



Quality Control of Polymer Production Processes

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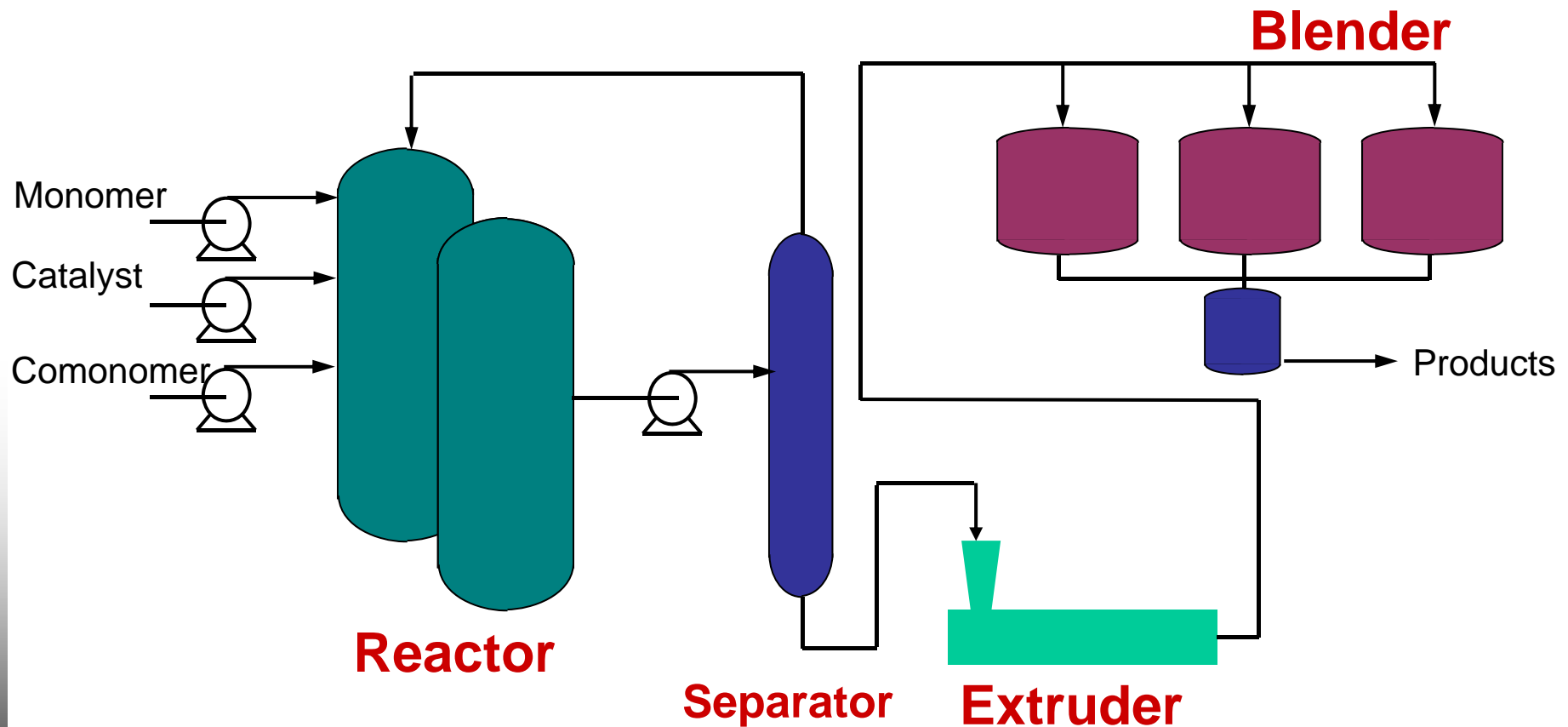
Introduction

- ❑ Polymer plant operation
 - Grade transition
 - Maximizing production
 - Safe operation of reactor

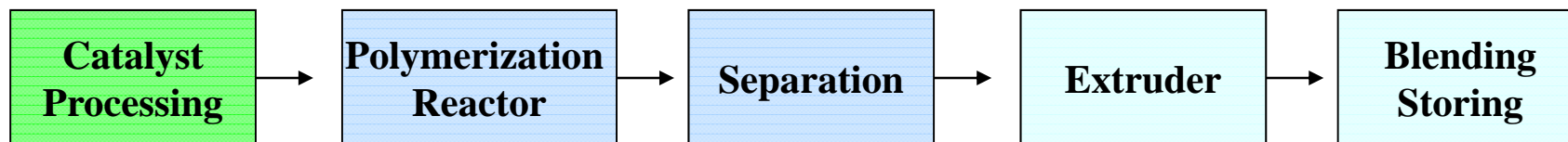
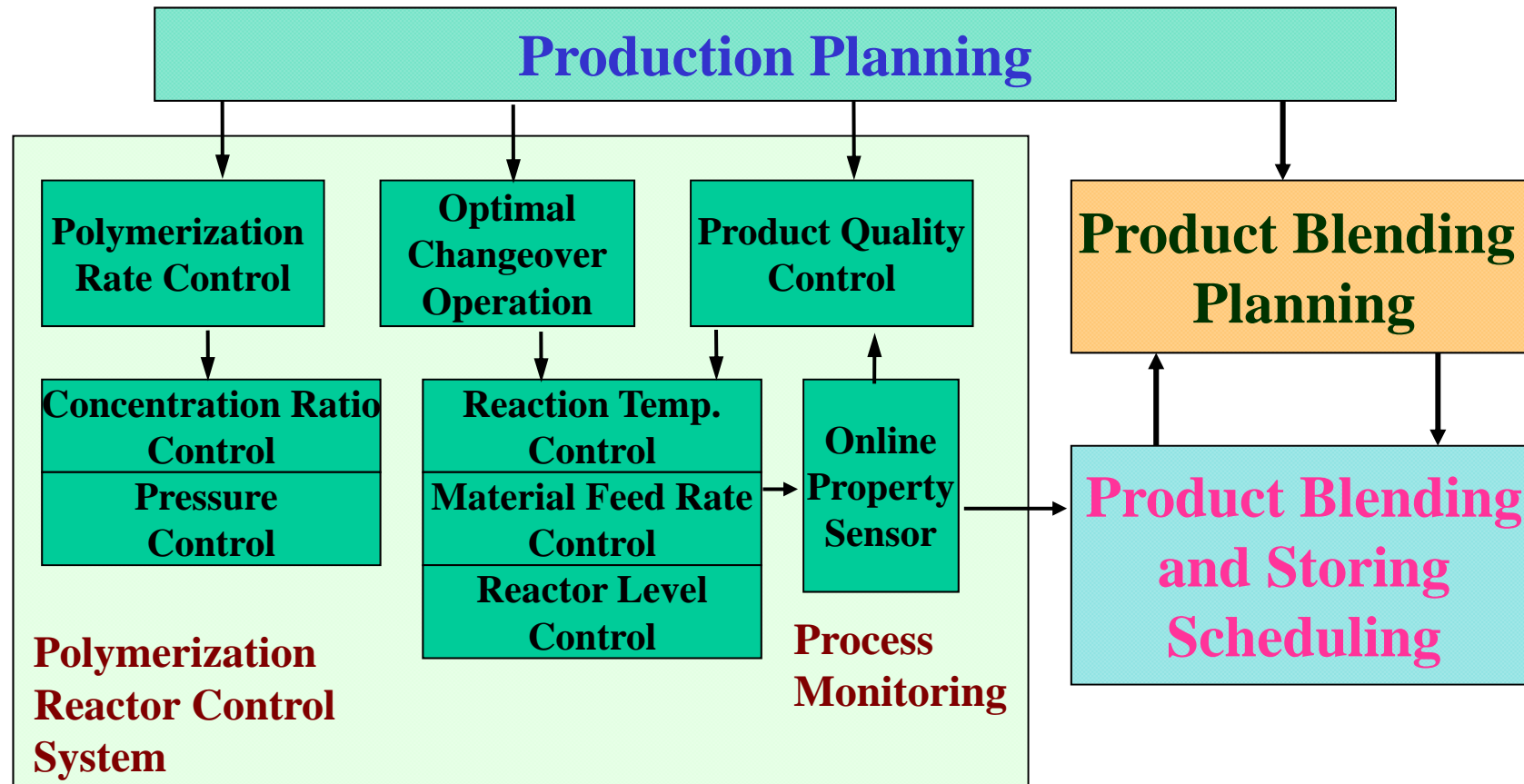
- ❑ Quality control for the objectives

- ❑ On-line **soft sensing** and optimal grade changeover **control**

Polymer Production Plant



Prospective Control System



Needs for Quality Modeling

Micro-scale \longrightarrow Macroscale

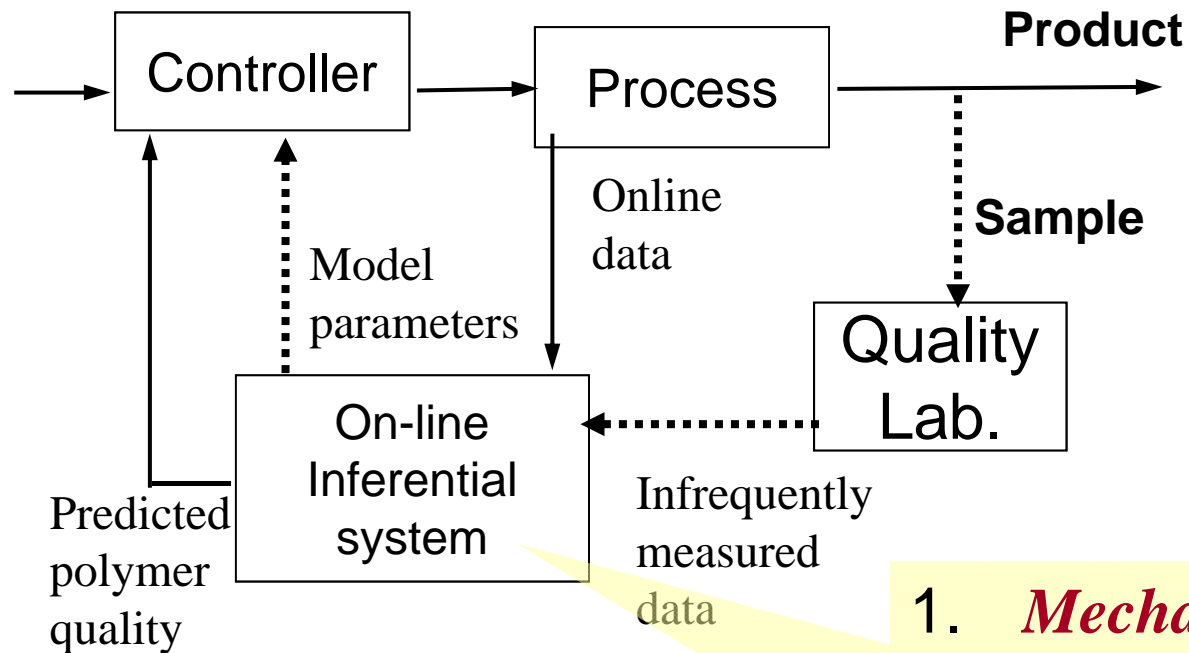
<i>Low-Order Structure</i>	<i>Distributed Parameter</i>	<i>High-Order Structure</i>	<i>Polymer Properties</i>	<i>End-User Properties</i>
Chain Branching LCB SCB	MWD	Morphology	Melt Index	Color
Stereoregularity Isotactic Sindiotactic Atactic	PSD	Molecular Mobility	Density	Mechanical property
	CCD	Crystal Structure	Shear Viscosity	Strength
			Melting Point	Electrical property



Process & Plant

Residence Time Distribution

Basic Structure of Inferential System



1. ***Mechanistic model*** derived from first principles
2. ***Empirical model*** derived from lab. data
3. ***Black box model*** by neural nets & statistical methods

An Examples of Three Kinds Model

□ Mechanistic model (McAuley & MacGregor, 1991)

$$\ln(MI_i) = 3.5 \ln \left(k_0 + k_1 \frac{[H_2]}{[C_2]} + k_2 \frac{[C_3]}{[C_2]} + k_3 \frac{[C_4]}{[C_2]} + k_4 \frac{[R]}{[C_2]} \right) + k_5 \left(\frac{1}{T} - \frac{1}{T_0} \right)$$
$$\frac{d MI_C(t)^{-0.286}}{dt} = \frac{1}{\tau(t)} MI_i(t)^{-0.286} - \frac{1}{\tau(t)} MI_C(t)^{-0.286}$$

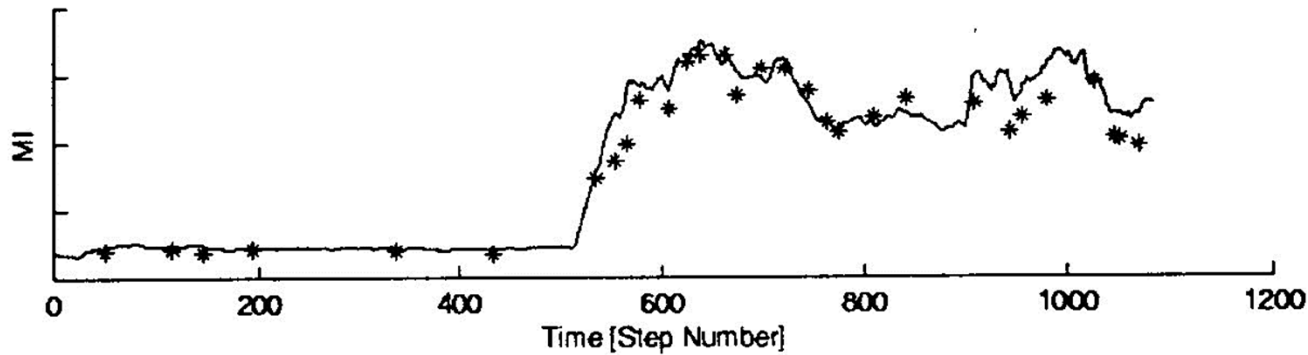
□ Empirical model (Watanabe et. al., 1993)

$$\log(MI_i) = \beta + \alpha_1 \log \frac{[H_2]}{[C_2]} + \alpha_2 \log \frac{[H_2]}{[C_2]} + \alpha_3 \log \frac{[C_3]}{[C_2]} + \alpha_3 \log \frac{[C_4]}{[C_2]}$$
$$+ \alpha_4 \log[R] + \alpha_5 \log(T)$$
$$\frac{d \log(MI_C(t))}{dt} = \frac{1}{\tau(t)} \log(MI_i(t)) - \frac{1}{\tau(t)} \log(MI_C(t))$$

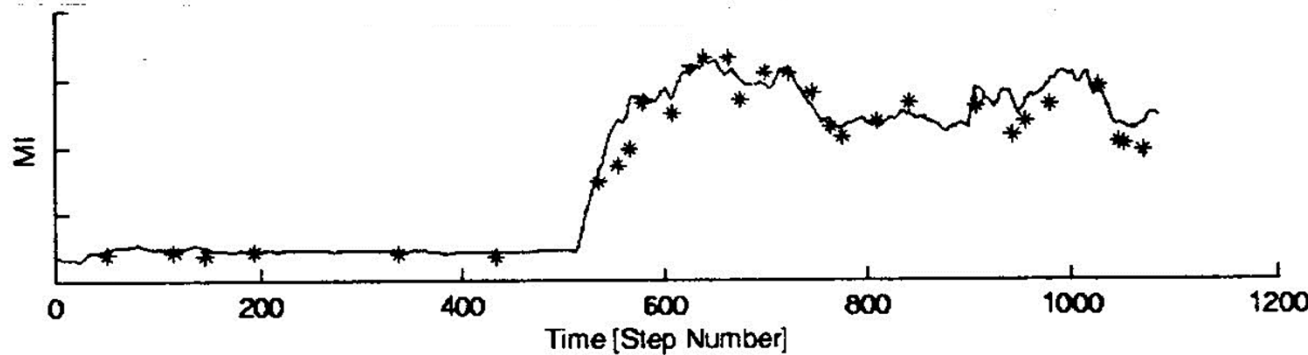
□ Neural net model (Koulouris, 1995)

$$MI_i^{-0.286} = \text{Wave-Net} \left(\frac{[H_2]}{[C_2]}, \frac{[C_2]}{[C_2]}, \frac{[C_6]}{[C_2]}, \frac{[R]}{[C_2]} \right)$$

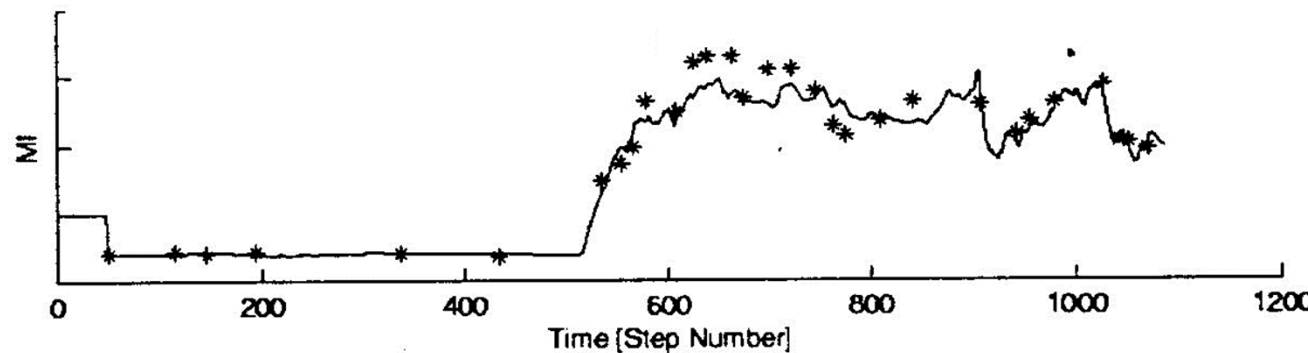
MI Estimation by Models



Mechanistic
model

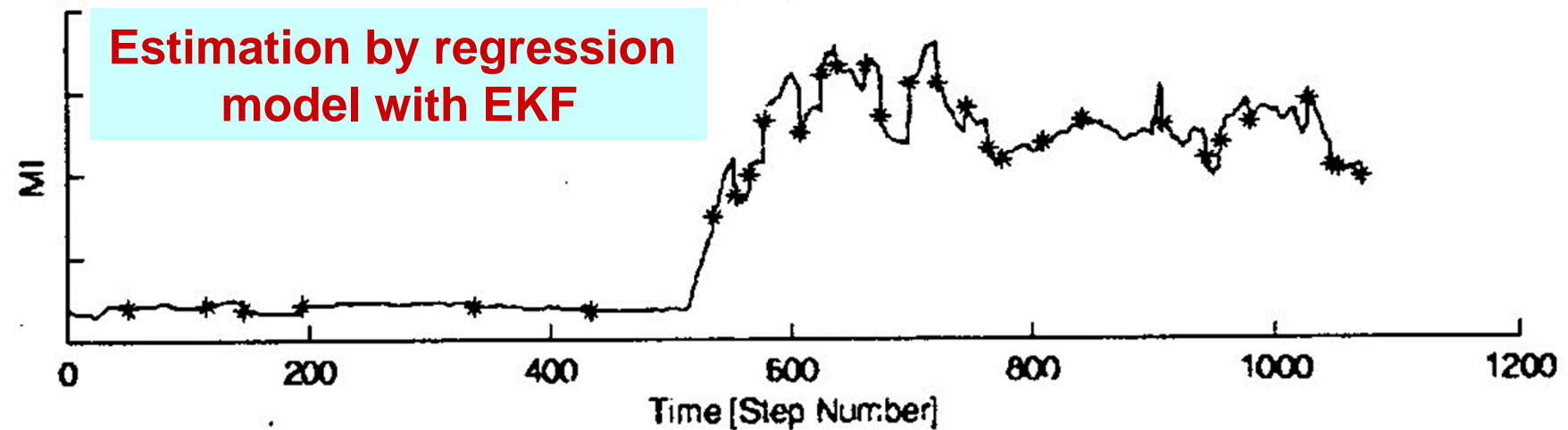
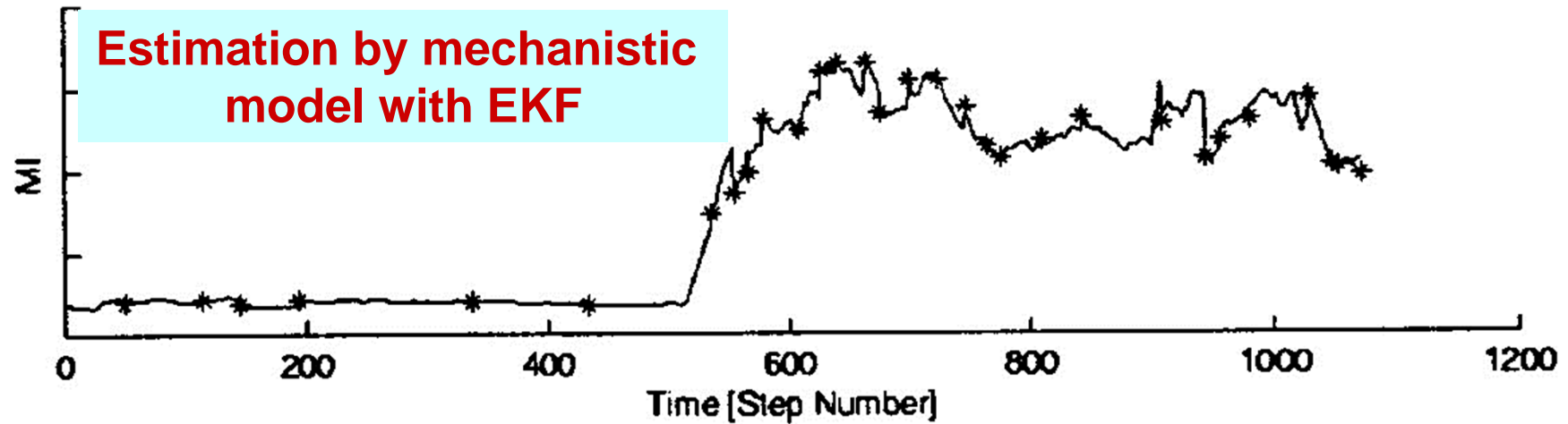


Regression
model

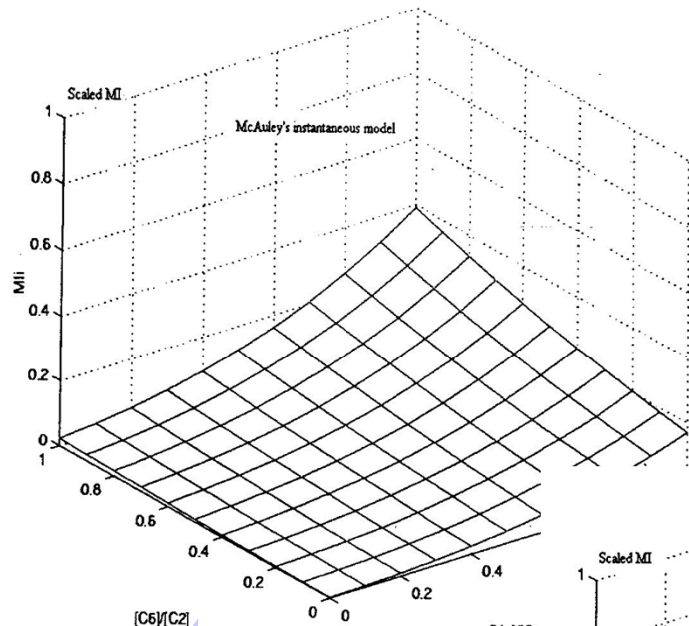


Neural net
model

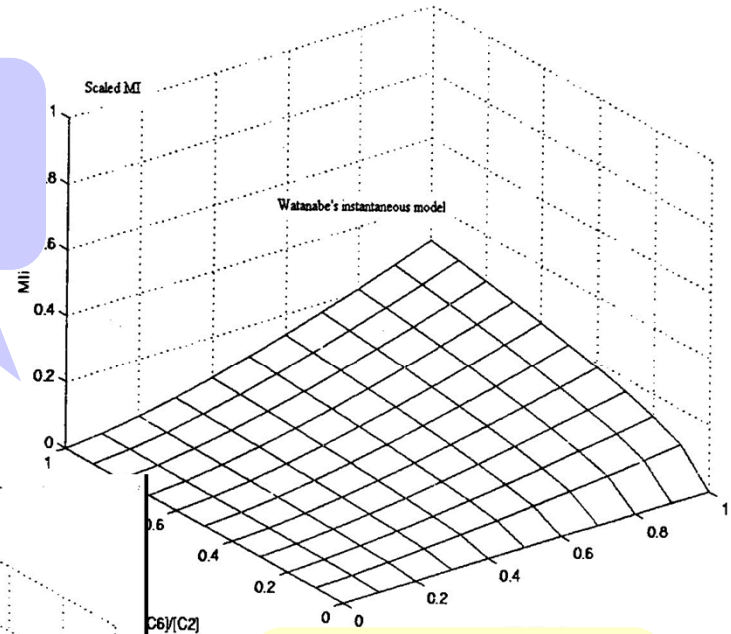
MI Estimation with EKF



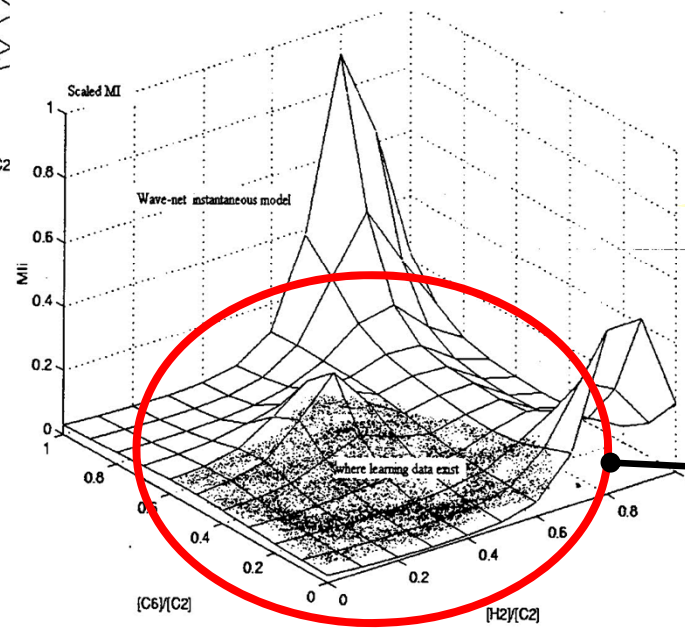
Risk of Extrapolation



Regression model



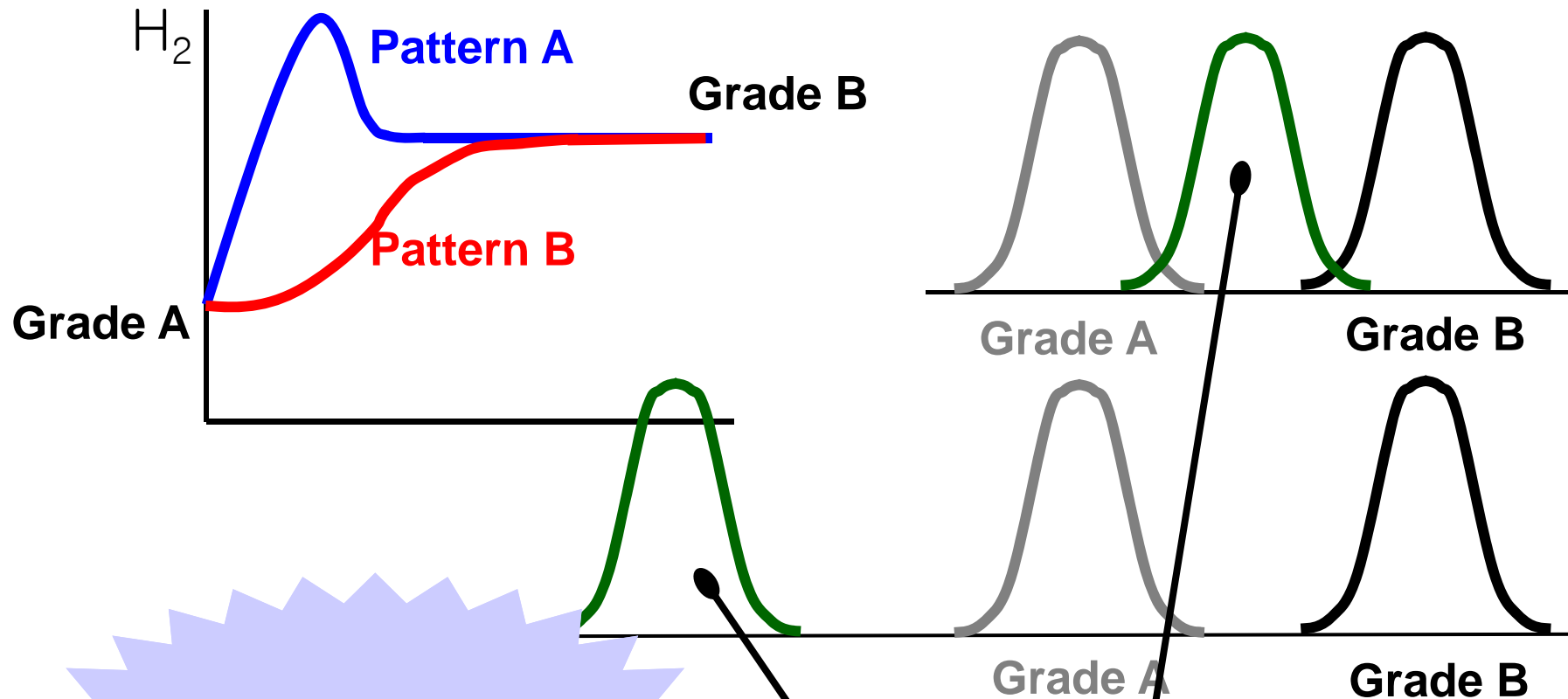
Mechanistic model



Neural net model

Learning data

Grade Changeover Operation



1. Not time but grade optimal operation
2. Runaway reaction

Instantaneous grade

Control System

□ Iterative open-loop optimization

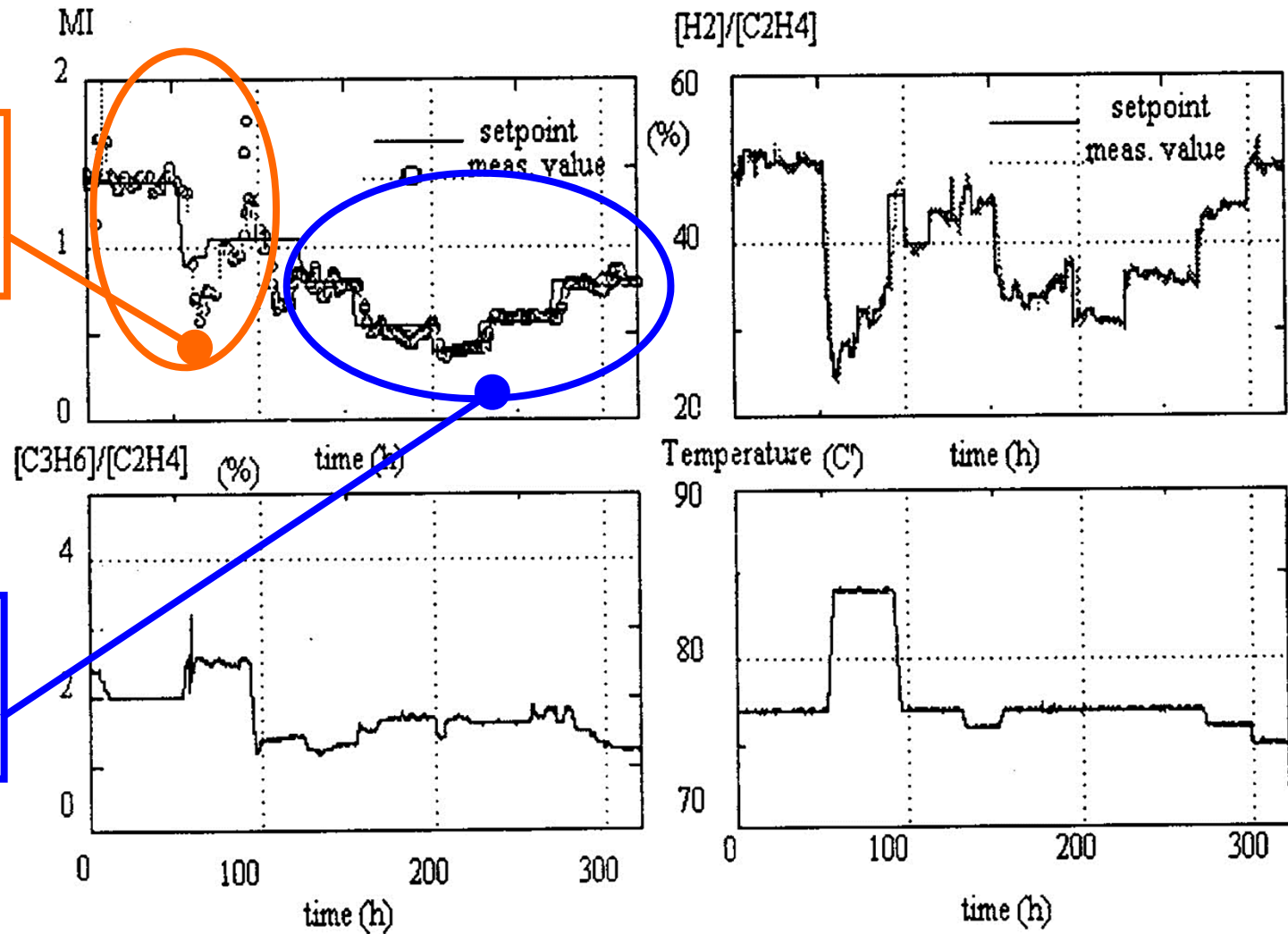
- A new optimal trajectory is recomputed
- The first input action is implemented at every new measurements

□ Combination of FF&FB controllers

- A optimal trajectory is pre-calculated of both MV & CV
- MV is introduced to the plant in a FF manner
- **CV is deviated from the desired optimal trajectory, FB controller is activated to compensate the deviation**

Results of Control

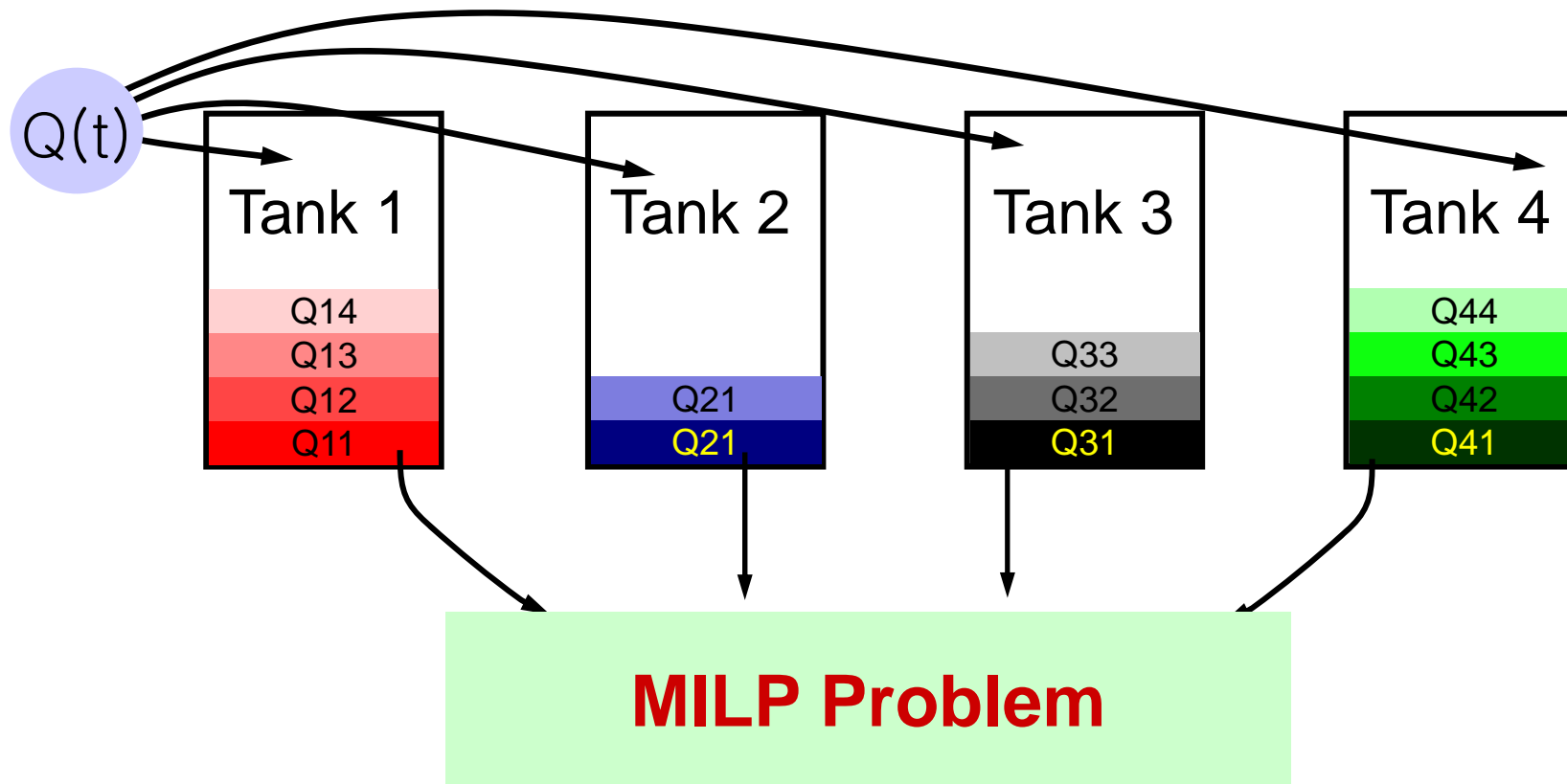
Manual operation



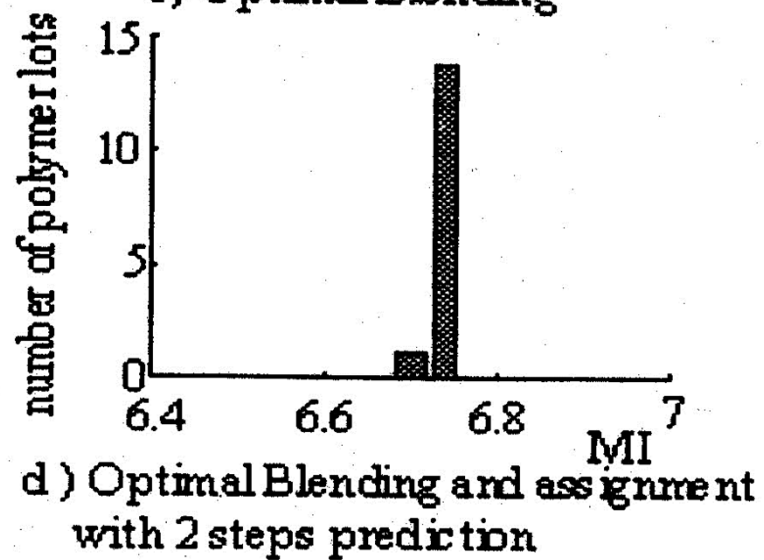
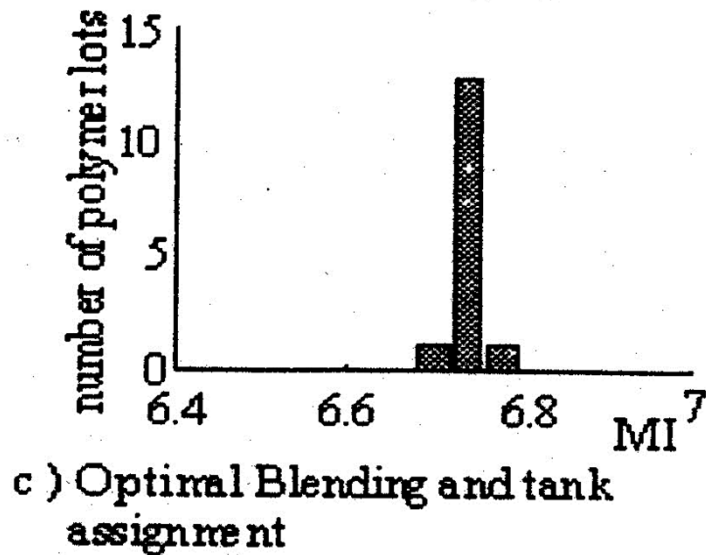
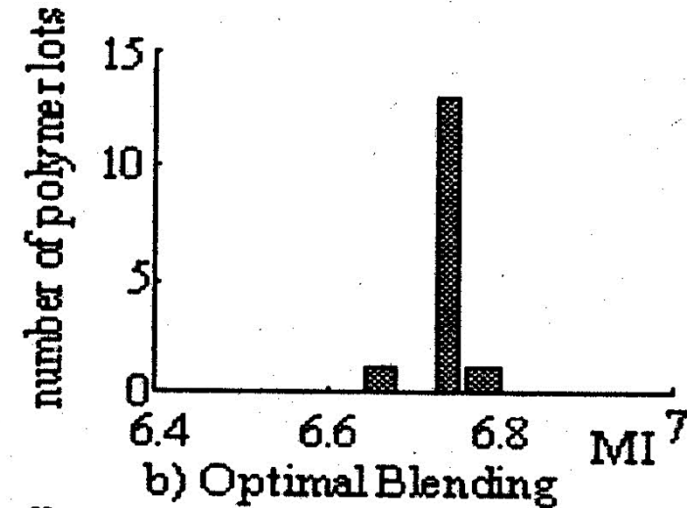
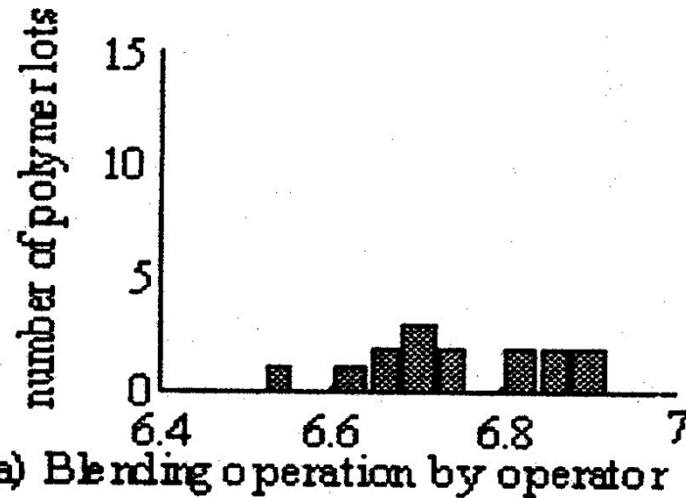
Control is activated

Optimal Blending

Reactor control is not good enough to satisfy the customer's demands



Blending Optimization Result



Conclusion

- ❑ Integration of process control, sensing and optimization is indispensable
- ❑ Most important factor is quality modeling