Biological-Chemical Reactor Control

Principles and Methods for Improving Product Quality and Optimizing Production Rate
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Top Ten Things You Don’t Want to Hear in a Project Definition Meeting

- (10) I don’t want any smart instrumentation talking back to me
- (9) Let’s study each loop to see if the valve really needs a positioner
- (8) Let’s slap an actuator on our piping valves and use them for control valves
- (7) We just need to make sure the control valve spec requires the tightest shutoff
- (6) What is the big deal about process control, we just have to set the flow per the PFD
- (5) Cascade control seems awfully complex
- (4) The operators can tune the loops
- (3) Let’s do the project for half the money in half the time
- (2) Let’s go with packaged equipment and let the equipment supplier select and design the automation system
- (1) Let’s go out for bids and have purchasing pick the best deal
Introduction

- Biological and chemical process performance is largely determined by reactor performance. The stage for product quality and process efficiency and capacity is set by reaction yield and selectivity.
- An increase in yield can be used to increase production rate for same feed rate or used to decrease raw material costs for the same production rate.
- For batch reactors, an increase in yield can be taken as shorter cycle time for the same charges or as smaller charges for the same cycle time.
- A higher yield reduces downgraded products, recycle, and waste.
- Reactor type, reaction rate, and time available for reaction affect yield.
- Temperature, concentration, and sometimes pressure affect reaction rate.
- Inventory and feed rate determines the amount of time reactants are in reactor (residence time), which determines time available for reaction.
- Process control of temperature, concentration, pressure, inventory, and feed rate is essential to achieve reaction rate and time for maximum yield.
- Endpoint control inherently prevents the accumulation of excess reactants.
- Valve position control increases reactant feed rate to limits of utility systems.
- Valve position control increases rangeability of utility systems.
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* - Additional control besides temperature and pressure control
Valve position controller (VPC) setpoint is the maximum throttle position. The VPC should turn off integral action to prevent interaction and limit cycles. The correction for a valve position less than setpoint should be slow to provide a slow approach to optimum. The correction for a valve position greater than setpoint must be fast to provide a fast getaway from the point of loss of control. Directional velocity limits in AO with dynamic reset limit in an enhanced PID that tempers integral action can achieve these optimization objectives.
Liquid Reactants (Jacket BFW)
Liquid Product Basic Control

- FC 1-1
- FT 1-1
- LT 1-8
- PT 1-5
- PC 1-5
- FT 1-5
- FC 1-7
- FT 1-7
- LC 1-8
- LY 1-8
- FY 1-6
- FT 1-2
- LC 1-9
- LT 1-9
- BFW

Reactant A: residence time calc
Reactant B: ratio calc
Vent: steam
Product:
Liquid Reactants (Jacket BFW) Liquid Product Optimization

ZC1-4 & ZC-9 are enhanced PID VPC
Gas Reactants (Jacket **BFW**)  
Gas Product Optimization

Fast reaction, short residence time, and high heat release prevents inverse response in manipulation of reactant feed rate for temperature control.

Temperature controller inherently maximizes reactant feed rate to amount permitted by the number of BFW coils in service.
Gas & Liquid Reactants (Jacket CTW)
Liquid Product End Point Control

Pressure control inherently prevents an excess of gas reactant providing endpoint control for liquid product in continuous and fed-batch reactors.
Gas & Liquid Reactants (Jacket CTW)
Gas Product End Point Control

Level control inherently prevents an excess of liquid reactant providing endpoint control for gas product in continuous reactors.
Liquid Reactants (Jacket CTW)
Gas & Liquid Products Basic Control
Liquid Reactants (Jacket CTW)
Gas & Liquid Products Optimization

ZC1-4, ZC-5, & ZC-10 are enhanced PID VPC
A flow controller in the recycle path from reactant in product back as recovered reactant is necessary to prevent a snowballing effect and divergence of reactant concentration. In this case the flow controller is on the reactor discharge and recovery column distillate receiver level controller provides fresh makeup of recycled reactant as needed.
The product discharge flow controller setpoint, which sets reactor production rate can be increased by a VPC to the maximum throttle limit of coolant system valve.
Jacket CTW
Outlet Temperature Control
Jacket CTW
Inlet Temperature Control
Jacket CTW with Steam Injection
Outlet Temperature Control
Reactor Heat Exchanger
Recirc Temperature Control

TT 1-4

product

TC 1-4

CTW
ZC1-4 is an enhanced PID VPC
Jacket Steam & CTW Heat Exchanger
Inlet Temperature Control
Jacket CTW Heat Exchanger
Inlet Temperature Bypass Control
Jacket CTW Heat Exchanger
Inlet Temperature Bypass Optimization

ZC1-4 is an enhanced PID VPC
Reactor Inferential Measurements of Heat Transfer Rate and Conversion

Integration Period is continuous reactor residence time or batch reactor cycle time.
Batch Reactor Concentration Profile Slope Control

- **FY 1-6**: Reactant A feed
- **LY 1-8**: Reactant B feed
- **FT 1-1**: Flow controller
- **FT 1-2**: Flow controller
- **FC 1-1**: Flow controller
- **FC 1-2**: Flow controller
- **CAS 1-8**: Concentration sensor
- **LC 1-8**: Level controller
- **LT 1-8**: Level controller
- **PT 1-5**: Pressure transmitter
- **PC 1-5**: Pressure controller
- **TT 1-3**: Temperature transmitter
- **TC 1-3**: Temperature controller
- **TT 1-4**: Temperature transmitter
- **TC 1-4**: Temperature controller
- **FT 1-1**: Flow transmitter
- **FT 1-2**: Flow transmitter
- **FT 1-7**: Flow transmitter
- **FC 1-7**: Flow controller
- **AC 1-6**: Accumulator
- **DT**: Deadtime
- **DIV**: Divider
- **SUB**: Subtractor
- **ΔPV/Δt**: Slope
- **ΔPV**: Differential pressure
- **ΔPV**: Differential pressure
- **Loop Deadtime**: Loop deadtime
- **product**: Product
- **return**: Return
- **vent**: Vent
- **makeup**: Make up
- **residence time calc**: Residence time calculation
- **ratio calc**: Ratio calculation

The diagram illustrates the flow and control system for a batch reactor, including flow control, concentration monitoring, level measurement, temperature control, and pressure monitoring. The system also includes components for venting and returning material, as well as product extraction.
Innovative PID System to Optimize Ethanol Yield and Carbon Footprint

Production Rate Enhanced PID

Average Fermentation Time Enhanced PID

Fermentable Starch Correction

Feedforward

Backset Recycle

Lag and Delay

Predicted Fermentable Starch

Coriolis Meter
Mammalian Bioreactor With Enhanced DO and pH Control

Inoculums

37 °C

wireless

AT 1-1
pH

AT 1-2
DO

Heater

AC 1-1
0.002 g/L

AC 1-2

Bicarbonate

MFC - Mass Flow Controller
VSD - Variable Speed Drive

AC1-1 and AC1-2 are Enhanced PID

7.0 pH

0.002 g/L

Bioreactor

spargers

OFF-gas

Calc

Glucose

Glutamine

Media

AT 1-9
Mass Spec

Spec

Calc

AT 1-4s1
Glucose

AT 1-4s2
Glutamine

AT 1-6
Product

MFC - Mass Flow Controller

VSD - Variable Speed Drive

CO₂

MFC

O₂

MFC

Air

O₂

MFC

Product

AT 1-5x2
Dead Cells

AT 1-5x1
Viable Cells

Viable

Cells

Dead

Cells

0.002 g/L

7.0 pH

37 °C

AC 1-1

AC 1-2

Splitter

AY 1-1

AY 1-2

AY 1-1

AC 1-1

AC 1-2

AY 1-2

AY 1-2

AY 1-1
Mammalian Bioreactor With Enhanced Substrate Control

- MFC - Mass Flow Controller
- VSD - Variable Speed Drive

Substrate (Glutamine/Glucose) Ratio Control with OUR Feedforward
Top Ten Reasons Why an Automation Engineer Makes a Great Spouse or at Least a Wedding Gift

- (10) Reliable from day one
- (9) Always on the job
- (8) Low maintenance (minimal grooming, clothing, and entertainment costs)
- (7) Many programmable features
- (6) Stable
- (5) Short settling time
- (4) No frills or extraneous features
- (3) Relies on feedback
- (2) Good response to commands and amenable to real time optimization
- (1) Readily tuned
Enhanced PID Algorithm
Originally Developed for Wireless

- PID integral mode is restructured to provide integral action to match the process response in the elapsed time (reset time set equal to process time constant)
- PID derivative mode is modified to compute a rate of change over the elapsed time from the last new measurement value
- PID reset and rate action are only computed when there is a new value
- If transmitter damping is set to make noise amplitude less than communication trigger level, valve packing and battery life is dramatically improved
- Enhancement compensates for measurement sample time suppressing oscillations and enabling a smooth recovery from a loss in communications further extending packing/battery life

Link to Enhanced PID White Paper

Hyclone 100 liter Single Use Bioreactor (SUB)
Rosemount WirelessHART gateway and transmitters for measurement and control of pH and temperature. (pressure monitored)
BioNet lab optimized control system based on DeltaV
Wireless Bioreactor pH
Gain 30 Reset 1200
Wireless Bioreactor Temperature
Gain 40 Reset 500

Output comes off high limit at 36.8 °C
0.30 °C overshoot
Wireless Bioreactor Temperature
Gain 40 Reset 5000

Output comes off high limit at 35.9 °C

0.12 °C overshoot
Wireless Bioreactor Temperature
Gain 40 Reset 10000

0.13 °C overshoot
Output comes off high limit at 36.1 °C
Wireless Bioreactor Temperature
Gain 40 Reset 15000

0.20 °C overshoot
Output comes off high limit at 36.4 °C
Wireless Bioreactor Temperature
Gain 80 Reset 15000

Best Tuning: < 0.01 °C overshoot for Gain = 80 Reset = 5000

0.11 °C overshoot
Output comes off high limit at 36.1 °C
Mammalian Bioreactor With Viable Cell and Product Profile Control

- MFC - Mass Flow Controller
- VSD - Variable Speed Drive
- AC - Air Compressor
- AY - Air Y-Piece
- VSD - Variable Speed Drive
- TC - Temperature Controller
- TT - Temperature Transmitter
- LT - Level Transmitter
- AT - Air Transmitter
- Glucose
- Glutamine
- pH
- DO
- BIocarbonate
- Splitter
- Bioreactor
- Off-gas
- Mass Spec
- MFC - Mass Flow Controller
- Wireless
- Enhanced PID
- O2
- CO2
- Dead Cells
- Viable Cells
- Calc
- MPC
- OUR
- Product
- Growth Rate
- Product Formation Rate
- Calc
Model Predictive Control (MPC)
Identified Responses for Profile
Model Predictive Control (MPC) Profile Control Test
Model Predictive Control (MPC) Profile Control Cycle Time Reduction
Model Predictive Control (MPC) Profile Control Improved Predictions
Loop Block Diagram (First Order Approximation)

First Order Approximation: \( \theta_o \cong \theta_v + \theta_{p1} + \theta_{p2} + \theta_{m1} + \theta_{m2} + \theta_c + \tau_v + \tau_{p1} + \tau_{m1} + \tau_{m2} + \tau_{c1} + \tau_{c2} \)

(set by automation system design for flow, pressure, level, speed, surge, and static mixer pH control)

Delay <=> Dead Time
Lag <=> Time Constant

For integrating processes: \( K_i = K_v \cdot (K_p / \tau_{p2}) \cdot K_m \)

100% / span

½ of Wireless Default Update Rate
Open Loop Response of Self-Regulating Process

% Controlled Variable (%PV)

or

% Controller Output (%CO)

For CSTR $\tau_o >> \theta_o$ process response appears to ramp for 10 $\theta_o$ and is termed a “near-integrating” process.

For plug flow reactor and the manipulation of feed $\theta_o >> \tau_o$ process response is a transport delay and is termed “deadtime dominant”.

$K_o = \frac{\Delta%PV}{\Delta%CO}$

Self-regulating process gain (%/%)
Open Loop Response of Integrating Process

Response to change in controller output with controller in manual

\[ K_i = \left\{ \left[ \frac{\%PV_2}{\Delta t_2} \right] - \left[ \frac{\%PV_1}{\Delta t_1} \right] \right\} / \Delta\%CO \]

Integrating process gain (%/sec/%)

- % Process Variable (%PV)
- % Controller Output (%CO)

Maximum speed in 4 deadtimes is critical speed

Wireless Trigger Level > Noise

Wireless Default Update Rate

- Ramp rate is \( \Delta\%PV_1 / \Delta t_1 \)
- Ramp rate is \( \Delta\%PV_2 / \Delta t_2 \)

- Observed total loop deadtime

- Time (seconds)

Wireless default update rate must be fast enough that excursion for maximum ramp rate is less than wireless trigger level that is set just larger than measurement noise
Open Loop Response of Runaway Process

% Process Variable (%PV) or % Controller Output (%CO)

Wireless presently not advisable for runaway

Tests are terminated before a noticeable acceleration leading to characterization as an integrating process

\[
K_o = \frac{\Delta PV}{\Delta CO}
\]

Runaway process gain (%/%)

Acceleration

Maximum speed in 4 deadtimes is critical speed

For safety reasons, tests are terminated after 4 deadtimes

1.72\(\Delta PV\)

\(\Delta CO\)

Observed total loop deadtime

\(\theta_o\)

\(\tau_o^p\) must be \(\tau_{p2}^p\)

Runaway process open loop positive feedback time constant

Time (seconds)

Response to change in controller output with controller in manual

Maximum speed in 4 deadtimes is critical speed
Near Integrator Gain Approximation

For “Near Integrating” gain approximation use maximum ramp rate divided by change in controller output.

The maximum ramp rate is found by passing filtered process variable (PV) through a deadtime (DT) block to create an old process variable. The deadtime block uses the total loop deadtime ($\theta_o$) for the time interval ($\Delta t$). The old process variable is subtracted from the new process variable and divided by the time interval to get the ramp rate. The maximum of a continuous train of ramp rates updated each module execution over a period of 3 or more deadtimes is selected to compute the near integrating process gain. For an inverse response or large secondary time constant, the computation may need to continue for 10 or more deadtimes.

$$K_i = \frac{K_o}{\tau_o} = Max(\Delta\%PV / \Delta t) / \Delta\%CO$$

The above equation can be solved for the process time constant by taking the process gain to be 1.0 or for more sophistication as the average ratio of the controlled variable to controller output.

Tuning test can be done for a setpoint change if the PID gain is > 2 and the PID structure is “PI on Error D on PV” so you see a step change in controller output from the proportional mode.
The near integrating test time (3 deadtimes) as a fraction of the self-regulating test (time to steady state is taken as 98% response time $T_{SR} = T_{98} = \theta_o + 4 \tau_o$) is:

$$T_{NI} = \frac{3 * \theta_o}{\theta_o + 4 * \tau_o} * T_{SR}$$

If the process time constant is greater than 6 times the deadtime

$$\tau_o \geq 6 * \theta_o$$

Then the near integrating tuning test time is reduced by > 90%:

$$T_{NI} \leq 0.1 * T_{SR}$$

For example:

$$\tau_o = 100 \text{ sec} \quad \theta_o = 4 \text{ sec}$$

The near integrator tuning time is reduced by 97%!

$$T_{NI} \leq 0.03 * T_{SR}$$
K_o = PV_0 / CO_0 process gain approximation
\( \tau_o = K_o / K_i \) negative feedback time constant
\( \tau'_o = K_o / K_i \) positive feedback time constant

Methodology extends beyond loops to any process variable that can be measured and any variable that can be changed

For the manipulation of jacket temperature to control vessel temperature, the near integrator gain is

\[ K_i = \frac{(U * A)}{(C_p * M_o)} \]

Since we generally know vessel volume (liquid mass), heat transfer area, and process heat capacity, we can solve for overall heat transfer coefficient (least known parameter) to provide a useful ordinary differential equation (ODE) for a first principle model (1).
The observed deadtime ($\theta_o$) and integrator gain ($K_i$) are identified after a change in any controller output (e.g. final control element or setpoint) or any disturbance measurement. The identification of the integrator gain uses the fastest ramp rate over a short time period (e.g. 2 dead times) at the start of the process response.

The models are not restricted to loops but can be used to identify the relationship between any variable that can be changed and any affected process variable that can be measured.

The models are used for processes that are have a true integrating response or slow processes with a “near integrating” response ($\tau_o > 5*\theta_o$). The process deadtime and integrating process gain can be used for controller tuning and for plant wide simulations including but not limited to the following types of models:

Model 1: Hybrid ordinary differential equation (ODE) first principle and experimental model
Model 2: Integrating process experimental model
Model 3: Slow self-regulating experimental model
Model 4: Slow non-self-regulating positive feedback (runaway) experimental model

Patent disclosure filed on 3-1-2010
Peak error is proportional to the ratio of loop deadtime to 63% response time
(Important to prevent SIS trips, relief device activation, surge prevention, and RCRA pH violations)

Total loop deadtime that is often set by automation design

\[ E_x = \frac{\theta_o}{(\theta_o + \tau_o)} \times E_o \]

Largest lag in loop that is ideally set by large process volume

Integrated error is proportional to the ratio of loop deadtime squared to 63% response time
(Important to minimize quantity of product off-spec and total energy and raw material use)

\[ E_i = \frac{\theta_o^2}{(\theta_o + \tau_o)} \times E_o \]

Wireless default update rate affects ultimate performance limit because ½ of default update rate is additional loop deadtime
Peak error decreases as the controller gain increases but is essentially the open loop error for systems when total deadtime $\gg$ process time constant

$$E_x = \frac{1}{(1 + K_o * K_c)} * E_o$$

Integrated error decreases as the controller gain increases and reset time decreases but is essentially the open loop error multiplied by the reset time plus signal delays and lags for systems when total deadtime $\gg$ process time constant

$$E_i = \frac{T_i + \Delta t_x + \tau_f}{K_o * K_c} * E_o$$

Rise time (time to reach a new setpoint) is inversely proportional to controller gain

$$T_r = \frac{\Delta SP}{(K_i \min(|\Delta CO_{max}|, SP_{ff} + K_c * \Delta SP)) + \theta_o}$$
## Fastest Controller Tuning
(Reaction Curve Method*)

### For self-regulating processes:

* - Ziegler Nichols method closed loop modified to be more robust and less oscillatory

\[ K_c = 0.4 \times \frac{\tau_o}{K_o \times \theta_o} \]

\[ T_i = 4 \times \theta_o \]

\[ T_d = \tau_{p1} \]

Near integrator (\( \tau_{p2} \gg \theta_o \)):

\[ K_c = 0.4 \times \frac{1}{K_i \times \theta_o} \]

\[ T_i = 4 \times \theta_o \]

\[ T_d = \tau_{p1} \]

### For integrating processes:

\[ K_c = 0.5 \times \frac{1}{K_i \times \theta_o} \]

\[ T_i = 4 \times \theta_o \]

\[ T_d = \tau_{p1} \]

### For runaway processes:

\[ K_c = 0.6 \times \frac{\tau'_o}{K_o \times \theta_o} \]

\[ T_i = 40 \times \theta_o \]

\[ T_d = 2 \times \tau_{p1} \]

Near integrator (\( \tau'_{p2} \gg \theta_o \)):

\[ K_c = 0.6 \times \frac{1}{K_i \times \theta_o} \]

These tuning equations provide maximum disturbance rejection but will cause some overshoot of setpoint response

Wireless default update rate affects fastest controller tuning because \( \frac{1}{2} \) of default update rate is additional loop deadtime

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* - Ziegler Nichols method closed loop modified to be more robust and less oscillatory

1.0 for Enhanced PID if Wireless Default Update Rate > Process Response Time!
Effect of Wireless Measurement Update Time and Interval on Performance

\[ E_x = \frac{\theta_o + \theta_w + \theta_v}{T_{63}} \times E_o \]
\[ E_i = \frac{(\theta_o + \theta_w + \theta_v)^2}{T_{63}} \times E_o \]
\[ T_{63} = \theta_o + \theta_w + \tau_o \]

\[ \theta_w = \text{Min}(\theta_{\Delta T}, \theta_S) \]
\[ \theta_{\Delta T} = 0.5 \times \Delta T_w \]
\[ \theta_S = \frac{0.5 \times S_m}{(\Delta \% PV / \Delta t)_{\text{max}}} \]

\[ (\Delta \% PV / \Delta t)_{\text{max}} = K_i \times (E_o / K_o) \]
\[ K_i = \frac{K_o}{\tau_o} \]
\[ (\Delta \% PV / \Delta t)_{\text{max}} = \frac{E_o}{\tau_o} \]

\[ \theta_S = \frac{0.5 \times S_m \times \tau_o}{E_o} \]
Additional Deadtime from Valve Stick-Slip, Resolution, or Deadband

\[
\theta_v = \frac{0.5 \times S_v}{(\Delta\% CO / \Delta t)_{\text{max}}}
\]

\[
(\Delta\% CO / \Delta t)_{\text{max}} = K_c \times (\Delta\% PV / \Delta t)_{\text{max}}
\]

\[
K_c = \min \left[ \frac{K_x \times \tau_o}{K_o \times \theta_o}, \frac{S_v}{\max[(N_m - S_m), 0.002]} \right]
\]

\[
(\Delta\% PV / \Delta t)_{\text{max}} = \frac{E_o}{\tau_o}
\]

\[
(\Delta\% CO / \Delta t)_{\text{max}} = \frac{K_x \times E_o}{K_o \times \theta_o}
\]

\[
\theta_v = \frac{0.5 \times S_v \times K_o \times \theta_o}{K_x \times E_o}
\]

Increase in process gain from elimination of controller reaction to noise by wireless trigger level or PID threshold sensitivity setting decreases deadtime from valve stick-slip, resolution, or deadband.
Nomenclature
(Process Dynamics & Performance)

$\Delta CV =$ change in controlled variable (change in process variable in % of scale)
$\Delta CO =$ change in controller output (%)
$K_c =$ controller gain (dimensionless)
$K_i =$ integrating process gain (%/sec/% or 1/sec)
$K_p =$ process gain (dimensionless) also known as open loop gain
$DV =$ disturbance variable (engineering units)
$MV =$ manipulated variable (engineering units)
$PV =$ process variable (engineering units)
$\Delta SP =$ change in setpoint (engineering units)
$SP_{ff} =$ setpoint feedforward (engineering units)
$\Delta t =$ change in time (sec)
$\Delta t_x =$ execution or update time (sec)
$\theta_o =$ total loop dead time (sec)
$\tau_f =$ filter time constant or well mixed volume residence time (sec)
$\tau_m =$ measurement time constant (sec)
$T_{p2} =$ primary (large) self-regulating process time constant (sec)
$\tau_{p2} =$ primary (large) runaway process time constant (sec)
$\tau_{p1} =$ secondary (small) process time constant (sec)
$T_i =$ integral (reset) time setting (sec/repeat)
$T_d =$ derivative (rate) time setting (sec)
$T_r =$ rise time for setpoint change (sec)
$\tau_o =$ oscillation period (sec)
$\lambda =$ Lambda (closed loop time constant or arrest time) (sec)
$\lambda_f =$ Lambda factor (ratio of closed to open loop time constant or arrest time)
Nomenclature
(Wireless Dynamics & Performance)

\( E_i \) = integrated error for unmeasured load disturbance (% sec)
\( E_x \) = peak error for unmeasured load disturbance (%)
\( E_o \) = open loop error (loop in manual) for unmeasured load disturbance (%)
\( K_i \) = near integrator process gain (% per % per sec)
\( K_o \) = open loop gain (product of valve, process, and measurement gains) (dimensionless)
\( K_x \) = detuning factor for controller gain (dimensionless)
\( N_m \) = measurement noise (%)
\( \Delta \% CO/\Delta t \) = rate of change in PID % controller output (% per sec)
\( \Delta \% PV/\Delta t \) = rate of change in PID % process variable (% per sec)
\( \Delta T_w \) = wireless default update rate (update time interval) (sec)
\( S_m \) = wireless measurement trigger level (threshold sensitivity) (%)
\( S_v \) = valve stick-slip, resolution, or deadband (%)
\( T_{63} \) = 63% process response time (sec)
\( \theta_o \) = original loop deadtime (sec)
\( \theta_{\Delta t} \) = additional deadtime from default update rate (sec)
\( \theta_s \) = additional deadtime from wireless trigger level (sec)
\( \theta_v \) = additional deadtime from valve (sec)
\( \theta_w \) = additional deadtime from wireless measurement (sec)
\( \tau_o \) = self-regulating open loop time constant (largest time constant in loop) (sec)
\( \tau'_o \) = runaway open loop time constant (largest time constant in loop) (sec)
Key Insights

- A liquid or solids phase reaction without a continuous liquid or solids discharge flow is the distinguishing characteristic of batch and fed-batch.
- There is generally no level control except perhaps in terms of a high level override or high level shutdown of feeds in batch and fed-batch reactors.
- In batch reactors, the reactants are fed sequentially and shutoff when charge tank weight or flow totals indicate the total charged is complete.
- In fed-batch operation, the reactants are fed simultaneously under flow control at a rate determined by a control system.
- Many of the same controls used for continuous reactors are applicable to fed-batch except typically there is no level or residence time control.
- There is a profile of temperature, physical properties, and composition with respect to length for a plug flow reactor and with respect to batch time for a fed-batch vessel. In both types of reactors opportunities exist for profile control and optimization. The temperature may be controlled at various setpoints depending upon length and time. Since composition generally goes in one direction only with length and time, the slope is controlled at points in length and time for composition profile control.
Key Insights

- Gas phase reactors are generally continuous with a short tight residence time.
- The process deadtime from transportation delay of gas reactants is small compared to the lags from catalyst heat capacity and thermowell design.
- Fast temperature control is possible by manipulation of gas reactant flows.
- Mature high capacity products (e.g. oil, gas, and petrochemicals) tend to use continuous reactors whereas new high value processes (e.g. specialty chemical and biological) primarily use batch and fed-batch reactors.
- The fastest and simplest implementation is batch with quantities charged sequentially mimicking lab experiments. As knowledge is gained batch reactors can become fed-batch reactors and eventually continuous reactors if there is enough demand and chemistry permits a variable residence time.
- Candidates for continuous reactors are products with a low profit margin, high volume requirement, fast reaction, minimal adverse reactions, preventable buildup of inhibitors and inactive components, and an extensive R&D history.
- Candidates for batch reactors are products with a high profit margin, low volume requirement, slow reaction, significant side effects, and minimal R&D.
Key Insights

- Reactors have 3 types of dynamic responses observed when the PID is put in manual and a step change is made in PID output with no disturbances.
  - If the response lines out at a steady state, the process is “**self-regulating**.”
  - If the response continues to ramp (no steady state), the process is “**integrating**.”
  - If the response continues to accelerate, the process is “**runaway**.”
- Inverse response can occur in any of the above responses when the initial response is in the opposite direction of eventual response.
  - Temperature control by manipulation of cold feed can exhibit an inverse response.
- A CSTR has a slow self-regulating response.
- A batch and fed-batch reactor has a slow integrating response.
- A plug flow and gas phase reactor has a fast self-regulating response.
- All of these reactors can develop a runaway response when the increase in reaction heat release with temperature exceeds the cooling capability.
Key Insights

- Reaction rate depends upon temperature and composition.
- To prevent an excess or deficiency of reactants, the reactant concentration must be in the ratio set by the stoichiometric equation for the reaction.
- High capacity products such as petrochemicals and intermediates greatly depend upon the added value of chromatographs because even a fractional percent increase in production rate is millions of dollars.
- Biological reactions utilize a wide variety of composition measurements including potentiometric and amperimetric electrodes for substrates and waste products, and dielectric spectroscopy and digital imagery for viable cell concentration, and near infrared (NIR) spectroscopy for compounds.
- The average amount of time reactants stay in contact is called residence time in continuous operations and is simply volume divided by flow rate.
- For fed-batch and batch, batch cycle time is used instead of residence time.
- In batch reactors, the batch cycle time is often longer than necessary.
- The process dynamics for vessels offer incredibly tight concentration, level, pH, pressure, and temperature control.
Resource

Advanced Temperature Measurement and Control - 2nd Ed has a lot of details on how to improve temperature sensor accuracy and temperature control of heat exchangers, reactors, and kilns.

Biological and Chemical Reactor Control is an ISA book whose kernel is the ISA Automation Week tutorial. The book will be available in December just in time for the holidays. Surprise your spouse with the book as a “gift that keeps on giving.” Your spouse will never let you forget it.