Applications of data-driven modeling on control and optimization of distillation process

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Outline

- Research background
- Integrated control and optimization strategy of distillation process
- Modeling for control of distillation process
- Modeling for optimization based on AHH method
- Applications on practical distillation process

Research Background

- Importance of distillation process
  - Widely used
  - One of the most energy-cost unit operations
- Problems in control of high-purity distillation process
  - Large delay
  - Large inertial lag



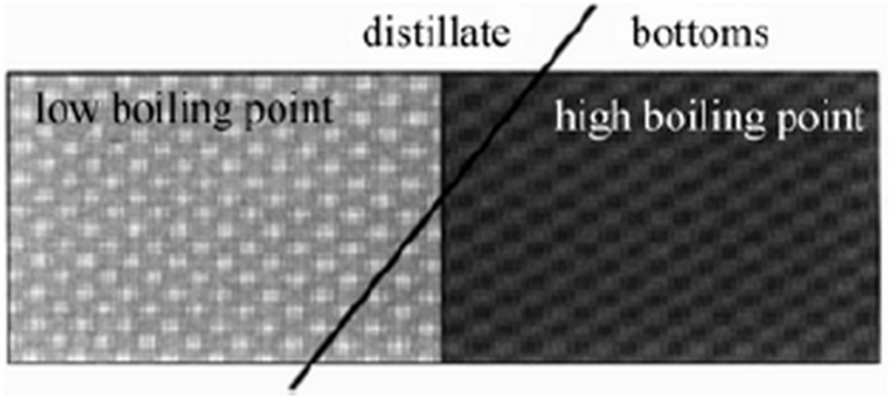
Modeling Based on First Principle

- Non equilibrium stage model (Kooijman, 1995)
  - for stage(or tray) *j* (*j*=1, …, *N*)
    - Material balance $\frac{\mathrm{d}M_j}{\mathrm{d}t} = F_j + L_{j-1} + V_{j+1} - L_j - V_j$ $\quad \frac{\mathrm{d}(M_j x_{i,j})}{\mathrm{d}t} = F_j z_{i,j} + L_{j-1}x_{i,j-1} + V_{j+1}y_{i,j+1} - L_j x_{i,j} - V_j y_{i,j}$
    - Energy balance $\frac{\mathrm{d}(M_j H_j^{\mathrm{L}})}{\mathrm{d}t} = F_j H_{\mathrm{F},j}^{\mathrm{L}} + L_{j-1}H_{j-1}^{\mathrm{L}} + V_{j+1}H_{j+1}^{\mathrm{V}} - L_j H_j^{\mathrm{L}} - V_j H_j^{\mathrm{V}}$
    - Rate $N_{i,j} = k_{\mathrm{eff},i,j}^{\mathrm{L}} A_{\mathrm{s},j}(x_{i,j}^{\mathrm{I}} - x_{i,j}) + x_{i,j}N_j$ $\quad E_j = h_j^{\mathrm{L}} A_{\mathrm{s},j}(T_j^{\mathrm{I}} - T_j^{\mathrm{L}}) + \sum_{i=1}^{2} N_{i,j}\overline{H}_{i,j}^{\mathrm{L}}$
      $N_{i,j} = k_{\mathrm{eff},i,j}^{\mathrm{V}} A_{\mathrm{s},j}(y_{i,j} - y_{i,j}^{\mathrm{I}}) + y_{i,j}N_j$ $\quad E_j = h_j^{\mathrm{V}} A_{\mathrm{s},j} \frac{\varepsilon_j^{\mathrm{V}}}{\exp(\varepsilon_j^{\mathrm{V}}) - 1}(T_j^{\mathrm{V}} - T_j^{\mathrm{I}}) + \sum_{i=1}^{2} N_{i,j}\overline{H}_{i,j}^{\mathrm{V}}$
    - Phase equilibrium $y_{i,j}^{\mathrm{I}} = K_{i,j}x_{i.j}^{\mathrm{I}}$
    - Sum $\sum_{i=1}^{2} x_{i,j}^{\mathrm{I}} - 1 = 0, \quad \sum_{i=1}^{2} y_{i,j}^{\mathrm{I}} - 1 = 0,$
      $\sum_{i=1}^{2} x_{i,j} - 1 = 0, \quad \sum_{i=1}^{2} y_{i,j} - 1 = 0$
    - Hydraulics $M_j = \rho_j^{\mathrm{L}} A_j (h_{\mathrm{w}j} + h_{\mathrm{ow}j})$ $\quad p_{j+1} - p_j = \lambda_j^{\mathrm{V}} \rho_{j+1}^{\mathrm{V}} \left(\frac{V_{j+1}}{\rho_{j+1}^{\mathrm{V}} A_{\mathrm{h},j}} \right)^2 + \lambda_j^{\mathrm{L}} \tilde{\rho}_j^{\mathrm{L}} g(h_{\mathrm{w}j} + h_{\mathrm{ow}j})$

Property of Dynamic Characteristic

- Large inertia of the response of composition
- Analysis based on first principle
  - Change of composition depends on molecular diffusion
  - Inertial lag of composition larger than that of flow rate
  - Inertia accumulated by *N* trays
- Analysis based on simulation
  - Settle time more than ten hours (Propene-Propane distillation process with twin towers, 90 trays each)

Analysis of Distillation Process



- (Svrcek, W. Y., etc., 2000)

- Function of distillation process
  - Split of material
  - Fractionation of component

Analysis of Distillation Process

- Material balance

$$F = D + B$$

$$Fz_F = Dx_D + Bx_B$$

$$\eta \overset{\Delta}{=} D/B = -\frac{z_F - x_B}{z_F - x_D}$$

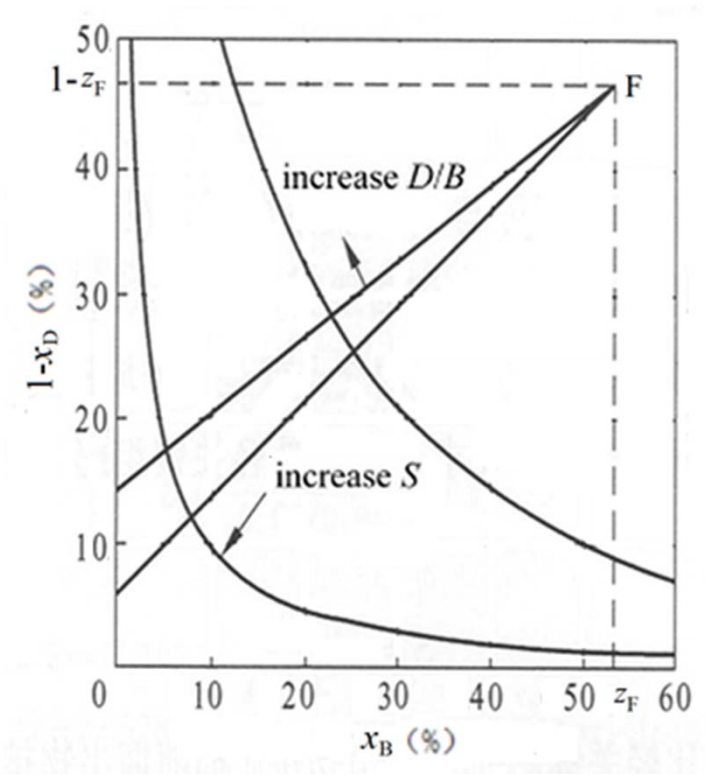
- Fenske equation

$$S = \frac{x_D/(1-x_D)}{x_B/(1-x_B)}$$

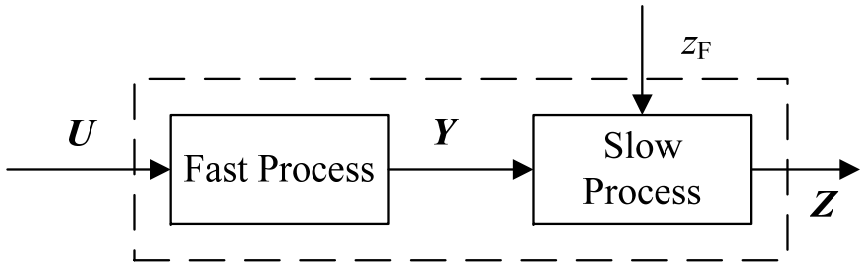
$$x_D = f(\eta, S, z_F)$$

$$x_B = g(\eta, S, z_F)$$

(Shinskey, F. G., 1998)



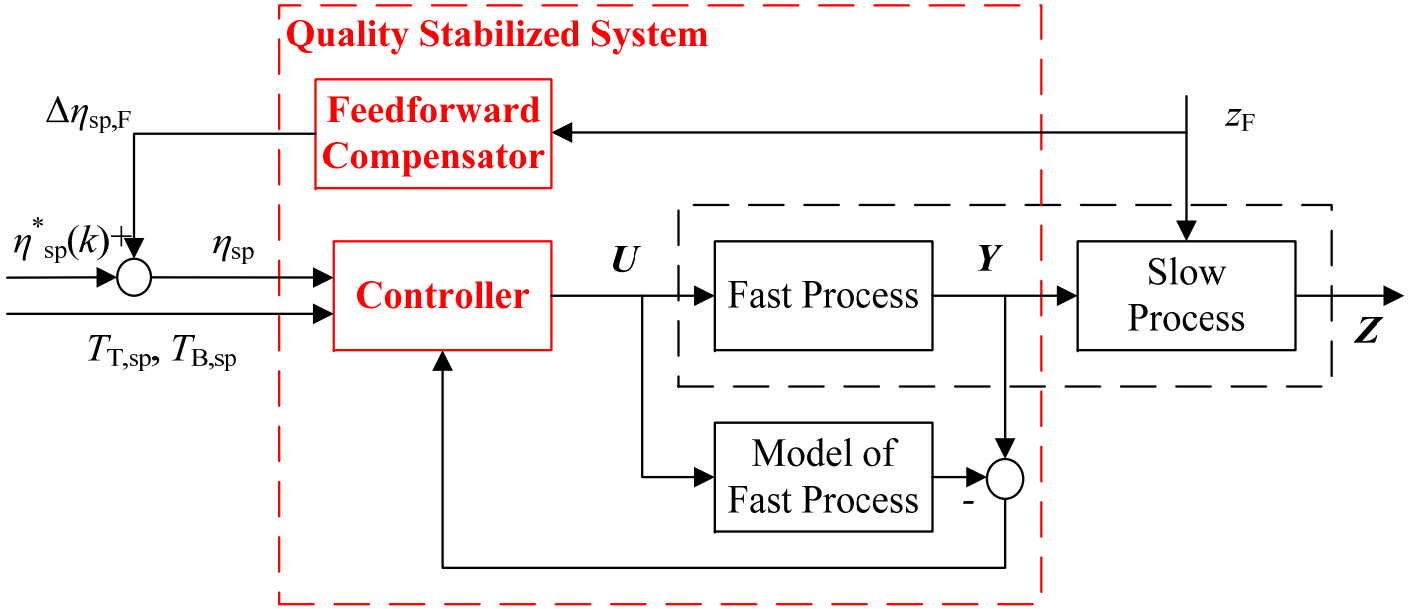
Structure Decomposition



- ***U*** : Reflux, Reboiling duty rated by feed
- ***Y*** : Split ratio (D/B), Temperatures of top and bottom trays (Reflecting separation factor)
- ***Z*** : composition of both products
- z_F : composition of feed

- Conclusion
  - Steady state of ***Z*** depends on steady state of z_F and ***Y***
  - ***Y*** should be regulated according z_F to maintain a stable ***Z***

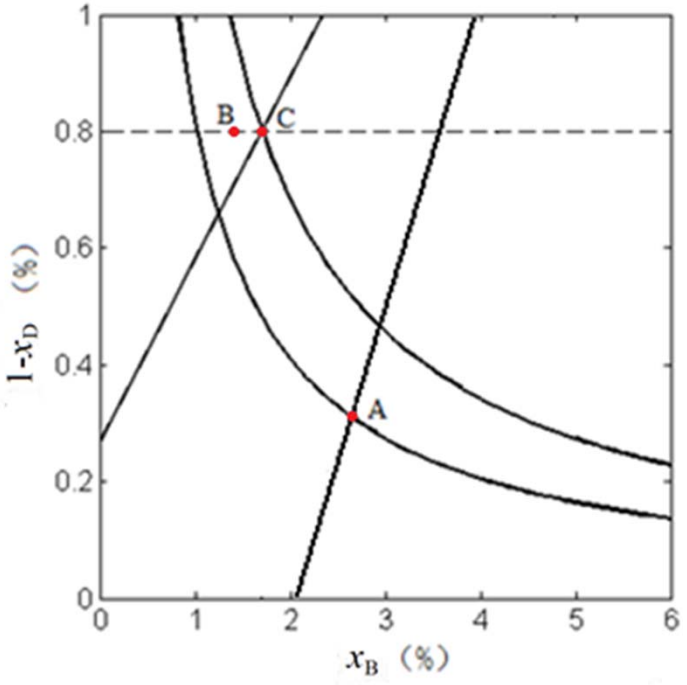
Quality Stabilized Control



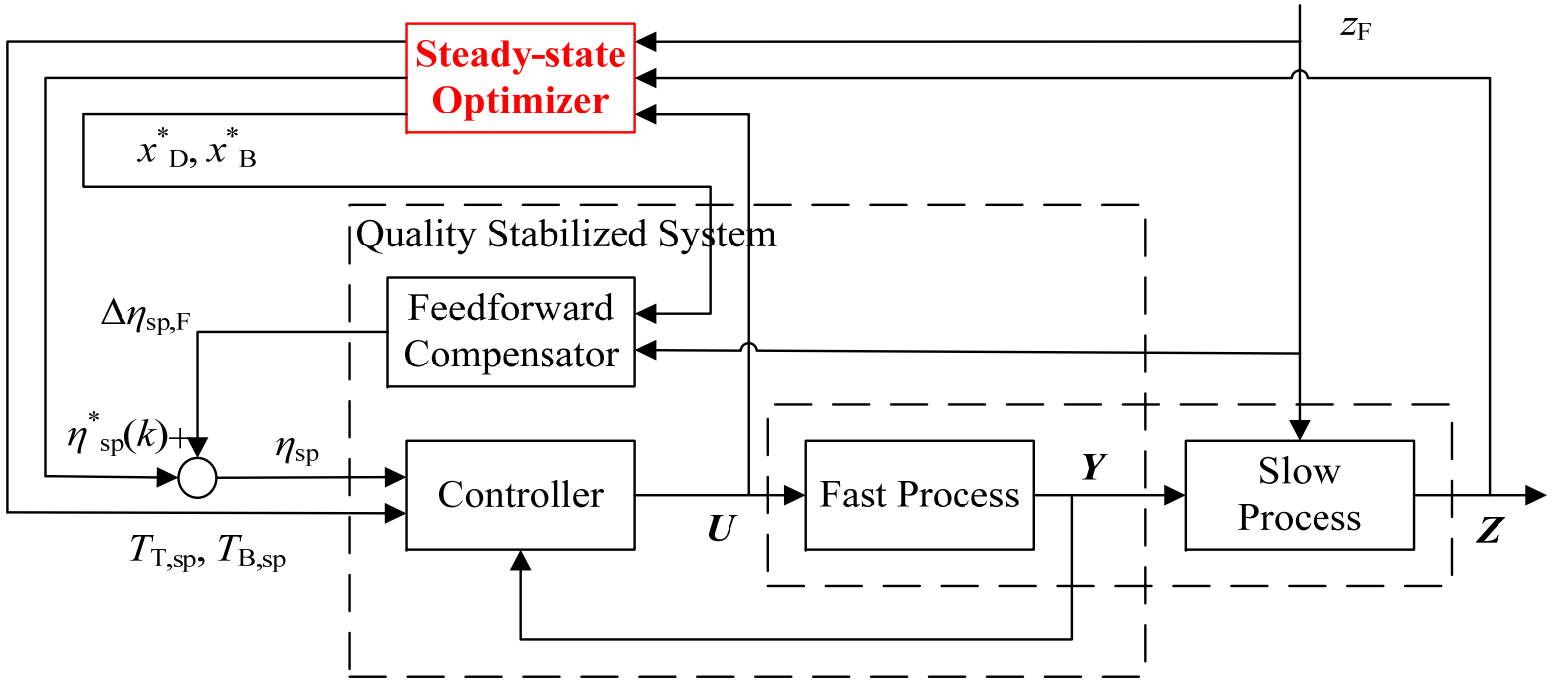
- $\boldsymbol{U} = [R/F,\ Q/F]^T$, $\boldsymbol{Y} = [\eta,\ T_T,\ T_B]^T$, $\boldsymbol{Z} = [x_D,\ x_B]^T$
- Feedforward compensation based on $\eta = D/B = -\dfrac{z_F - x_B}{z_F - x_D}$

Optimization of the Operation Point

- (Assume the distillate with higher price)
  - A (Over-distillation)
  - A→B (To increase yield of distillate)
    - Decrease the reflux ratio until the quality of distillate reaches its limit
    - Meanwhile, the energy cost and the loss of light component are both decreased
  - B→C (To balance the energy cost and the loss)
    - Maintain the quality of distillate
  - C (Optimized operation point)

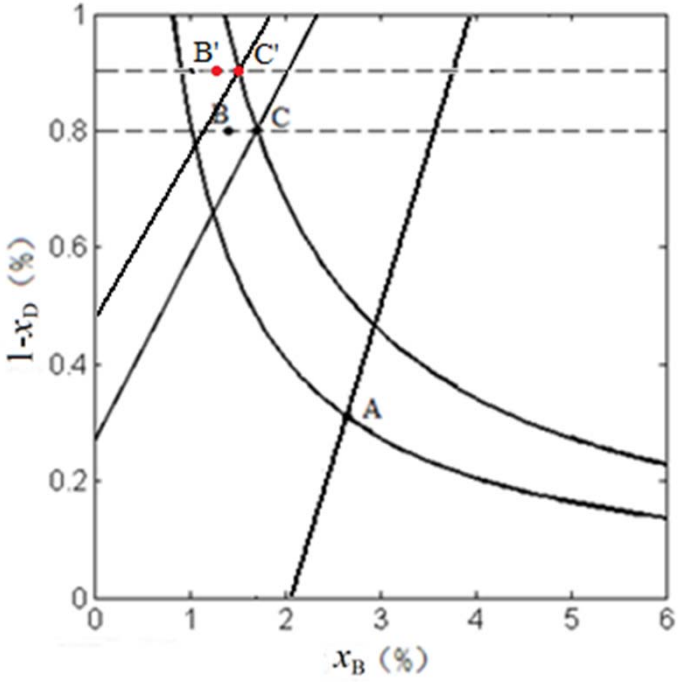


Integrated Control and Optimization Strategy

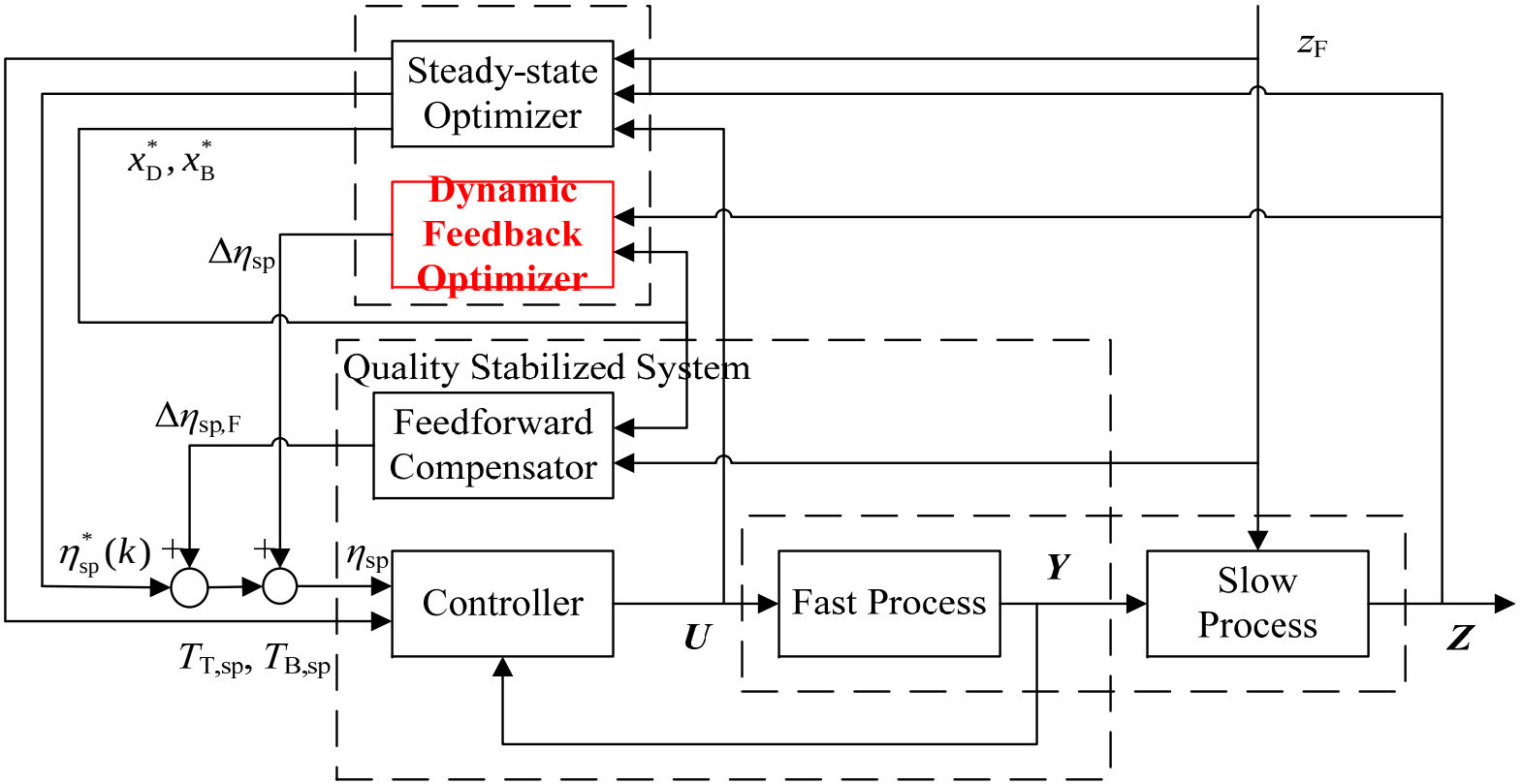


Introduction of Dynamic Feedback Optimization

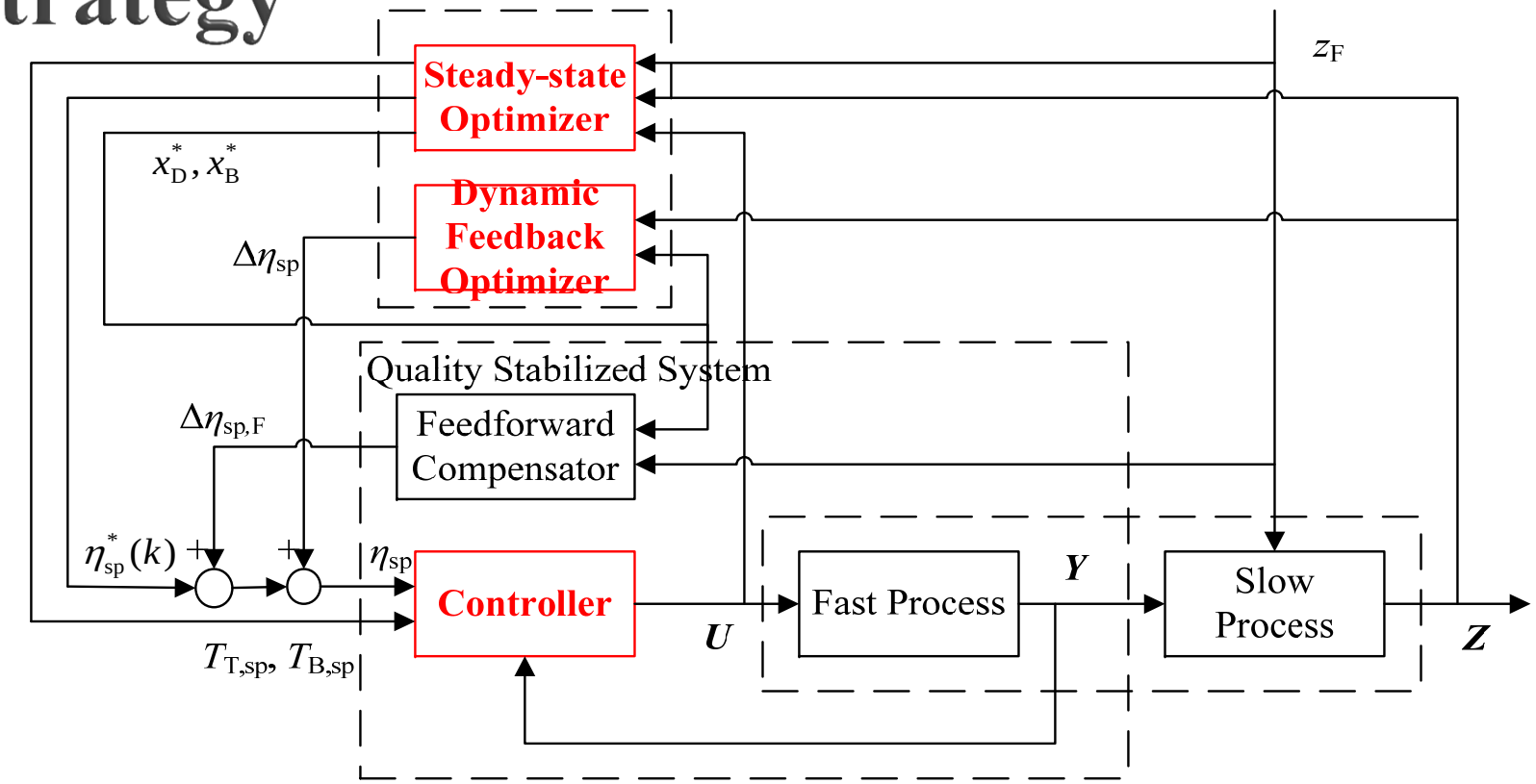
- Why?
  - Mismatch of model
  - Fast quality analyzer is realized
- Optimization based on feedback of quality information
  - Dynamic model
  - Prediction of steady state of quality
  - Model adjustment
- Decrease the margin between the actual limit and the required limit



Integrated Control and Optimization Strategy



Data-driven Models used by the Strategy



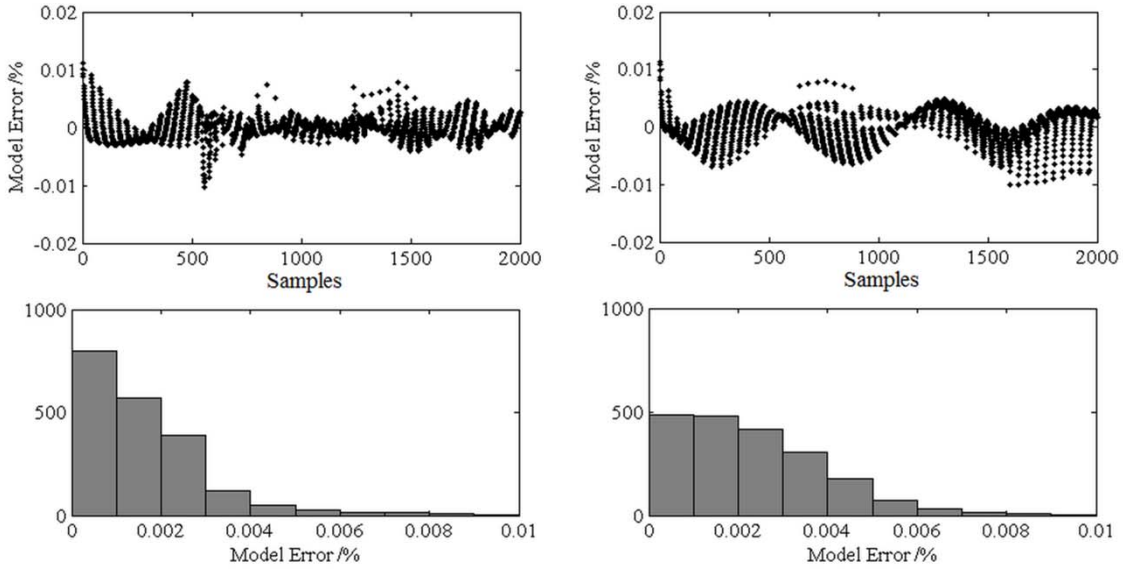
- 2 dynamic models (Controller, Dynamic feedback optimizer)
- 1 steady state model (Steady-state optimizer), namely surrogate model

Identification of Dynamic Model

- Traditional dynamic model
  - Multi-input-multi-output
  - Transfer function
  - Step response
- Traditional identification method
  - Least square
  - From MatLab

Build Surrogate Model

- RBF NN model
- AHH (Adaptive Hinging Hyperplanes) model



- AHH (25, 0.0022%) RBF (27, 0.0026%)
  - Smaller number of base function but with higher accuracy

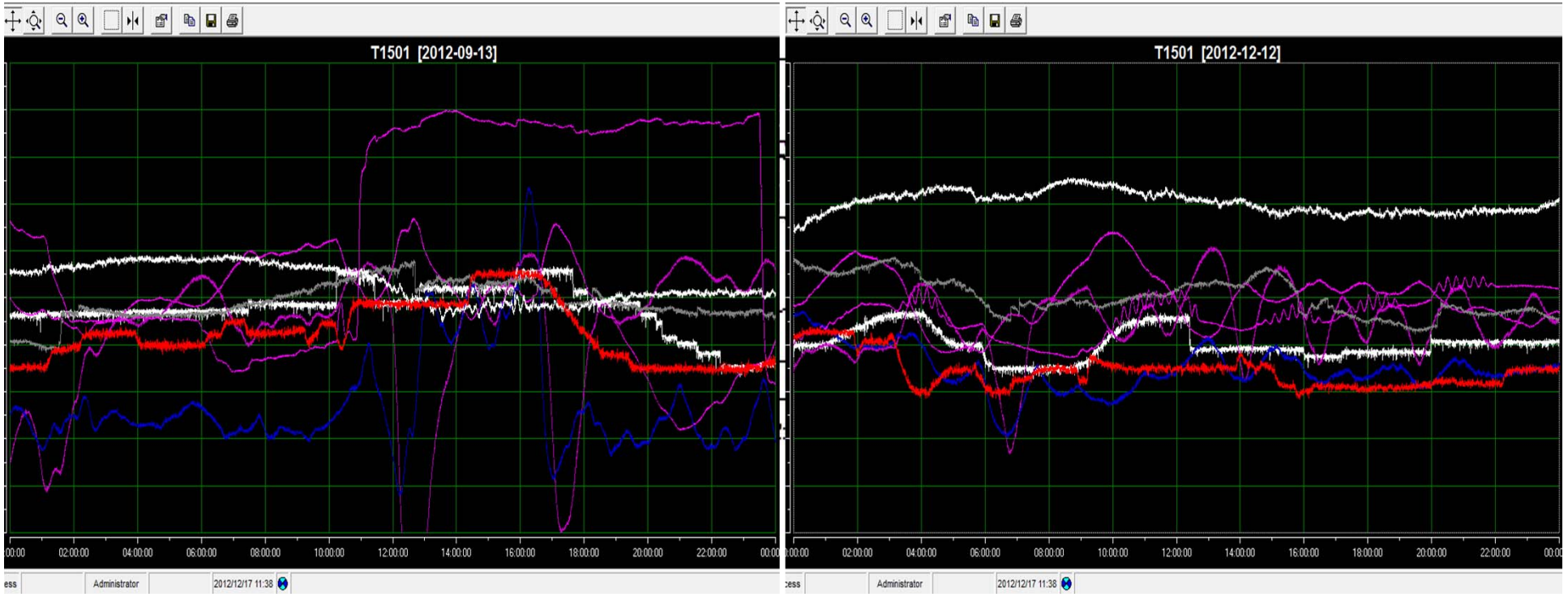
Solve the Optimization Problem

- DE (Differential Evolution) method
- PLP (Piecewise Linear Programming) method
  - Nonlinear optimization → Sequence of linear optimization
  - Decreased computation load
- Comparaison of computation time (18 times, optimization per 4 hours in 72 hours)

	AHH-PLP	RBF-DE
Average /s	10.381	53.830
Variance	0.127	1.061

Application Case 1

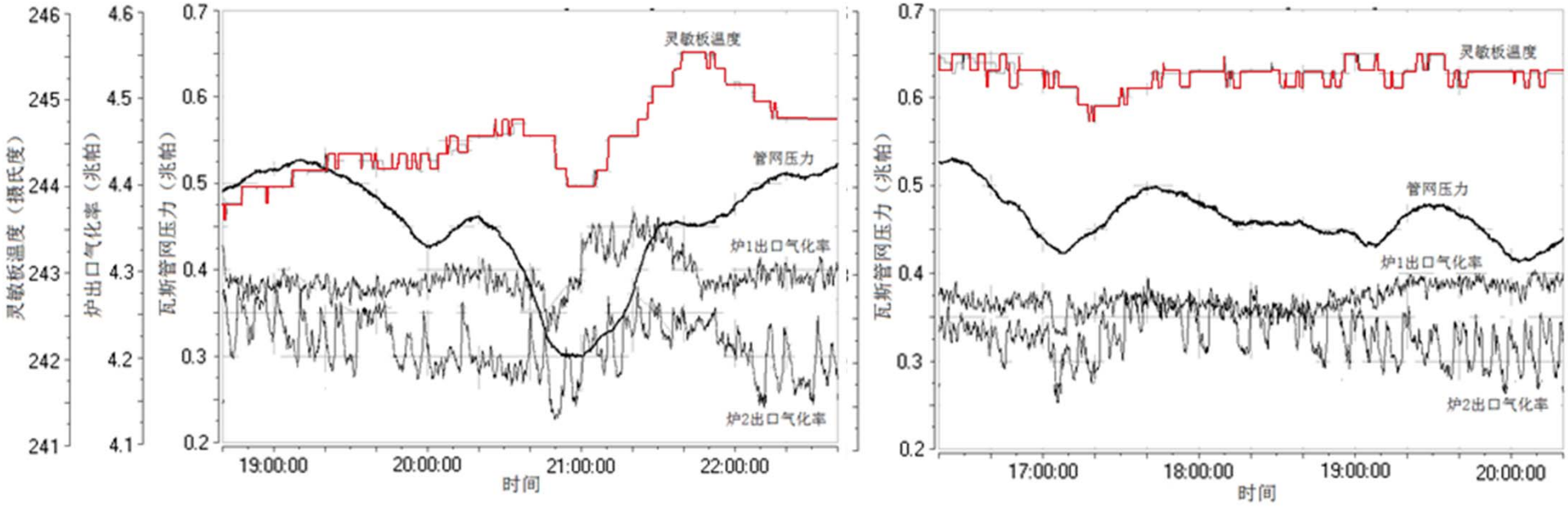
- Gas Fractionation (200 kilo ton/yr)



  - Benefit about 5.665 million yuan (11 months)
  - About 0.605 million yuan from energy saving

Application Case 2

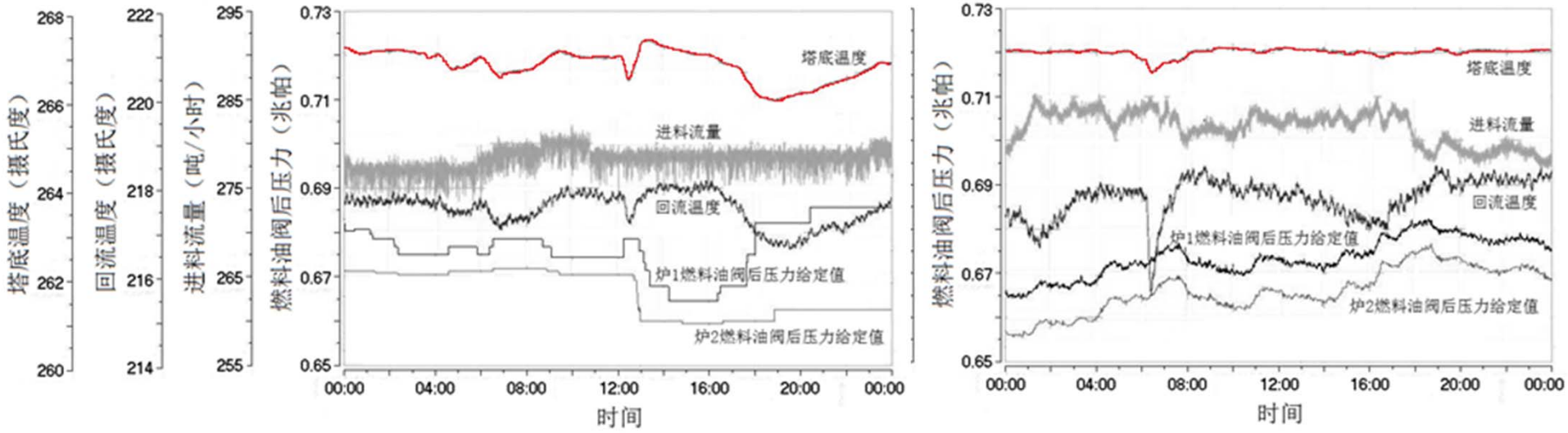
- Xylene distillation of aromatic hydrocarbon production (400 kilo ton/yr)



- PID APC
  - Energy cost decreased by 8.2 (kg Oil)/ton (i.e. 3.38%), Fuel oil saving about 3.28 kilo ton/yr

Application Case 3

- Xylene distillation of PX production (450 kilo ton/yr)



PID APC

- Energy cost decreased by 6.318 (kg Oil)/ton
- Benefit above 13.027 million yuan/yr
- About 5.6862 million yuan/yr from energy saving

Thank you very much!