Polymerization Reactor Control Under Uncertainty

REU Final Project Presentation

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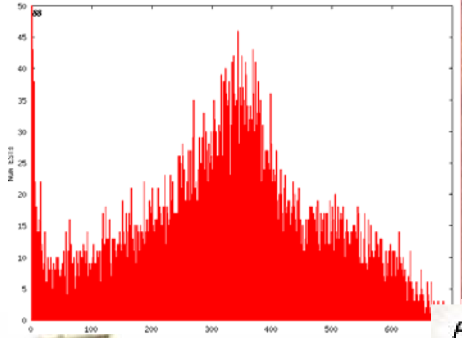
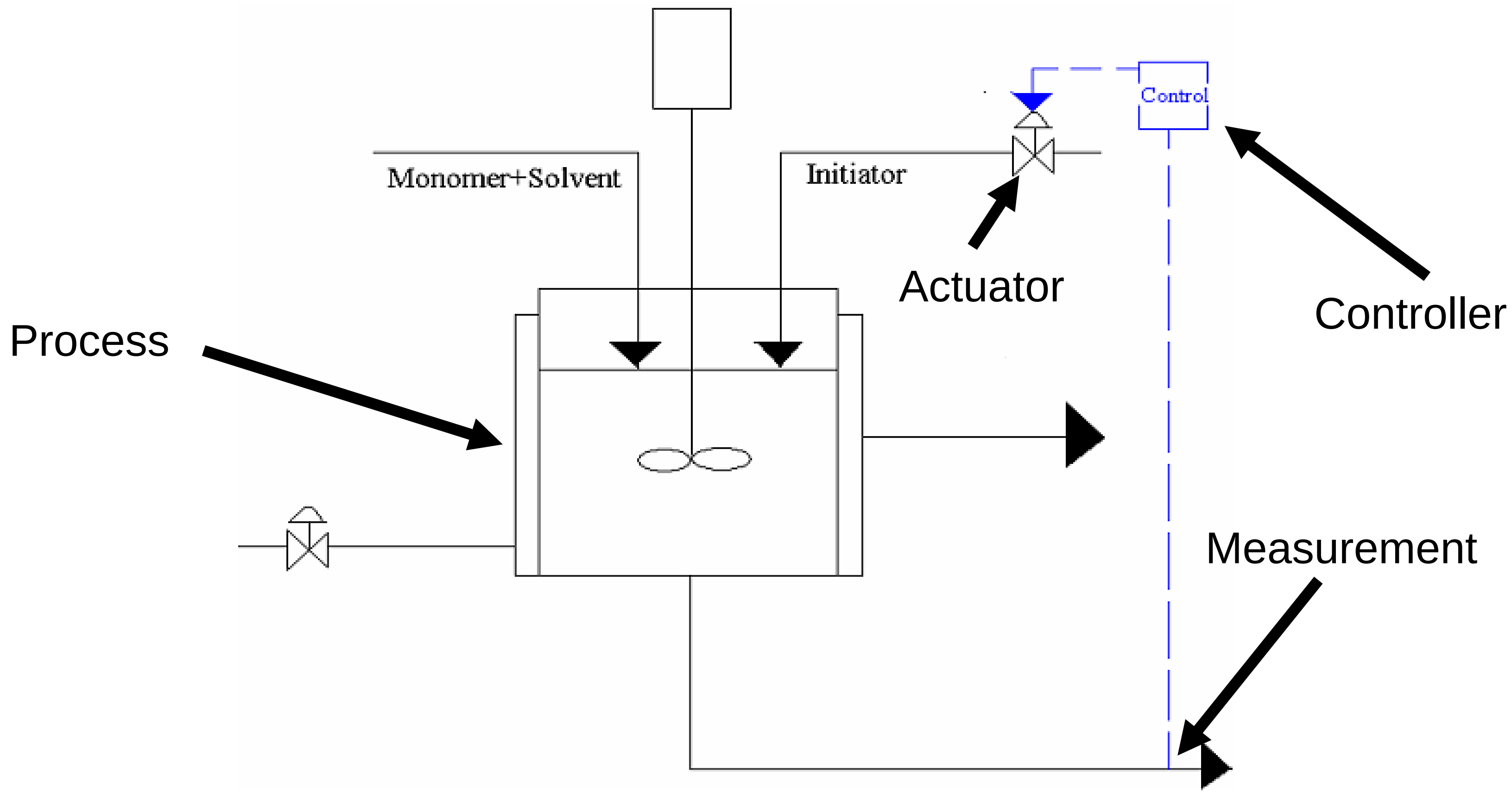
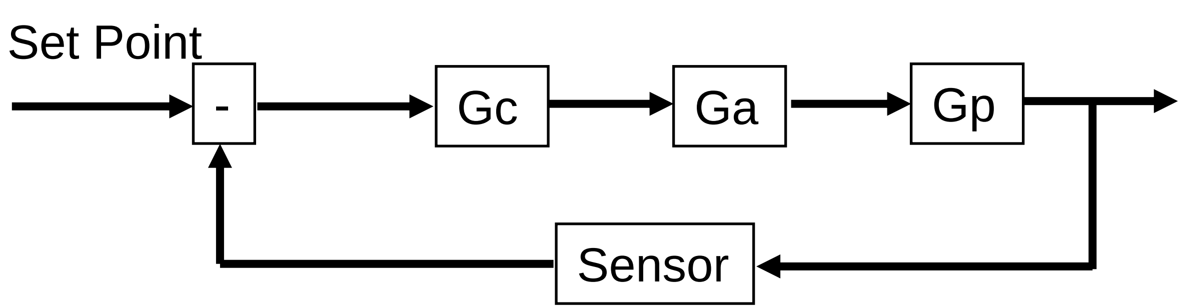
Uncertainty in Chemical Manufactuaring

- **What is uncertainty?**
  - **Operational (pumps)**
  - **Property (density, heat capacity)**
  - **Model (Equilibrium point, order of reaction)**
- **Why do we care?**
  - **Quality**
  - **Safety**
  - **Profit**
- **How do we deal with it?**
  - **Design**
    - » **Effectiveness Factor**
    - » **Volume**
  - **Control**
  - **Simultaneous design and control?**
- **How will I use it?**
  - **To determine control robustness and economic feasibility**



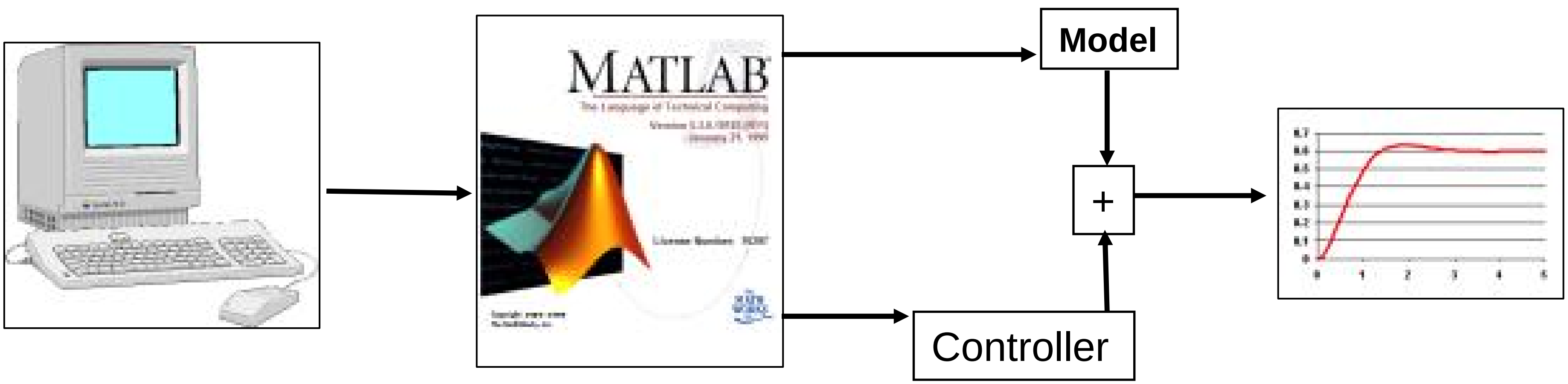
Feedback Control





Methodology

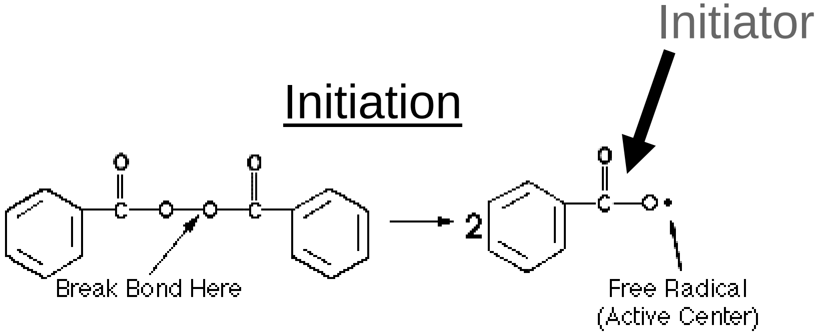
- **Find how the process reacts to uncertainty**
- **Develop different controllers to minimize uncertainty**
- **Compare process estimations of different controllers**
- **AIM: <u>Quantify the cost of uncertainty under control</u>**



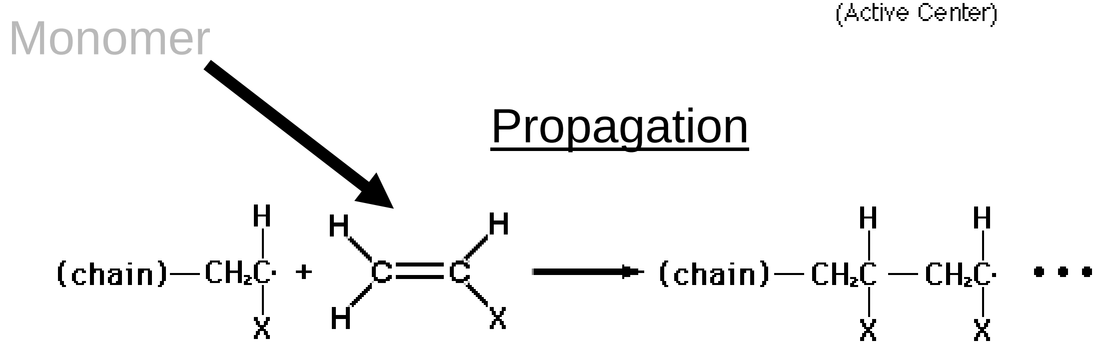
Background of Polymerization Reaction

- **How are polymers made?**
  - **Free-Radical Polymerization**
    - » **Initiator**
    - » **Monomer**
- **Reaction (Exothermic)**
  - **Initiation**
  - **Propagation**
  - **Termination**
- **For this case study, the desired quality is 25,000 ±100 kg/kmol.**

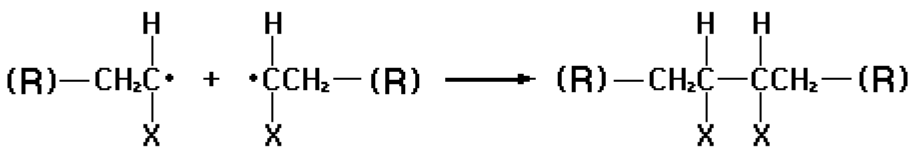
Initiation



Propagation

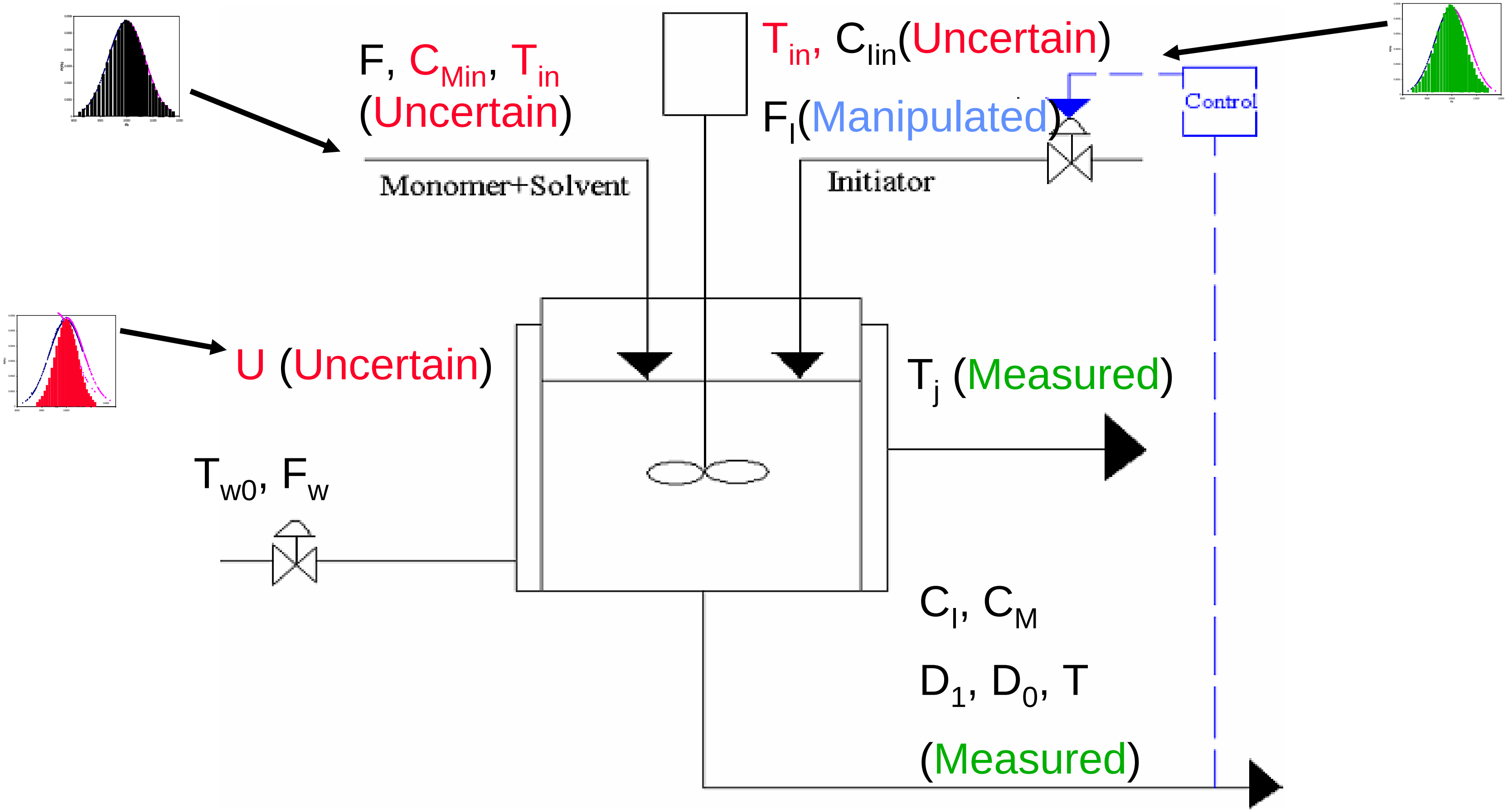


Termination



From http://plc.cwru.edu/tutorial/enhanced/files/polymers/synth/synth.htm

Case Study: The Polymerization Reactor



Desired Quality=25,000 ±100kg/kmol

Balances

Reaction

- Accumulation = input – output + generation – consumption

Mass

$$\frac{dC_I}{dt} = -k_I \cdot C_I + \frac{(F_I \cdot C_{I_{in}}) - (F \cdot C_I)}{V}$$

Initiator Concentration

$$\frac{dC_m}{dt} = -(k_p + k_{f_m}) \cdot C_m \cdot P_0(C_1, T) + \frac{F \cdot (C_{m_{in}} - C_m)}{V}$$

Monomer Concentration

$$\frac{dD_0}{dt} = (0.5 \cdot k_{T_c} + k_{T_d}) \cdot [P_0(C_1, T)]^2 + k_{f_m} \cdot C_m \cdot P_0(C_1, T) - \frac{F \cdot D_0}{V}$$

Mass Concentration

$$\frac{dD_1}{dt} = M_m \cdot (k_p + k_{f_m}) \cdot C_m \cdot P_0(C_1, T) - \frac{F \cdot D_1}{V}$$

Molar Concentration

Energy

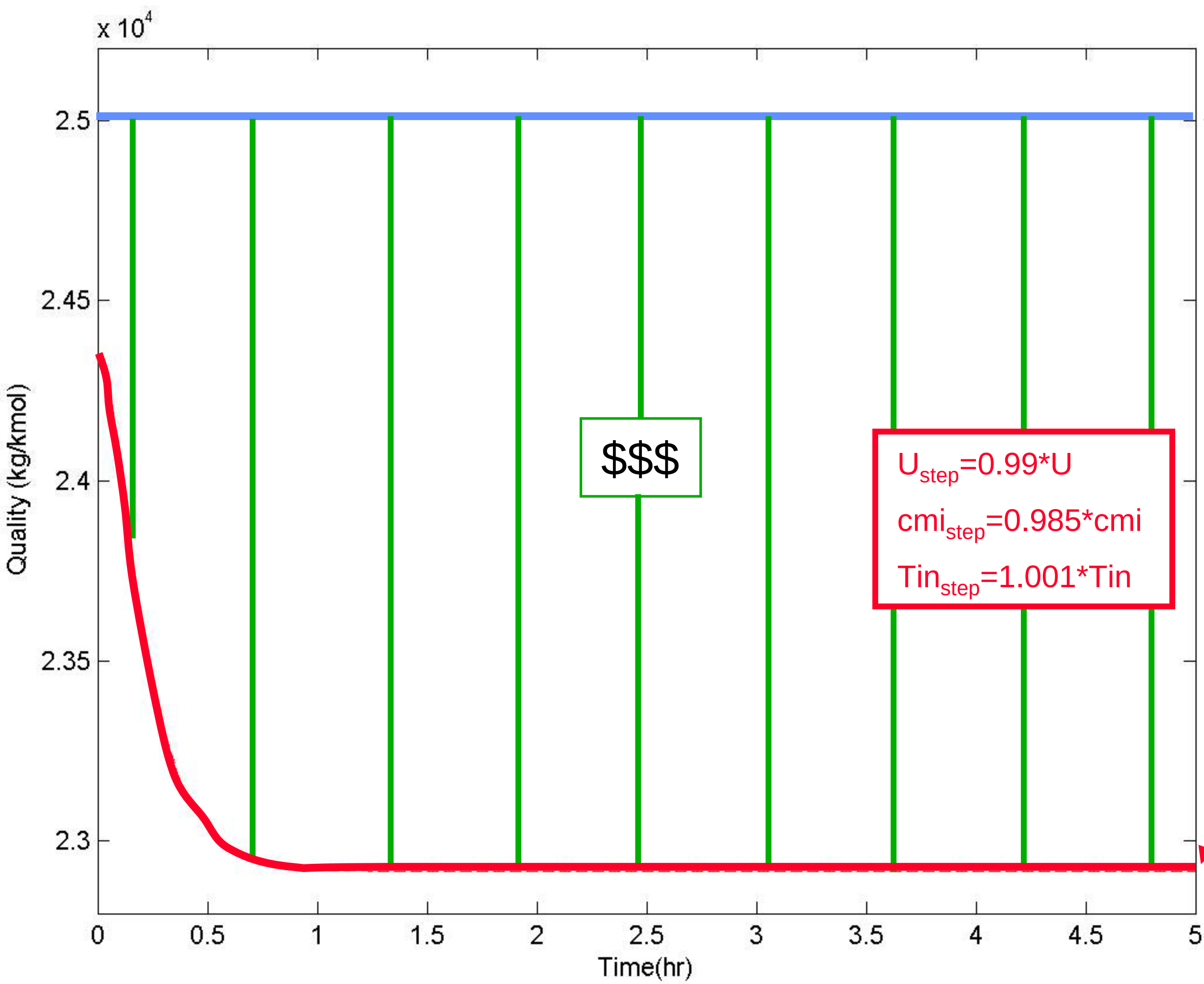
$$\frac{dT}{dt} = k_p \cdot C_m \cdot \frac{(-\Delta H_P)}{\rho \cdot C_p} \cdot P_0(C_1, T) - \frac{U \cdot A}{\rho \cdot C_p \cdot V}(T - T_j) + \frac{F \cdot (T_{in} - T)}{V}$$

Reactor Temperature

$$\frac{dT_j}{dt} = \frac{F_{cw}}{V_o} \cdot (T_{w_o} - T_j) + \frac{U \cdot A}{\rho_w \cdot c_w \cdot V_o}(T - T_j)$$

Cooling Jacket Temperature

Dynamic Model



Desired Quality

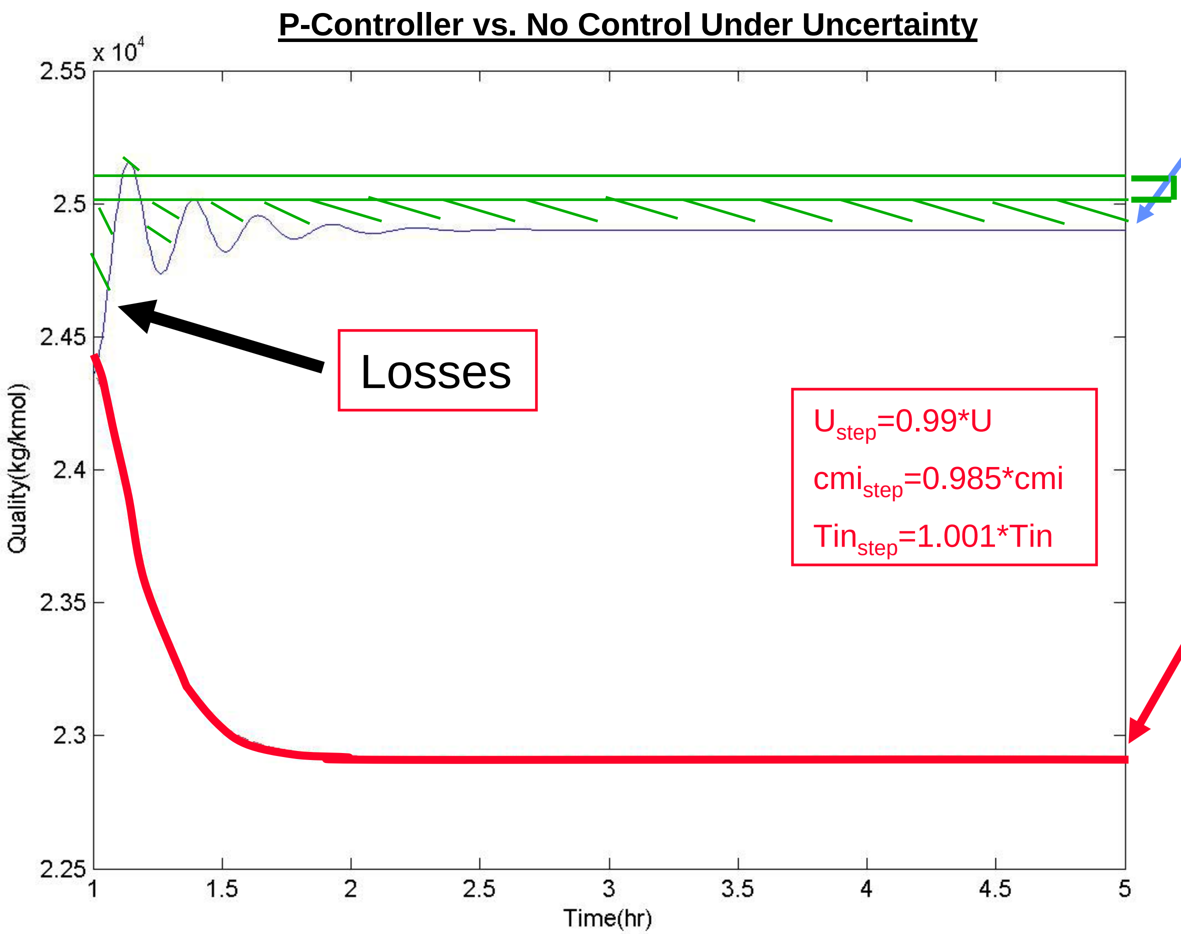
25,000 kg/kmol

Quality without control

22,900 kg/kmol

Uncertainty → Disturbances → Costs you money!

Proportional-Controller



Quality with Control

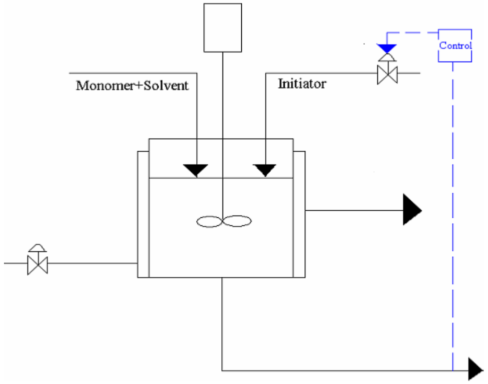
24,900 kg/kmol

Acceptable Quality Region

25,000±100 kg/kmol

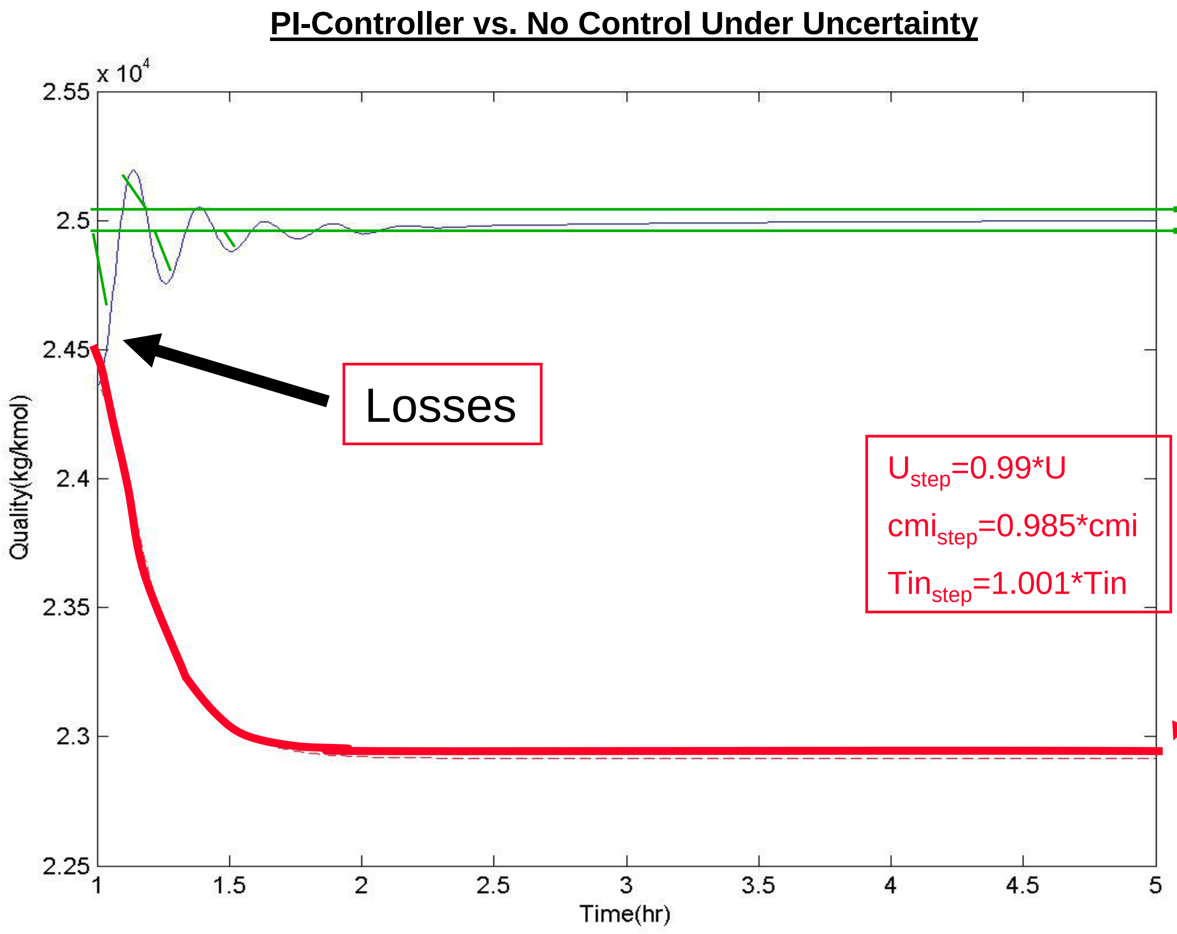
Quality without control

22,900 kg/kmol



Uncertainty → Disturbances → Control → Saves you money!

Proportional-Integral Controller



Quality with Control

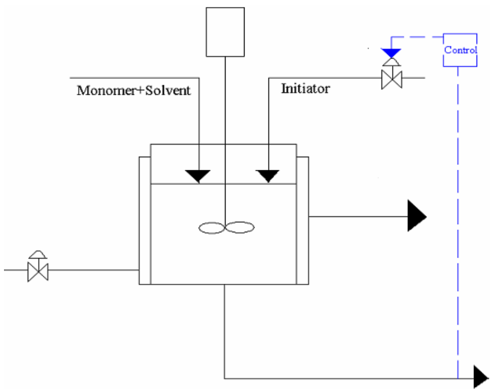
25,000 kg/kmol

Acceptable Quality Region

25,000±100 kg/kmol

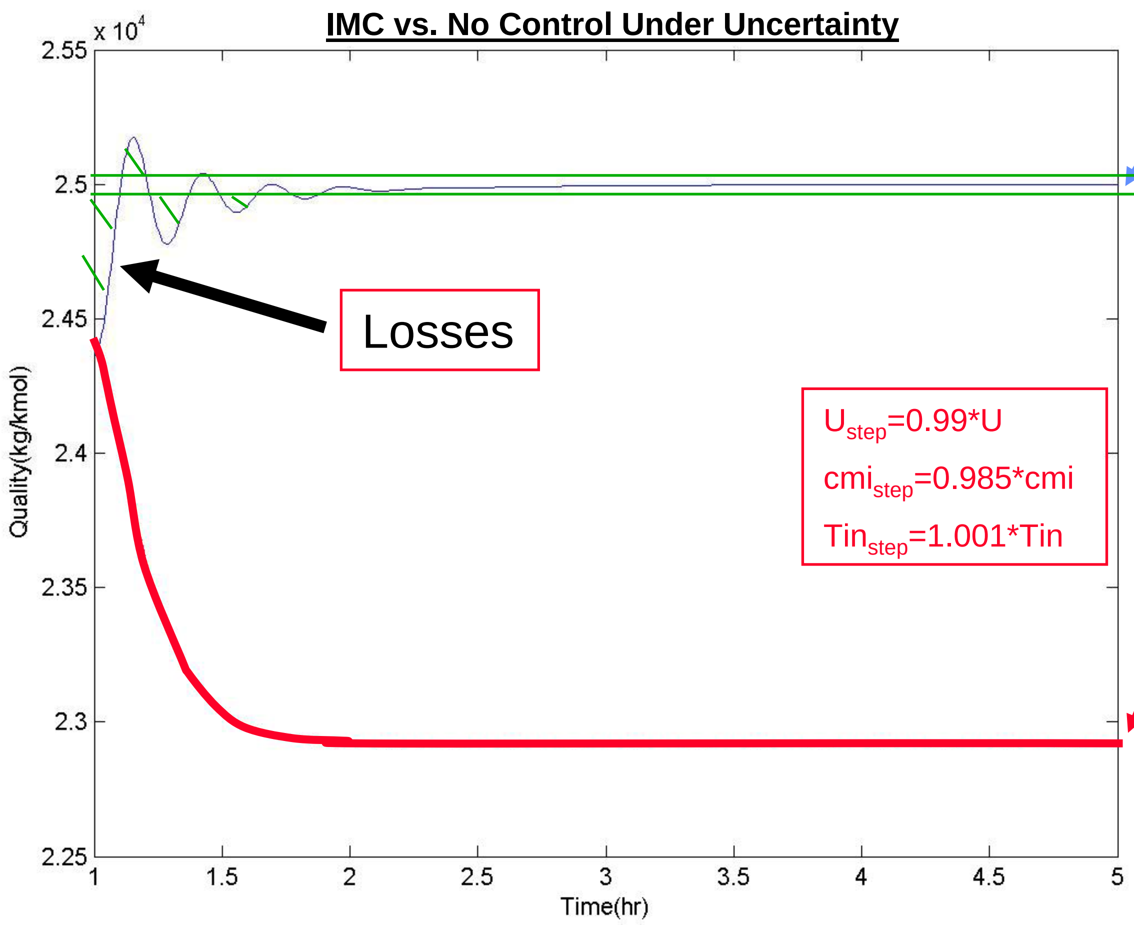
Quality without control

22,900 kg/kmol



Uncertainty → Disturbances → Control → Saves you money!

IMC



Quality with Control

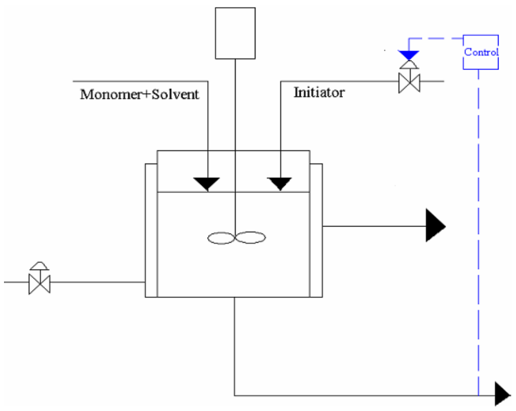
25,000 kg/kmol

Acceptable Quality Region

25,000±100 kg/kmol

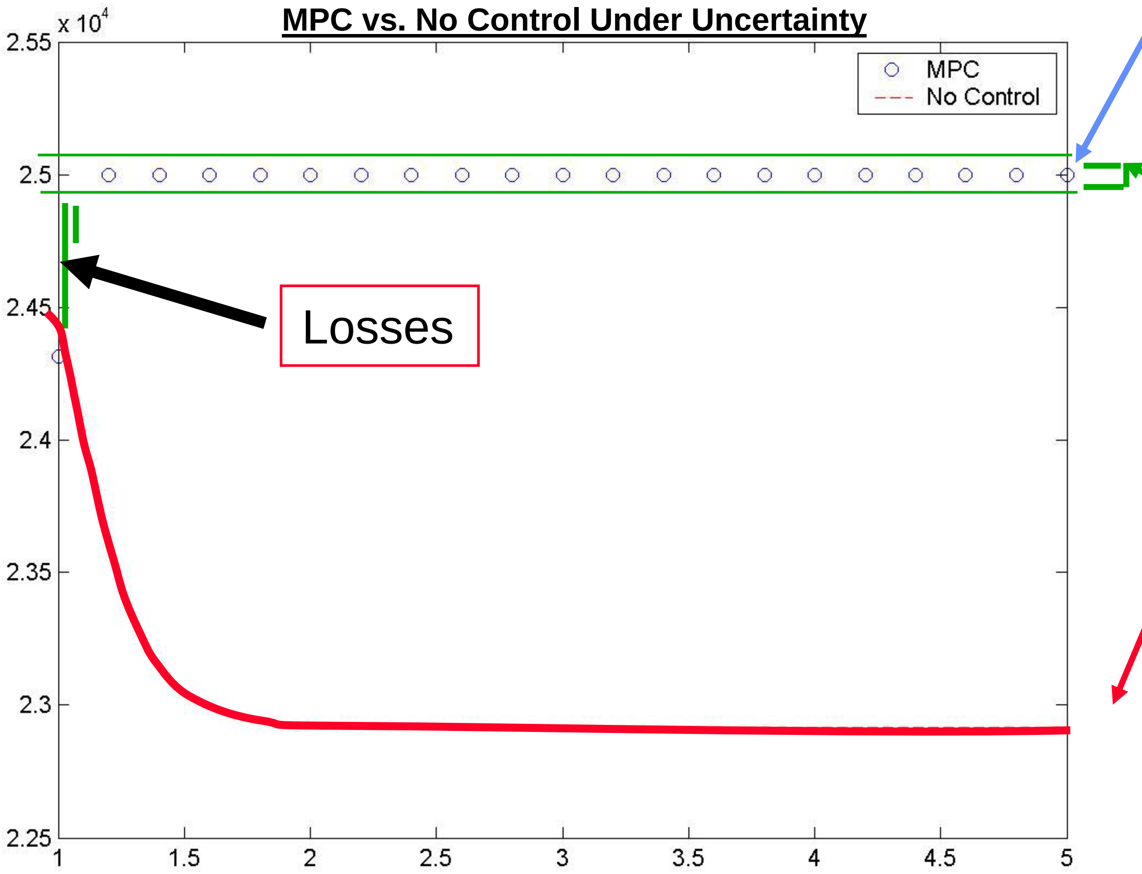
Quality without control

22,900 kg/kmol



Open-loop response → Response Parameters → "One-Tuning" Controller (λ)

MPC Controller



Quality with Control

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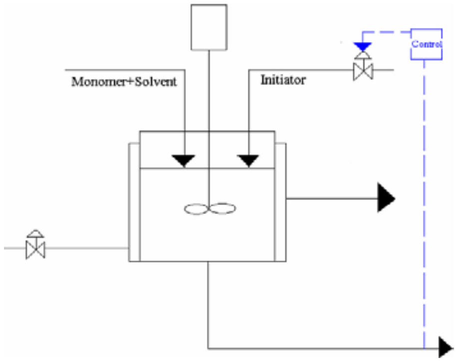
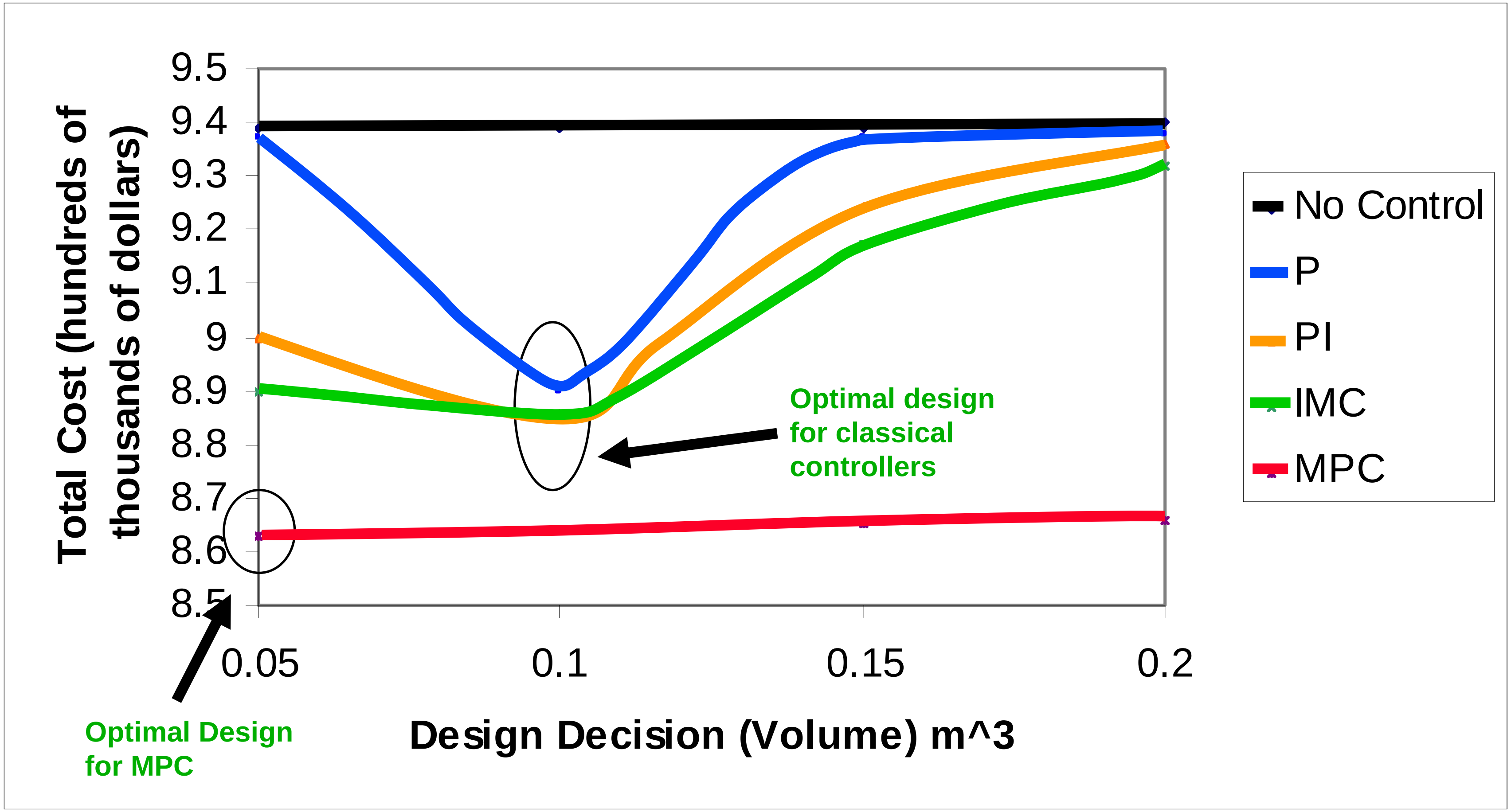


- MPC solves an optimization problem at each time step
- Can handle multiple manipulated variables – classic control can't!

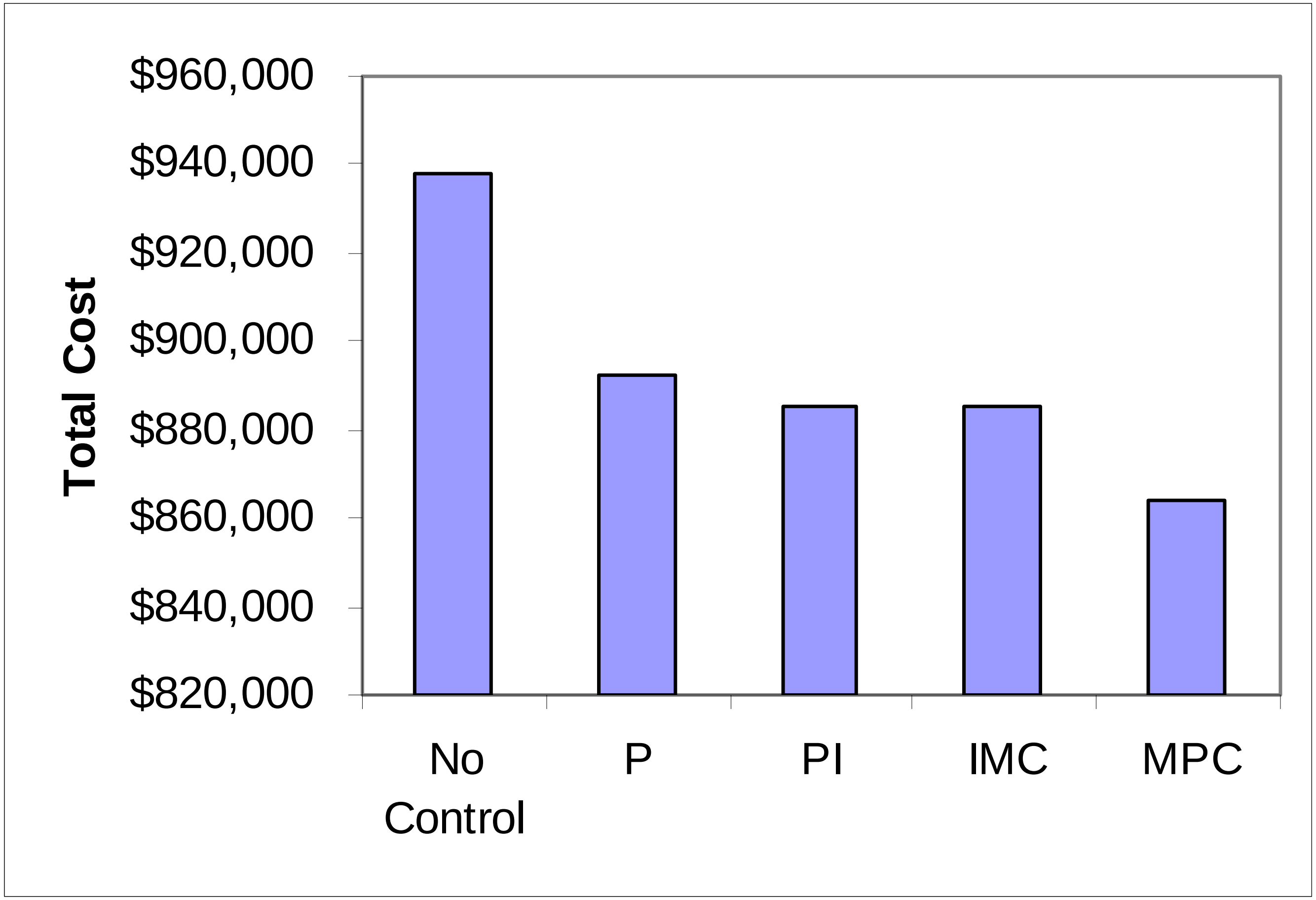
Process Costs



Total Cost = Operating Costs + Capital Costs - Profit

- Operating Costs: Initiator, Monomer
- Capital Costs: Reactor, Control, Heat Exchanger

Approximate Cost Model



Bottom Line

Under given process conditions, the optimal design *and* control can be determined simultaneously – do not have to be done separately!

Conclusions

- **Dynamic models show how the system responds under uncertainty**
- **Controls require more capital, but decrease total costs**
- **MPC outperforms all classical controllers**
- **MPC can also control and optimize many manipulated variables**
- **It is possible to determine an optimal design *and* control scheme for a given set of process conditions simultaneously.**

Future Work

- **Introducing time-dependent uncertainty**

- **Applying other optimization techniques (Six Sigma)**

- **Find optimal design and control for each volume to determine which is the overall optimal volume**

References/Acknowledgements

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- **Chawankul, N.; Budman, H.; Douglas, P.L.: The integration of design and control: IMC control and robustness, *Comp. Chem. Eng.* 2005, *29*, 261-271.**
- **Daoutidis, P. *et al*: Feedforward/Feedback Control of Multivariable Nonlinear Processes, *AIChE J*. 1990, *36*, 1471-1484.**
- **Maner, B. R. *et al*: Nonlinear Model Predictive Control of a Simulated Multivariable Polymerization Reactor Using Second-order Volterra Models, *Automatica*. 1996, *32,* 1285-1301.**
- **"Polymer Synthesis,"**

  http://plc.cwru.edu/tutorial/enhanced/files/polymers/synth/synth.htm. June 24th, 2005.