

An Introduction to Mechanistic Models and Control Theory

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Outline



- Mechanistic (first-principles) modeling.
- Control engineering concepts (with emphasis on feedback control).
- Brief thoughts on
 - Dynamic modeling using system identification.
 - Model Predictive Control.



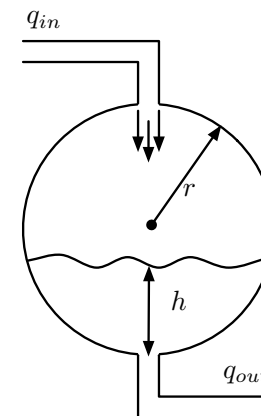
About this talk



- We will rely on a representative example to describe how mechanistic modeling and control theory can be used to “manage” the dynamic behavior of systems.
- Talk will be focused on concepts; not a survey.
- Main conclusions:
 - Control theory offers a means to alter the behavior of uncertain, nonlinear dynamical systems from *undesirable* to *desirable*, and to *transfer variability* from an expensive system resource to a less expensive one.
 - Biased / “erroneous” models can be good for control design, when sensibly used.
 - *System identification* can be used to obtain models needed for control under conditions involving noise and uncertainty.



“Fishbowl” Modeling and Control



- Manipulate the volumetric rate of inflow q_{in} in a spherical tank (aka a “fishbowl”) to keep level h at a desired value, despite varying and unpredictable changes in the volumetric outflow q_{out} .



- Can you find a spherical tank in this picture?

- A mechanistic model is a set of equations based on known physical and chemical relationships that can be used to *predict* the behavior of a system.
- The accuracy requirements for the model will be influenced by the intended application and its performance requirements.
- Also referred to as *white-box* or *first-principles* models.

- Mechanistic dynamical models of systems can be classified according to the following criteria:
 - linear vs. nonlinear;
 - continuous-time vs. discrete-time,
 - lumped parameter vs. distributed parameter.
- *Conservation* and *accounting* of extensive properties form the basis for mechanistic modeling of physical systems.

- Conserved properties of a system include:
 - Total Mass
 - Total Energy
 - Net Charge
 - Linear Momentum
 - Angular Momentum
- Quantities such as species mass, mechanical energy, thermal energy, electrical energy, and entropy are not conserved in a system, but nonetheless these can be *accounted*.

Accounting Principle:

$$\begin{array}{rcl} \text{Accumulation within} & = & \text{Inflow through} \\ \text{the System} & & \text{the System} \\ & & \text{Boundaries} \\ & + & \text{Generation within} \\ & & \text{the System} \\ & - & \text{Outflow through} \\ & & \text{the System} \\ & & \text{Boundaries} \\ & - & \text{Consumption} \\ & & \text{within the System} \end{array}$$

Conservation Law:

$$\begin{array}{rcl} \text{Accumulation within} & = & \text{Inflow through} \\ \text{the System} & & \text{the System} \\ & & \text{Boundaries} \\ & - & \text{Outflow through} \\ & & \text{the System} \\ & & \text{Boundaries} \end{array}$$

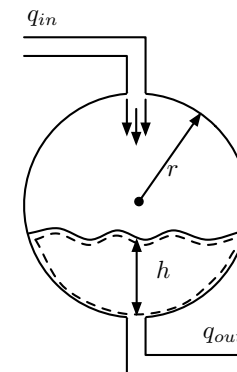
The model's purpose will highlight the relevant properties that need to be conserved or accounted for:

- How does pressure change in a closed vessel with increasing gas inflow?
 - *Conservation of mass*
- How does level change in a tank when pump speed is increased?
 - *Conservation of mass*
- How does temperature change in a tank when heater current is increased?
 - *Conservation of energy*
- How does concentration of a reactant A change in a chemical reactor (where $A \rightarrow B$)?
 - *Accounting of species A*

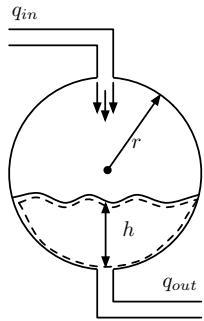
- Define the extensive property (or properties) that we need to account for.
- Define the system(s) that we wish to analyze, with system boundaries.
- Define the time period for the analysis.
- Apply the general accounting statement or conservation law, as appropriate.

Note: differential ("rate") and integral ("accumulation") forms exist and one statement may be more useful than the other, depending on the problem being analyzed.

- Take advantage of constitutive relationships and make reasonable assumptions to express the model in a suitable working form.



- Modeling goal: to predict how level (h) changes as a result of changes in the volumetric inflow q_{in} and outflow q_{out} .
- Relevant conserved property: total mass.
- System: mass m_T in the tank; time scale: minutes to hours.



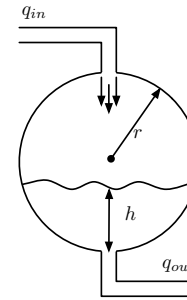
$$\frac{dm_T}{dt} = m_{in} - m_{out}$$

$$\frac{d(V\rho)}{dt} = \rho q_{in} - \rho q_{out}$$

$$V = \frac{\pi}{3} h^2 (3r - h)$$

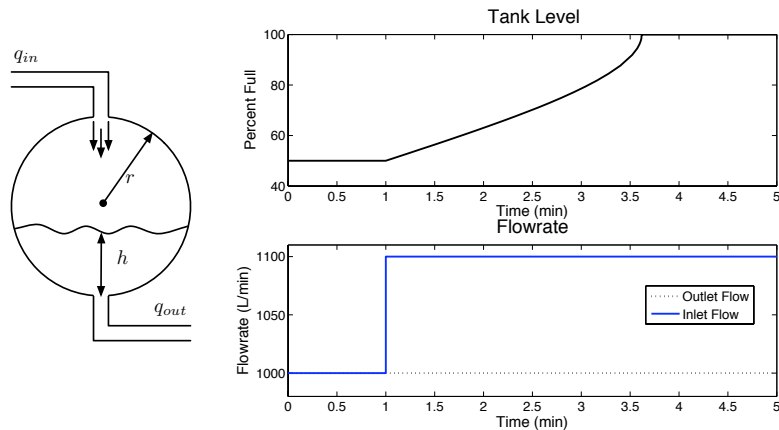
ρ = Density

- The rate statement for the conservation of mass states that the rate of accumulation (dm_T/dt) is equal to the rate of mass inflow m_{in} minus the rate of mass outflow m_{out} .
- Assume constant density ρ for all streams and a flat liquid surface (i.e., ignore “waviness”).
- The constitutive relationship between volume V and level h is needed.

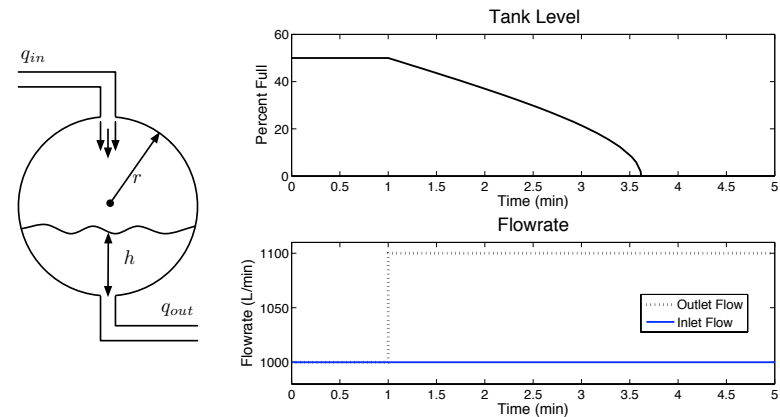


$$\frac{dh}{dt} = \frac{q_{in} - q_{out}}{\pi h (2r - h)}$$

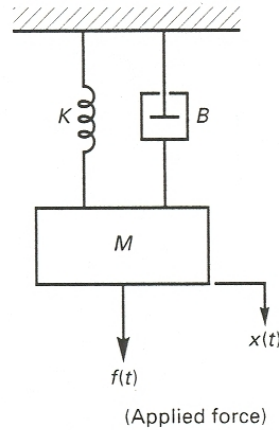
- Applying the Chain Rule and a little algebra yield an ordinary differential equation (ODE) that describes the effect of system inputs (volumetric inflow q_{in} and outflow q_{out}) to the system output (level h).
- The ODE is the basis of a *lumped parameter* model representation amenable to numerical integration and further analysis, such as linearization.
- The model is *nonlinear* in nature since the system inputs, outputs, and states are not in a linear combination.



- Tank with $r = 0.5$ m initially at 50% full with $q_{in} = q_{out} = 1000$ L/min. An step inlet flow change of 100 L/min is applied at time = 1 min. Tank becomes full after ~2.6 min.

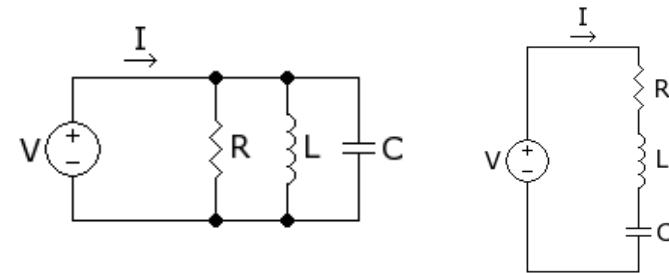


- Tank with $r = 0.5$ m initially at 50% full with $q_{in} = q_{out} = 1000$ L/min. An step outlet flow change of 100 L/min is applied at time = 1 min. Tank is empty after ~2.6 min.

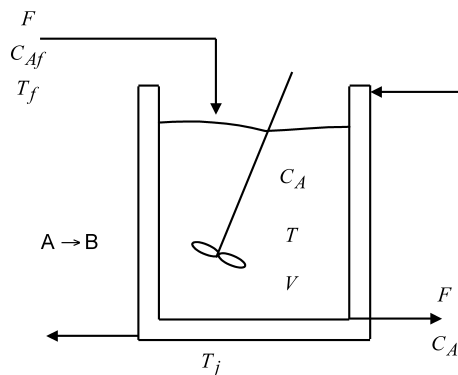


$$M \frac{d^2 x}{dt^2} = f(t) - B \frac{dx}{dt} - Kx$$

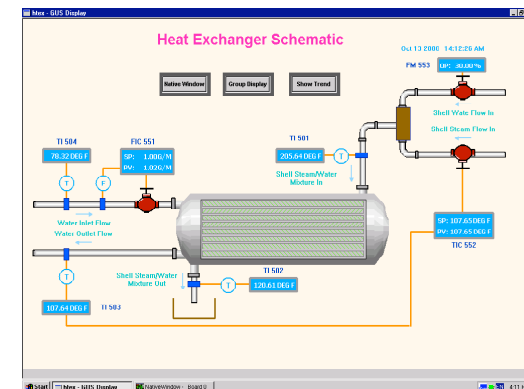
- Need to model how position $x(t)$ varies as a result of an applied force $f(t)$.
- Dynamic modeling relies on the conservation of linear momentum.



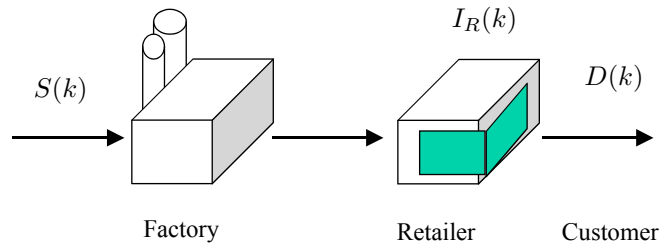
- Kirchoff's Laws that describe electrical networks stem from the conservation of charge and accounting for electrical energy, respectively.



- Modeling a continuously-stirred jacketed chemical reactor involves two systems (the contents of the reactor and the contents of the jacket).
- Conservation of mass, conservation of energy, and accounting of species A lead to three coupled differential equations describing the dynamics of volume, temperature, and concentration in this process.



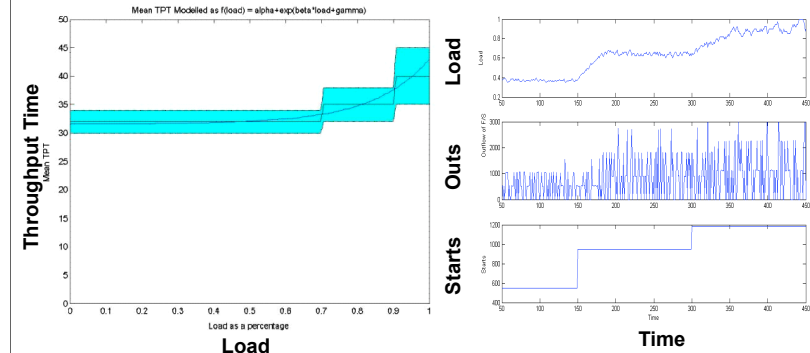
- Modeling involves the conservation of mass and energy.
- This is an example of a *distributed parameter system* where the primary system output (temperature) varies over time and space. Described by a system of partial differential equations (PDEs).



$$I_R(k+1) = I_R(k) + S(k-\theta) - D(k)$$

- Conservation of mass can be used to describe retailer inventory I_R at a time index k as a function of factory starts S and customer demand D .
- Discrete-time model that in practice displays a stochastic, nonlinear dependence between throughput time θ and factory load.

Fab manufacturing node properties Nonlinear and stochastic throughput time



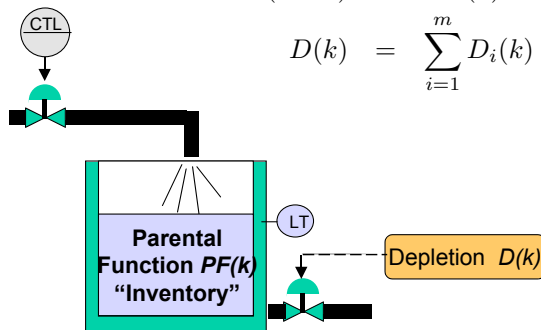
$$\text{Outs}(k) = K_{\text{yield}} \text{Starts}(k - \theta)$$

K_{yield} and throughput time θ are stochastic in nature

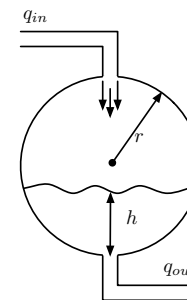
Rivera, D.E., M. D. Pew, and L.M. Collins, "Using engineering control principles to inform the design of adaptive interventions: a conceptual introduction," *Drug and Alcohol Dependence*, Vol. 88, Supplement 2, pgs. S32-S40, 2007.

Intervention $I(k)$ $PF(k+1) = PF(k) + K_I I(k-\theta) - D(k)$

$$D(k) = \sum_{i=1}^m D_i(k)$$

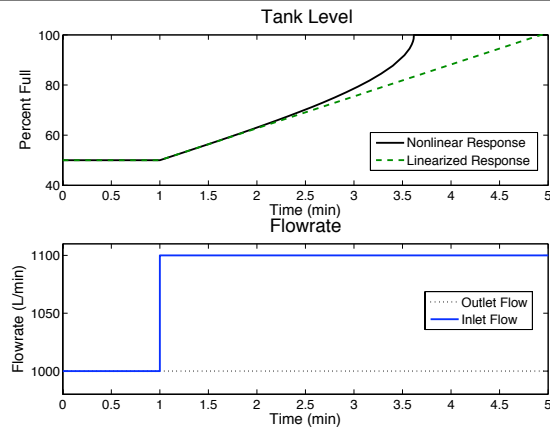


- Parental function $PF(k)$ is built up by providing an intervention $I(k)$ (frequency of home visits), that is potentially subject to delay, and is depleted by multiple disturbance factors $D(k)$.



$$\begin{aligned} \frac{d\Delta h}{dt} &= \frac{1}{\pi \bar{h} (2r - \bar{h})} (\Delta q_{in} - \Delta q_{out}) \\ &= K_P (\Delta q_{in} - \Delta q_{out}) \\ \Delta h &= h - \bar{h} \\ \Delta q_{in} &= q_{in} - \bar{q}_{in} \\ \Delta q_{out} &= q_{out} - \bar{q}_{out} \end{aligned}$$

- Model based on steady-state conditions $\bar{q}_{in}$, $\bar{q}_{out}$, and $\bar{h}$ and deviation variables Δq_{in} , Δq_{out} , and Δh .
- The process gain K_P is a key parameter.
- The linearized model is amenable to control design and analysis.



- Tank dimensions, operating conditions, and inlet flowrate change as before.
- The linearized model, while accurate over a neighborhood of the initial steady-state conditions, is inadequate for answering the question: how much time does it take for the tank to completely fill up?

Control engineering is the field that considers how to manipulate system variables so that its behavior over time is transformed from *undesirable* to *desirable*,

Open-loop: refers to system behavior without a controller or decision rules (i.e., MANUAL operation).

Closed-loop: refers to system behavior once a controller or decision rule is implemented (i.e., AUTOMATIC operation).

A well-tuned control system will effectively *transfer variability* from an expensive system resource to a less expensive one.



Manual



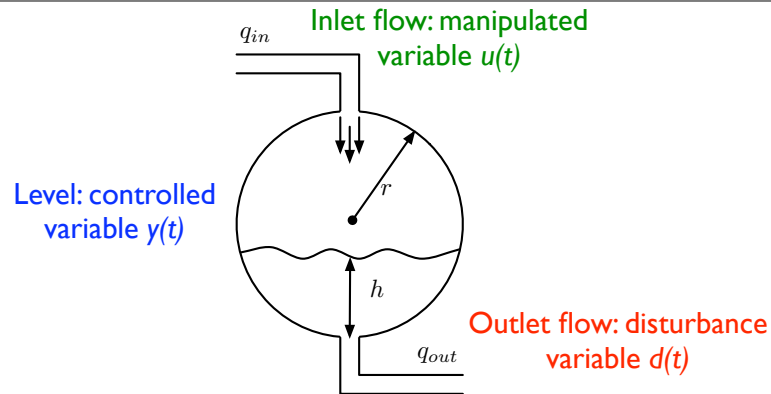
Automatic

- Climate control in automobiles is one of many illustrations of closed-loop control that can be found in daily life.

Controlled Variables (y): system variables that we wish to keep at a reference value (or goal), also known as the setpoint (r).

Manipulated Variables (u): system variables whose adjustment influences the response of the controlled variable; their value is determined by the controller/decision policy.

Disturbance Variables (d): system variables that influence the controlled variable response, but cannot be manipulated by the controller; disturbance changes are external to the system.



- Manipulate the volumetric rate of inflow q_{in} in a spherical tank (aka a “fishbowl”) to keep level h at a desired value, despite varying and unpredictable changes in the volumetric outflow q_{out} .

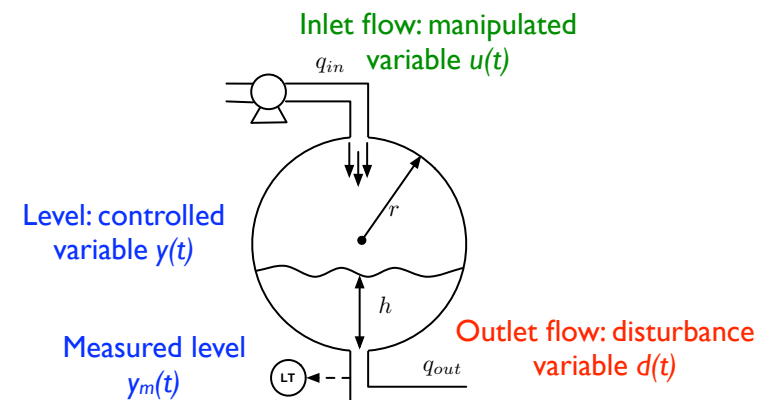
Setpoint Tracking. The ability of the control system to enable the controlled variable to follow a reference (setpoint) trajectory as closely as possible.

Disturbance Rejection. Refers to the ability of the control system to accomplish setpoint tracking, despite substantial variations in the disturbance variables.

Sensors: devices needed to measure the controlled and (possibly) the disturbance variables.

Actuators: devices needed to achieve desired settings for the manipulated variables

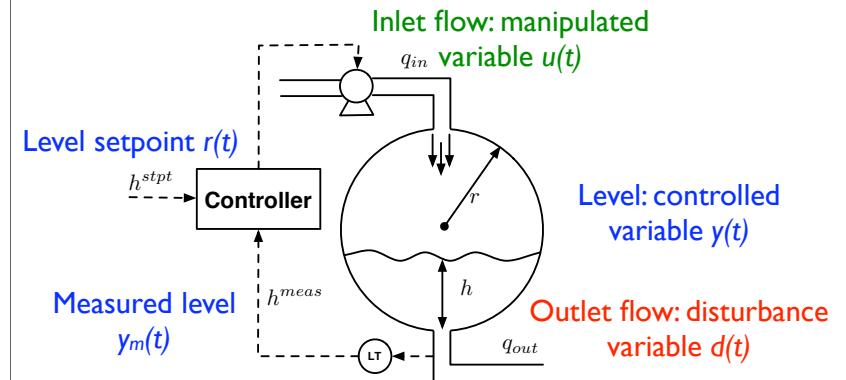
Controllers (i.e., decision rules). These relate current and prior controlled variable, manipulated variable, and disturbance measurements to a current value for the manipulated variable.



- A pump is used to manipulate the inlet flow q_{in} while a level transmitter (LT) is used to determine level h .

In feedback control:

- the controlled variable measurement (y_m) is compared to the reference setpoint r ,
- a control error $e_c = r - y_m$, representing the discrepancy between y and r is calculated.
- a control algorithm determines a current value for the manipulated variable (u) based on current and previous values of e_c and u .
- feedback does not rely on measuring the disturbance d , but rather on how disturbances affect y (and hence y_m).



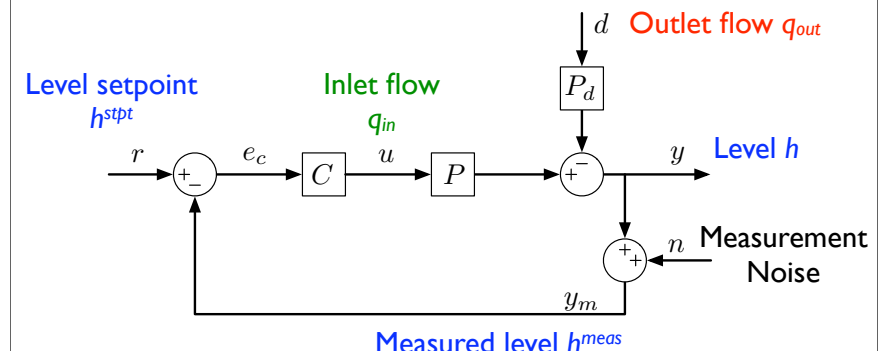
- Manipulate the volumetric rate of inflow q_{in} in a spherical tank (aka a “fishbowl”) to keep level h at a desired value, despite varying and unpredictable changes in the volumetric outflow q_{out} .

(Adapted from K.J. Åström’s “Challenges in Control Education” plenary talk at the 7th IFAC Symposium on Advances in Control Education, Madrid, Spain, June 21-23, 2006).

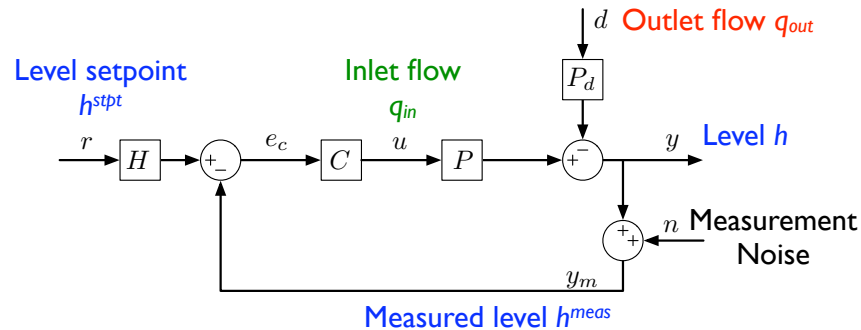
Feedback has some amazing properties:

- can create good systems from bad components,
- makes a system less sensitive to disturbances and component variations,
- can stabilize an unstable system,
- can create desired behavior, for example, linear behavior from nonlinear components.

Major drawback: it can cause instability if not properly tuned.

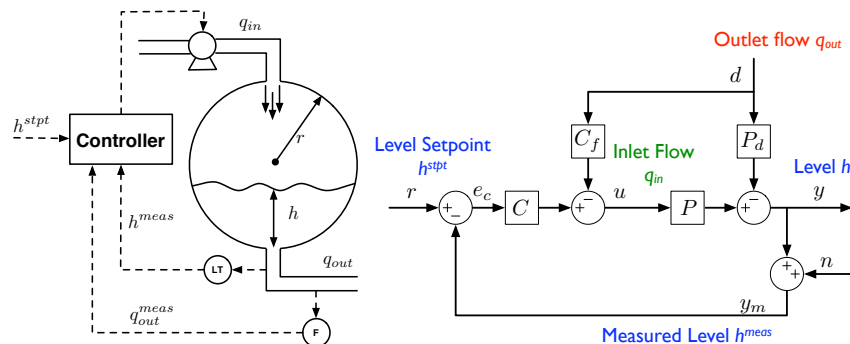


- The symbols P , P_d , and C represent plant, disturbance, and controller models, expressed in transfer function form. These can be in continuous-time (using Laplace transforms) or discrete-time (using z-transforms).
- Control engineering textbooks devote much of their attention to the analysis and design of closed-loop feedback systems using this representation.



- A two degree-of-freedom (2DoF) structure enables the design of a feedback control system that can independently meet performance criteria for setpoint tracking and disturbance rejection.
- Accomplished through the flexibility afforded by the setpoint prefilter H .

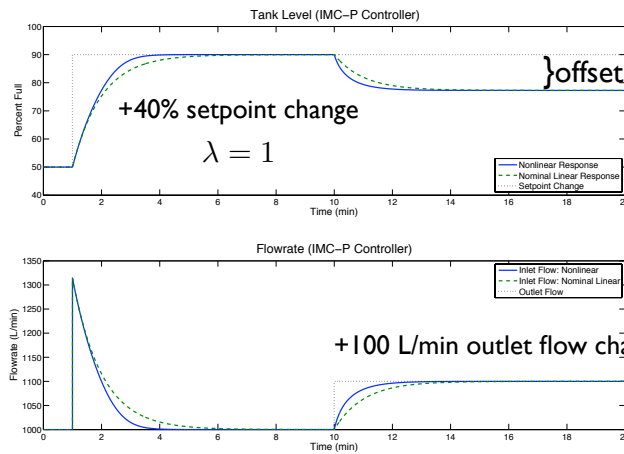
- In feedforward control, changes in the disturbance variable (d) are measured, and based on these changes a manipulated variable (u) is chosen that counteracts anticipated changes in the controlled variable y as a result of d .
- Feedforward control is most beneficial when long delays exist between disturbances and controlled variables.
- Because disturbance measurement is not perfect (and because of uncertainty and plant-model mismatch), combined feedback-feedforward strategies are typically used in industrial practice.



- C_f denotes the feedforward controller, in transfer function form.
- Without the availability of an early forecast of the outlet flow disturbance, feedforward control action does not add much to this problem. All of the subsequent simulations in this talk will be done using feedback-only control.

- **Stability.** Many different notions exist, but “BIBO” stability (bounded inputs resulting in bounded outputs) is usually sufficient.
- Minimal effect of disturbances on controlled variables.
- Rapid, smooth (i.e., non-oscillatory) responses of controlled variables to setpoint changes.
- No offset. Control error e_c should go to zero at a finite time.
- Large variations (“moves”) in the manipulated variables should be avoided.
- Robustness, that is, performance should display little sensitivity to changes in operating conditions and model parameters.

In an optional “Step 3,” the augmented q_r , q_d , and q_f are expressed in classical feedback form as H , C , and C_f . This step may be needed for implementation purposes.



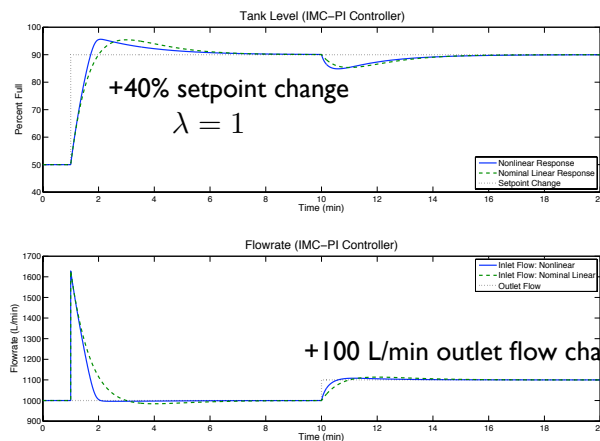
- Good setpoint tracking and low mismatch between the nonlinear and nominal linear response, but disturbance rejection displays offset.

- Applying the IMC design procedure to the linearized model for the performance requirements of
 - no offset to *ramp* disturbance changes,
 - smooth response

results in a model-based *tuning rule* for a Proportional-Integral (PI) controller with controller gain K_c and integral time τ_I

$$u(t) = K_c e_c(t) + \frac{K_c}{\tau_I} \int_0^t e_c(t') dt'$$

$$K_c = \frac{2}{K_p \lambda} \quad \tau_I = 2\lambda$$



- Offset eliminated, but setpoint tracking shows overshoot.

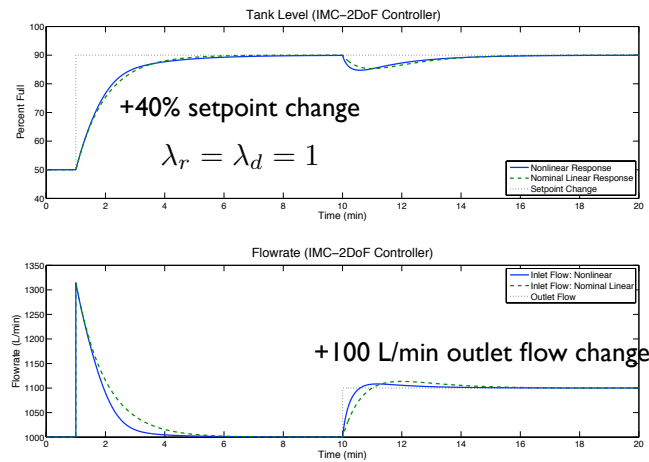
- Applying the IMC design procedure to the linearized model for the performance requirements of
 - no offset to both *step* and *ramp* changes,
 - smooth response, with no overshoot for setpoint changes.
 - independent adjustable parameters for setpoint tracking and disturbance rejection (λ_r and λ_d , respectively).

results in a *tuning rule* for a Proportional-Integral (PI) controller

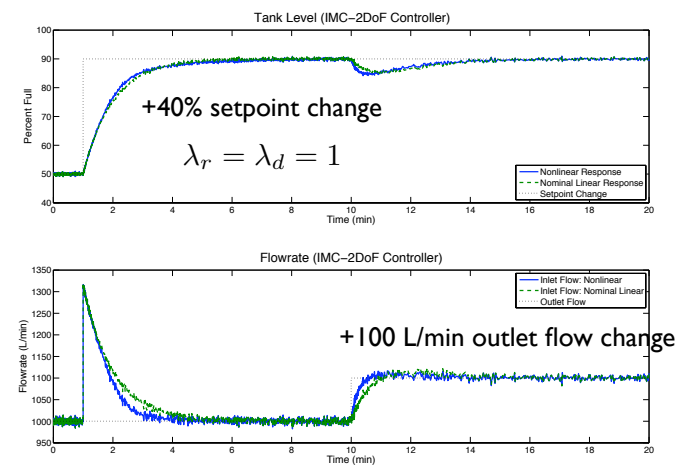
$$u(t) = K_c e_c(t) + \frac{K_c}{\tau_I} \int_0^t e_c(t') dt' \quad K_c = \frac{2}{K_p \lambda_d} \quad \tau_I = 2\lambda_d$$

with setpoint prefilter $H(s)$ (in Laplace transform form)

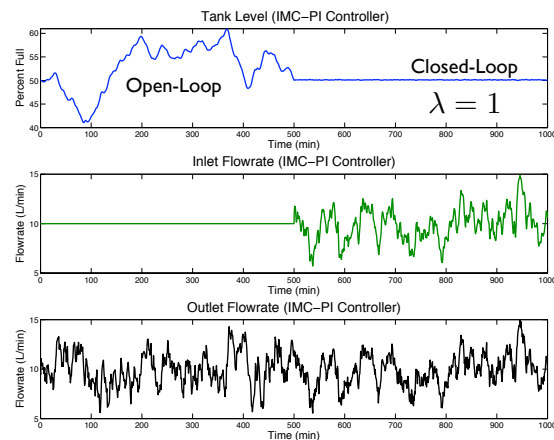
$$H(s) = \frac{(\lambda_d s + 1)^2}{(\lambda_r s + 1)(2\lambda_d s + 1)}$$



- No overshoot during setpoint tracking, while offset in the disturbance rejection response is eliminated.

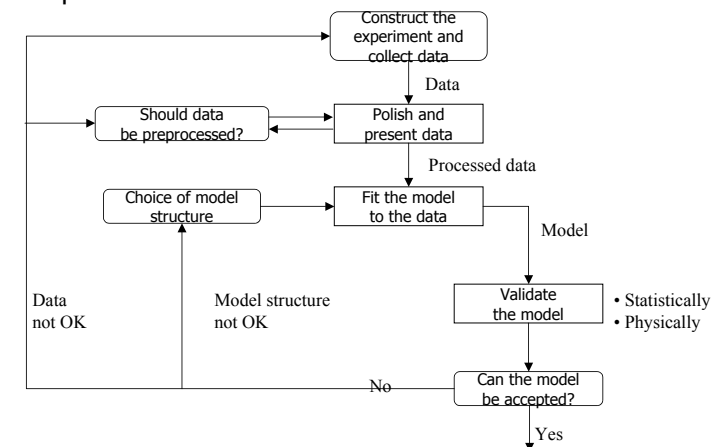


- High frequency but low variance noise; not a very demanding scenario...



- Autoregressive outlet flowrate changes result in autoregressive-integrated changes in level; closed-loop control enabled at $t=500$ min.
- Variability in the level is transferred to a cheaper resource, the inlet flowrate.

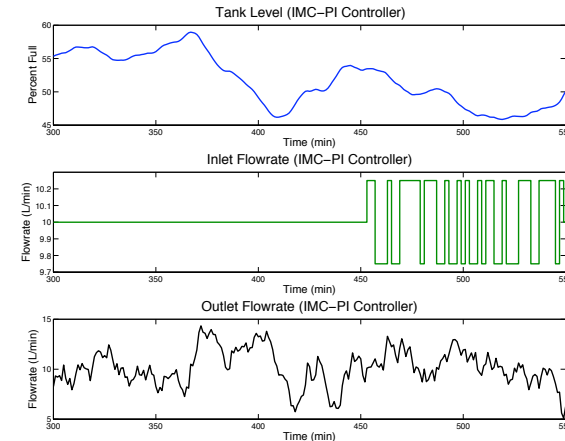
- Term first coined by Lofti Zadeh in 1962.
- System identification focuses on the modeling of dynamical systems from experimental data.



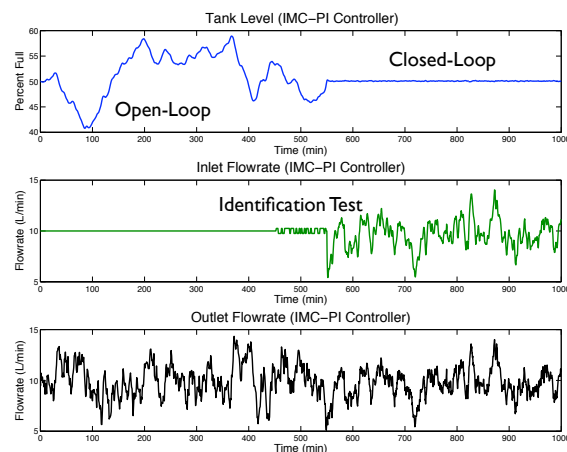
- Sampled-data representation corresponding to the linearized spherical tank model. T_s is the sampling time, k is the sampling index, and e_{pred} is the one-step-ahead prediction error:

$$h(k) - h(k-1) = K_p T_s q_{in}(k-1) + e_{pred}(k)$$

- Gain parameter K_p can be estimated through linear regression using an AutoRegressive with eXternal input (ARX) $-[0 \ 1 \ 1]$ model structure (after differencing the output time series).

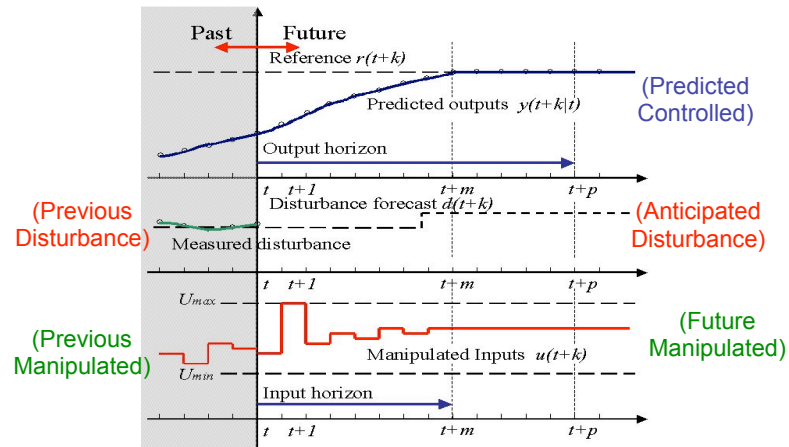


- Relies on the use of a random binary sequence (RBS) to accomplish a “plant-friendly” test conducive to “operations.”



- Estimated process gain K_p is 1.5469, which is 21.5% higher than the gain for the linearized plant model at 50% full ($K_p = 1.2732$).

- Optimization-based algorithm for multivariable, constrained control that originated from the chemical process industries.
- As an *optimizer*, MPC can minimize or maximize an objective function that represents a suitable metric for closed-loop performance, while enforcing constraints.
- As a *controller*, MPC can be tuned to achieve stability, performance, and robustness in the presence of plant/model mismatch, failures, and disturbances.
- Three major steps in MPC:
 - Prediction of the process output at future time instants (horizon) based on a model,
 - Optimization of a control sequence through minimizing an objective function,
 - Receding horizon strategy



Take Controlled Variables to Goal Penalize Changes in the Manipulated Variables

$$J = \sum_{\ell=1}^p Q_e(\ell) (\hat{y}(t+\ell|t) - r(t+\ell))^2 + \sum_{\ell=1}^m Q_{\Delta u}(\ell) (\Delta u(t+\ell-1|t))^2$$

- Mechanistic models arise from applying conservation and accounting principles to extensive system properties such as mass, energy, and momentum.
- Control theory offers a means to alter the behavior of uncertain, nonlinear dynamical systems from *undesirable* to *desirable*, and to *transfer variability* from an expensive system resource to a less expensive one.
- Biased / “erroneous” models can be good for control design, when sensibly used.
- *System identification* can be used to obtain models needed for control under conditions involving noise and uncertainty.

- Scott Occhuizzo, undergraduate, chemical engineering.
- Jay D. Schwartz, Ph.D. candidate, chemical engineering.
- Richard Steenis, Ph.D. student, electrical engineering.

- Some good process modeling and control texts:
 - Ogunnaik and Ray, *Process Dynamics, Modeling and Control*, Oxford University Press, 1994.
 - Seborg, Edgar, and Mellichamp, *Process Dynamics and Control*, Wiley, 2004.
 - Bequette, *Process Control: Modeling, Design and Simulation*, Prentice-Hall, 2001.
- The definitive text on Internal Model Control:
 - Morari and Zafiriou, *Robust Process Control*, Prentice-Hall, 1987.
- Good reference for Model Predictive Control:
 - Camacho and Bordons, *Model Predictive Control*, Springer, 2004.
- Good references on system identification:
 - Ljung and Glad, *Modeling of Dynamic Systems*, Prentice-Hall, 1994.
 - Ljung, *System Identification: Theory for the User*, Prentice-Hall, 1999.
- Identification and control, from a statistical perspective:
 - Box, Jenkins and Reinsel, *Time Series Analysis: Forecasting and Control*, Prentice-Hall, 1994.