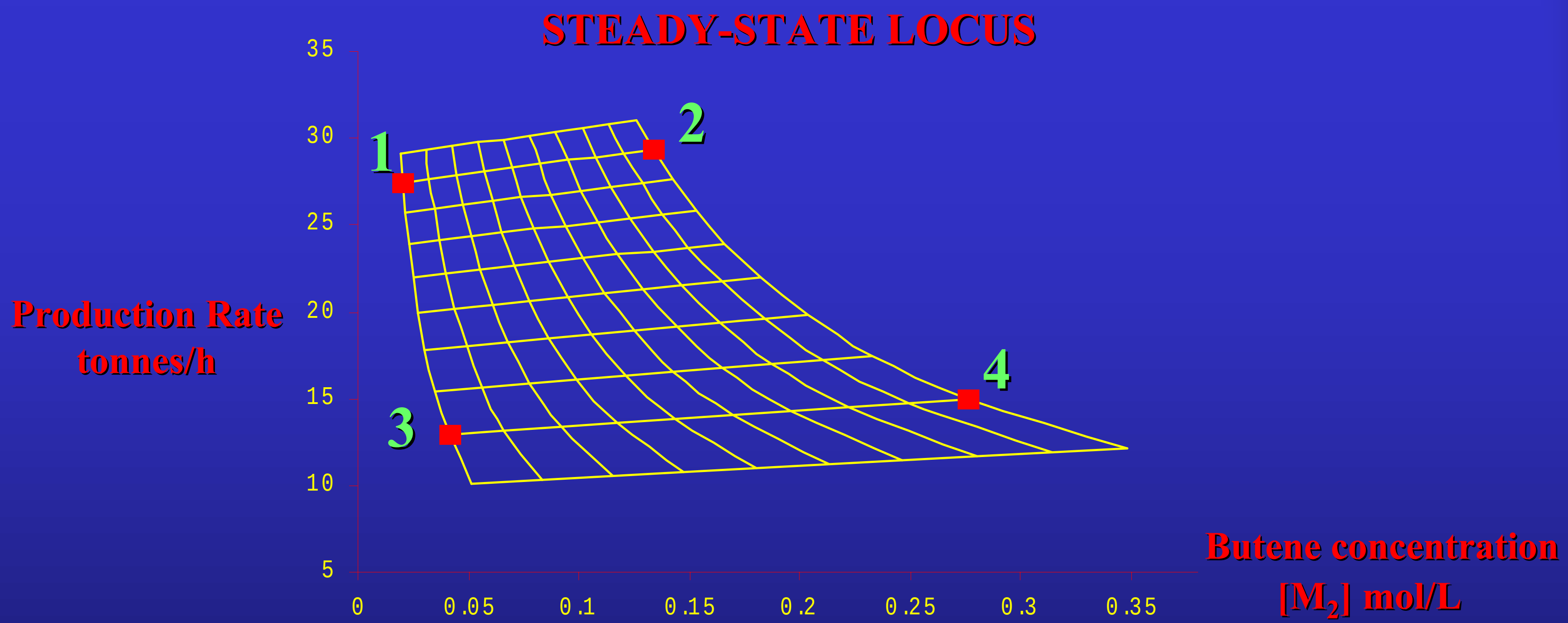


Point	RMS value
1	0.23
2	0.31

Visual inspection

- Point 1 shows the least curve in the constant input lines. Also most even spacing of lines.
- Point 2 has a bit more curve to the constant input line. Perhaps slightly more uneven spacing.

Visualizing Curvature - Example 2

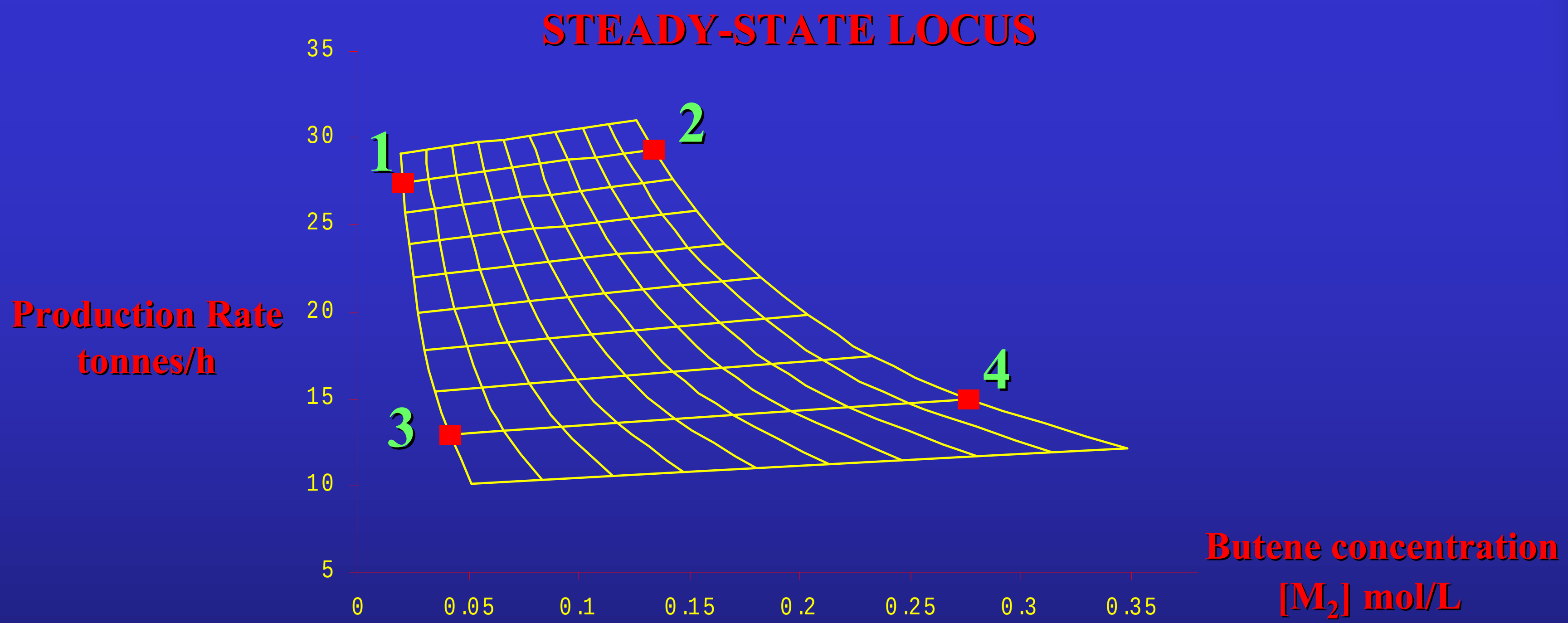


Visual inspection

- Point 3 shows more uneven spacing and more curve of constant input lines than at point 1

Point	RMS value
1	0.23
2	0.31
3	0.76

Visualizing Curvature - Example 2

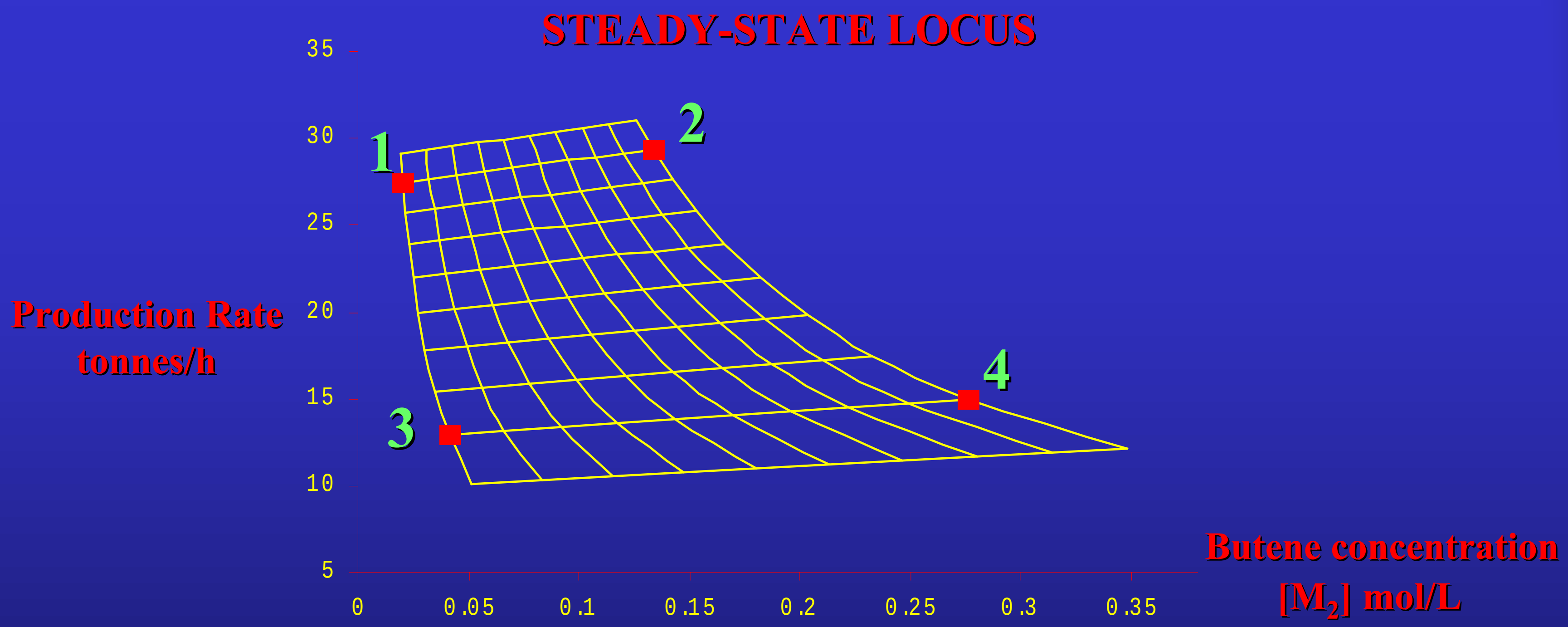


Visual inspection

- Point 3 shows more uneven spacing and more curve of constant input lines than at point 1
- Point 4 displays most curve and the most uneven spacing

Point	RMS value
1	0.23
2	0.31
3	0.76
4	1.90

Visualizing Curvature - Example 2



Point	RMS value
1	0.23
2	0.31
3	0.76
4	1.90

Control Expectations:

- If operating at point 1, linear control will suffice.
- If operating elsewhere on the locus, a nonlinear controller is highly recommended.

Curvature of the Full P.E. Model

- Polyethylene product property model
- The full PE reactor model consists of:
  - a dynamic gas mass balance of the form:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u})$$

  - a static output mapping of the form:

$$\mathbf{y} = \mathbf{h}(\mathbf{x})$$

» melt index

» density

» production rate

The Full Polyethylene Reactor Model

$$\frac{d[H_2]}{dt} = \frac{1}{Vg}\left(F_{H2} - k_H \cdot Y \cdot [H_2] - \frac{[H_2]\cdot b}{C_t} - gl \cdot [H_2] \right)$$

$$\frac{d[M_2]}{dt} = \frac{1}{Vg+Vs}\left(F_{M2} - k_{p2} \cdot Y \cdot [M_2] - \frac{[M_2]b}{C_t} - S[M_2]Y\left(k_{p1}[M_1]mw_1 + k_{p2}[M_2]mw_2\right) \right)$$

$$\frac{dY}{dt} = F_{cat} \cdot a_{cat} - \frac{Y^2\left(k_{p1}[M_1]mw_1 + k_{p2}[M_2]mw_2\right)}{Bw} - k_d Y$$

$$\ln(MI) = 3.5\ln\left(k_0 + k_1 \frac{[M_2]}{[M_1]} + k_3 \frac{[H_2]}{[M_1]} \right)$$

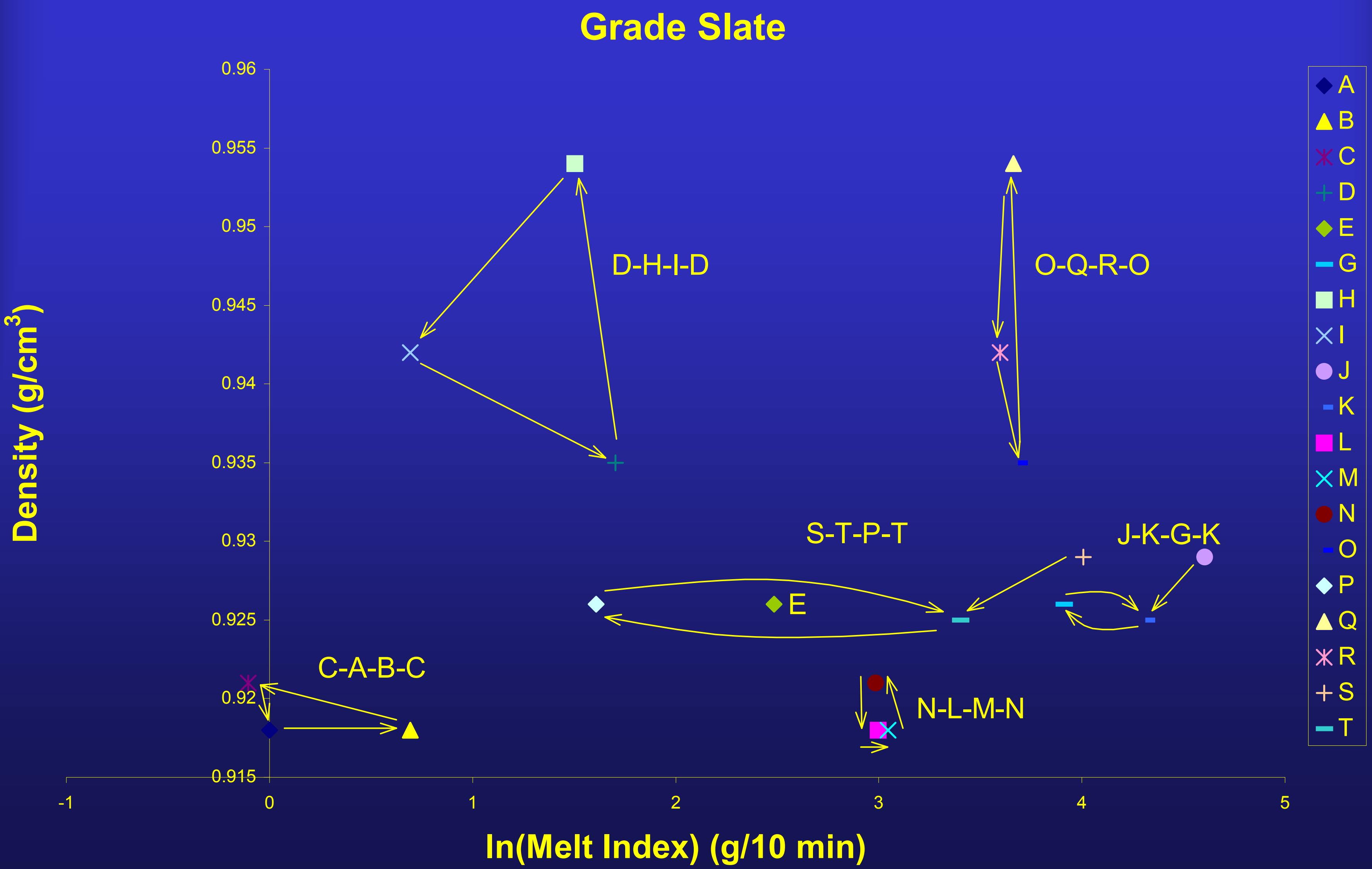
$$\rho = p_0 + p_1 \ln(MI) - \left(p_2 \frac{[M_2]}{[M_1]} \right)^{p_4}$$

$$PR = Y\left(k_{p1}[M_1]mw_1 + k_{p2}[M_2]mw_2\right)$$

Nonlinearity & Performance

- Is steady-state nonlinearity a good indicator of closed-loop performance degradation under linear control?
- Approach
  - design linear and nonlinear controllers
    - » linear output feedback - pole placement on tracking error trajectory
    - » input-output linearizing controller - pole placement on tracking error trajectory
  - simulate under setpoint tracking and disturbance rejection scenarios
  - compare relative performance

Polyethylene Grade Selection



Disturbances for Control Simulations

- 25% increase in a_{cat} (concentration of active sites)
  - due to batch to batch variation
- 25% increase in k_d (deactivation of active sites)
  - due to reactive impurities
- 25% decrease in b (bleed flow)
  - due to operator intervention or pressure changes downstream of the bleed valve

Melt Index Transformation

- Most practitioners use the following model form, because the logarithm transform is thought to provide better linear control:

$$\mathbf{y}(\mathbf{x}) = \begin{bmatrix} \ln(MI) \\ \rho \\ PR \end{bmatrix}$$

- As opposed to the nominal model (non-transformed model):

$$\mathbf{y}(\mathbf{x}) = \begin{bmatrix} MI \\ \rho \\ PR \end{bmatrix}$$

Calculating RMS Curvature

- Note the large difference in RMS curvature between the transformed model and the nominal model:

Grade Transition	Curvature Transformed Model	Curvature Nominal Model
S -T-P-T	0.813	117
D-H-I-D	0.951	14.0
C-A-B-C	1.70	6.70
J-K-G-K	2.77	89.6
O-Q-R-O	18.6	20.5
N-L-M-N	70.2	72.4

Linking Nonlinearity to Controller Performance

- have curvature of many regions on the output space
- use this information in comparative controller performance study
- determine if consistent relationship between curvature and linear control performance is observed

Performance Measure

- Designed an error measure that
  - Compares linear to nonlinear control performance
  - Is a generic normalized measure
  - Is based on IAE
- For grade transition simulations, compared the design trajectory to the actual trajectory
  - IAD_{norm}
- For regulatory control simulations, compared the actual output against the set point.
  - IAE_{norm}

Performance Measure

- IAD: Integral of the deviation between designed and actual trajectory
- IAE: Integral of the error between set point and actual trajectory
- Difference between deviations/errors of the linear and nonlinear controllers:
  - $IAD = IAD_{linear} - IAD_{nonlinear}$
  - $IAE = IAE_{linear} - IAE_{nonlinear}$

Performance Measure

- Normalize the performance measure with a nominal deviation/error value
  - For grade transitions:

$$IAD_{norm} = \frac{IAD_{linear} - IAD_{nonlinear}}{IAE_{nominal}}$$

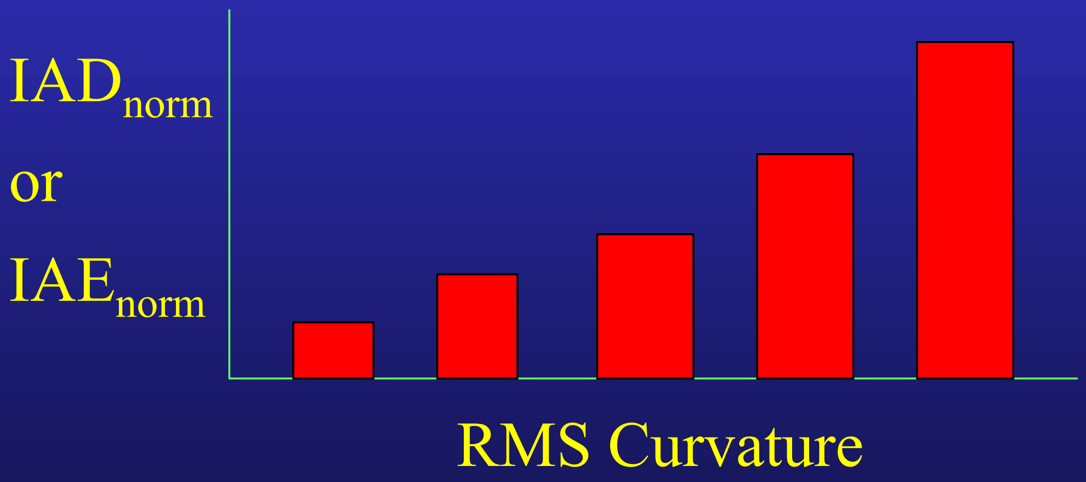
  - For disturbance rejection:

$$IAE_{norm} = \frac{IAE_{linear} - IAE_{nonlinear}}{IAE_{nominal}}$$

  - where $IAE_{nominal} = \int \left| \left(SP - CV_{design} \right) \right| dt$

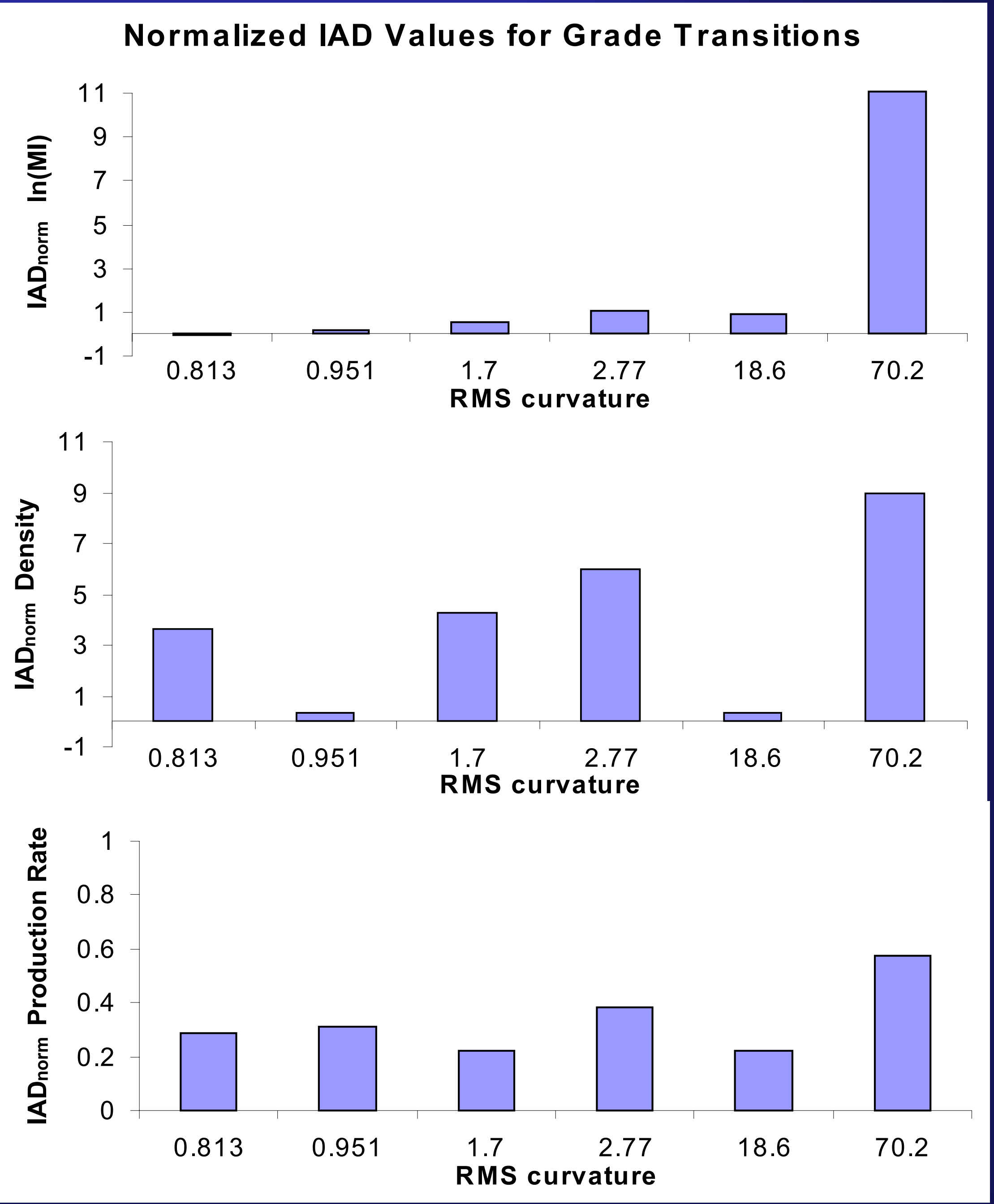
Nonlinearity and Controller Performance

- Expected Relationship:



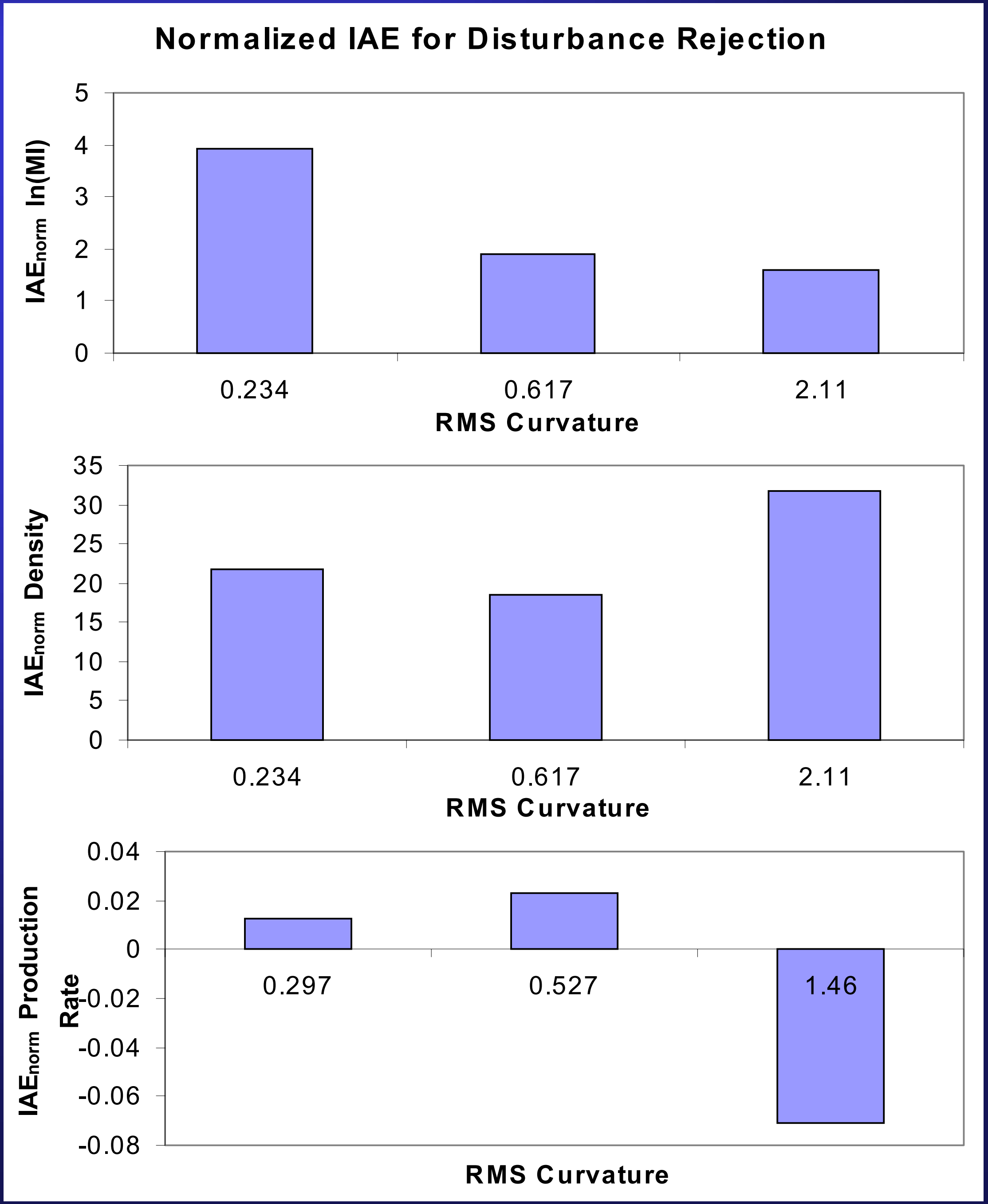
Results

- Grade Transition Simulations



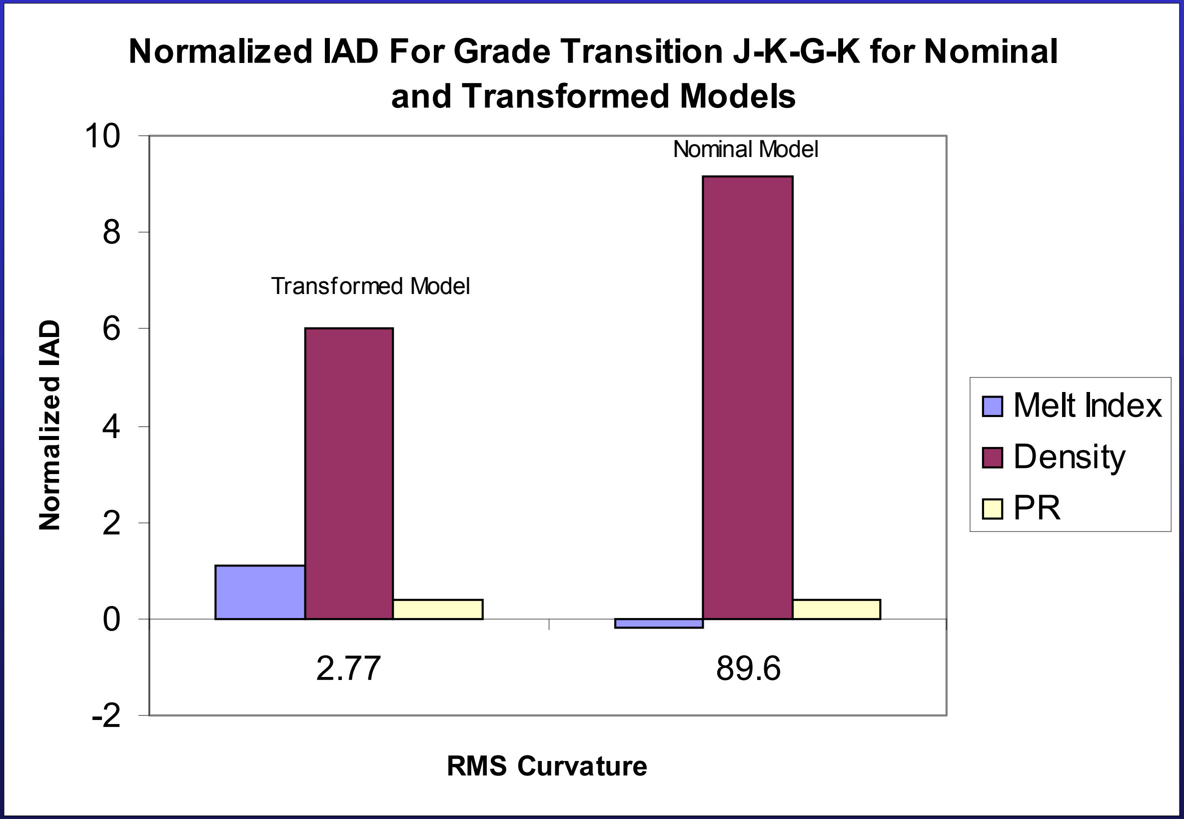
Results

- Disturbance Rejection Simulations



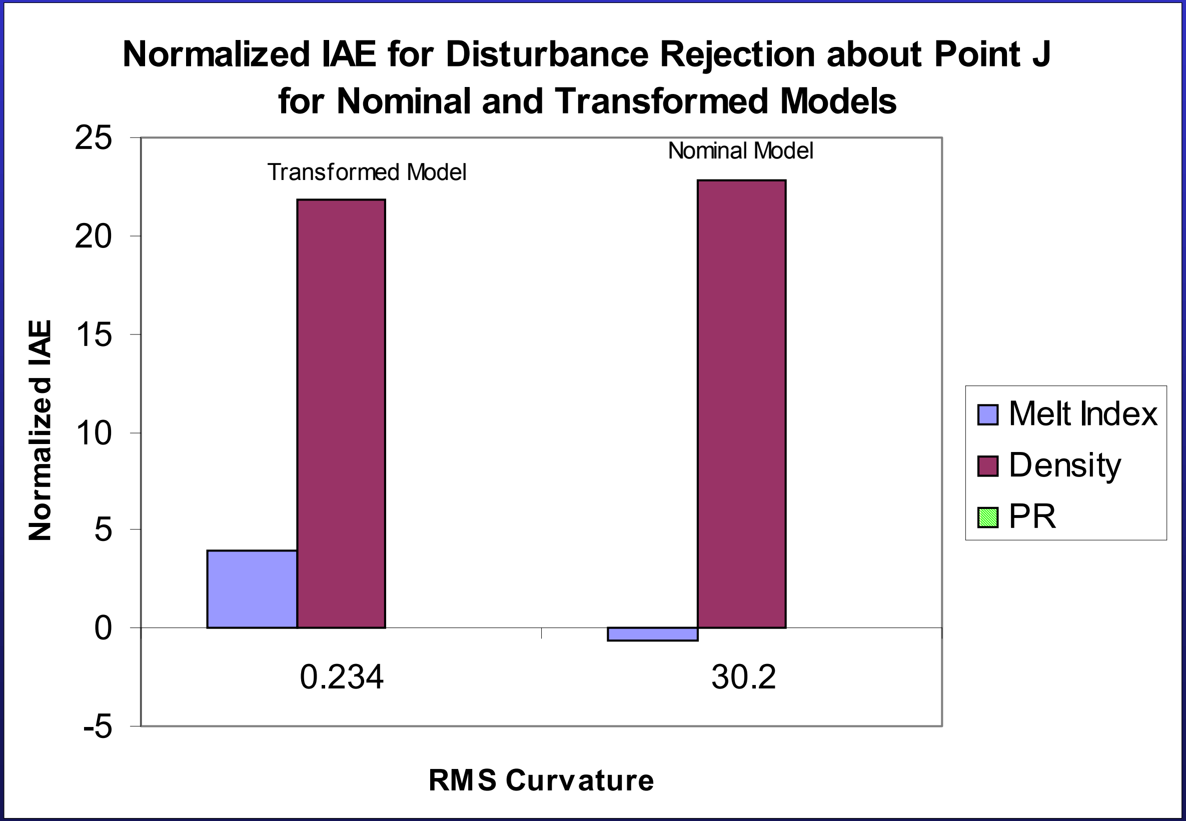
Results

- Grade Transition J-K-G-K
- Transformed vs. Nominal Model



Results

- Regulatory control about point J
- Transformed vs. Nominal Model



Result

- There is no consistent relationship between steady-state curvatures and performance for this example.
- Possible reasons
  - Manipulated Variable Saturation - investigated - no
  - Performance Measure Inappropriate - relative measure defined - consider L_2 measure?
  - Directionality Effects - investigated for specific directions
  - Dynamic vs. Steady-State Curvature?
  - Comparison Measure - accounting for MV action?

Summary

- Nonlinearity measures
- Scaling issues
- Polyethylene model
- Steady-state curvatures
- Curvature and performance depending on operating position and mode
    - grade transitions - “servo problem”
    - disturbance rejection
    - linear state feedback
    - input-output linearization + pole placement

Conclusions

- Mild to moderate nonlinearity was detected in the state (gas mass balance) model
- Mild to severe nonlinearity was detected in the output (full PE) model
- The nominal model (melt index) displays a higher degree of curvature than the transformed model (ln(MI))
- There is no consistent relationship between steady-state curvature and controller performance for this process example.
- Nonlinearity does not always imply degradation at a point
    - approximation error can produce output response with reduced performance cost
    - need to penalize MV input action

Acknowledgement

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