

How does One Develop First-Principles Dynamic Models?

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Question: How does One Develop First-Principles Dynamic Models?

Russ' Responses: Dynamic models describe how process responses evolve over time. This contrasts with steady state models, which just reveal the final settled response values (if by some magic, the inputs do not change while the process is settling!). There are several steps in developing a dynamic model. This pod will focus on unit operation processes that are described by ordinary differential equations (ODEs). The reader can find details and examples in my 2024 book "Nonlinear Model-Based Control, Using First-Principles Models in Process Control" published by ISA, <https://www.isa.org/products/nonlinear-model-based-control-using-first-principles>.

As the reader will see, developing first-principles models enhances understanding of the fundamental mechanisms in the process. This understanding will be beneficial in many process engineering tasks such as trouble shooting, optimization, design, and operational management.

1. Inventory

First, decide the inventory that accumulates. Tank level changes in time. But, level does not go into or flow out of a tank. Liquid material is the inventory that flows in or out or accumulates in the tank, and level is a response to the liquid inventory. If you want to model how tank level changes in time, describe how the liquid inventory changes in time. Similarly, pH (a measure of acidity) does not flow in or out of a tank. The acid and base material are the inventory components, and pH is a response. If you want a dynamic model of pH, describe how the acid and base inventories change in time. Table 1 lists some common process variables and the related inventory.

Table 1 – A list of some common relations.

If you want to model:	The inventory is:
Temperature	Thermal Energy
Charge	Electrons
Speed	Momentum
Pressure	Molecules and Thermal Energy of Gas
Liquid Level	Liquid Mass
Weight	Material Mass
pH	Acid, Base, Water Components
Concentration	Mass of Components
Conductivity	Ionic and Water Components

Depending on your community, variables in the left column of Table 1 could be termed response variables, process outputs, measurements, or state variables.

Variables representing the inventory on the right column can be either mass (or equivalently count of objects), energy (thermal or kinetic), or momentum.

2. Control Volume

Second, decide the space in which the inventory accumulates. This is called the control volume. For instance, liquid inventory accumulates in a tank. The space for liquid accumulation is the tank internal volume, which excludes the space occupied by mixers and baffles, and does not include the insulation on the outside of the tank nor the length of discharge pipe.

The material in the control volume should be of uniform properties (temperature, composition, etc.). For instance, in a distillation column, inventory of material accumulates on the trays. Each tray has its own composition and temperature. So, do not consider that the control volume is the overall column, because the material is not spatially uniform within the column. Consider the liquid volume on each tray as an individual control volume.

If the material in a control volume is not spatially uniform, then the dynamic model will be a partial differential equation. For example, as material flows through a heat exchanger tube it changes temperature (inventory of thermal energy); it does not have a uniform temperature within the tube. In such applications the modeling approach is to divide the nominal control volume into very small elements (differential elements along the tube) and consider that the material within each tiny element is spatially uniform. The modeling approach remains the same as is presented here, but the numerical solution is more complicated. I'll focus on macro volumes that can be considered spatially uniform.

3. K.I.S.S.

Third, assume conveniences. Do not consider secondary confounding effects. Stick to the K.I.S.S. principle and only consider dominant mechanisms. For instance, do not consider evaporation losses of material in an open vessel, do not consider ambient losses from an insulated heat exchanger, do not consider how material density or specific heat change with temperature, do not consider how fugacity coefficients change with composition. Your frenemies may want to claim your work is inferior if you do not include such minor effects. They may seek to goad you into the dead-end of overwhelming complexity. First, get the impressive dynamic model working. The complexities could be added later, if they are important. Balance perfection with sufficiency.

4. IOGA

Fourth, apply IOGA. This acronym is short for Inflow, Outflow, Generation, and Accumulation. Inflow is the quantity of inventory that goes into the control volume from outside, during a small time-interval. Outflow is the quantity of inventory that leaves the control volume and goes to the outside during a small time-interval. Generation is the quantity of inventory that is generated within the control volume during a small time-interval. For example, if a chemical reaction is happening, it may be generating heat and new molecules within the control volume. The reaction would also be depleting molecules and might be removing heat. In this case the "Generation" would be negative, and it might be termed "Depletion". (Some folks use the acronym IOGDA to explicitly include Depletion, but IOGA is easier to pronounce and uses less ink to print!) Lastly, the Accumulation

term is the quantity of inventory that accumulates within the control volume during the small time-interval. The equation concept is $I - O + G = A$.

Initially just list all the I, O, and G influences. There may be more than one of each. For instance, in adding a concentrate to a process fluid tank, both the main flow and concentrate flow are inflow terms.

Then using symbols to represent each influence, write the IOGA relation in terms of the symbols.

Define what you are using for the measure of inventory. For heat it might be BTU or calories or kilojoules. For mass it might be lbs, or g-moles. At each step in developing the model, check that the units on each term match the intent.

The accumulation term will be the quantity of inventory at the end of the time step minus the quantity at the beginning of the time step, $Q_{t+\Delta t} - Q_t$. Note: It is the incremental accumulation during the Δt time interval, not the total accumulation over time, $Q_t - Q_{t=0}$.

$$\dot{Q}_{Inflow,t}\Delta t - \dot{Q}_{Outflow,t}\Delta t + \dot{Q}_{InternalGen,t}\Delta t = Q_{t+\Delta t} - Q_t$$

The term Q indicates quantity of inventory, and \dot{Q} is the rate. The subscript $_t$ represents the time at the beginning of a time step, and $_{t+\Delta t}$ represents the time after the small time-interval.

IOGA is also termed a “Balance” equation.

Some folks use rates for the IOGA terms instead of quantity in a small time-interval. In my experience, using rates often leads to errors in the accumulation term. I recommend using quantity in a small time interval.

5. Constitutive Relations

These equations relate the state variables to the inventory. For instance, if the response is temperature, and the inventory is thermal energy, the K.I.S.S. constitutive relation between the response (T) and inventory of thermal energy (Q) is $Q = \rho C_p T$, where the reference T is zero. Rearrange to obtain the state variable from the inventory. $T = Q/\rho C_p$. If the response is pressure in a gas, and the inventory is the moles of gas, the K.I.S.S. constitutive relation for how pressure responds to inventory is $P = nRT/V$. Another first-principles relation, Newton’s Law of Cooling, states that the rate of accumulation of thermal energy is $\dot{Q} = UA\Delta T$, and the quantity of heat accumulated in a small time-interval would be $Q = \dot{Q}\Delta t = UA\Delta T\Delta t$. The specific rate of generation of a chemical molecule in a reaction might be $r = k_0 e^{-E/RT}[A][B]$, so the quantity of molecules generated in a small time-interval would be $n = rV\Delta t = V\Delta t k_0 e^{-E/RT}[A][B]$.

Insert the constitutive relations in the IOGA, and double check that the units on each term in IOGA are still the same as specified earlier.

You may need to include unit conversion factors, particularly g_c to convert mass units to force. For instance, pressure losses are usually modeled by the Moody-Darcy model, which is stated as

$\Delta P_{friction} = f \frac{L_{equ}}{d} \frac{1}{2} \rho v^2$. But the units on the right-hand side are not pressure. In SI units they are

Kg/m-s. Use $\Delta P_{friction} = f \frac{L_{equ}}{d} \frac{1}{2} \frac{\rho}{g_c} v^2$. Also, Reynolds Number, $Re = \frac{dv\rho}{\mu}$, may need g_c to be dimensionless.

The values of the state variables in the constitutive relations will change from the beginning of the small time-interval, Δt , to the end. Also, so may influences, such as flow rates. Don't try to model these secondary effects. Consider that all I, O, and G terms are constant over the small Δt interval, based on their values at the beginning of the time interval. This is termed an explicit model. Some folks use Δt ending values, which is termed an implicit model. Some want to use the average values, because they better represent what happens over the entire time interval. This is termed a semi-implicit model. Implicit and semi-implicit models are more difficult to solve numerically. And if the time step is small enough the results from explicit models are practically no different than implicit or semi-implicit models.

Use the subscript $_t$ for all I, O, and G variables that change in time.

6. Rearrange

Divide the IOGA equation by Δt , and place the accumulation term on the left side of the equal sign, and all the I, O, and G terms on the right-hand side. This presents the rate of accumulation as a function of the influences.

If you want to present the balance as a differential equation, take the limit as Δt goes to zero, and the finite difference in inventory accumulation will become a derivative. But there is no need to do so.

7. Initial State

Typically, the start time of a simulation is considered $t = 0$, but at that time, the tank may be half full or the contents at a temperature of 67 °F. The state variable initial values are not zero. Specify the initial values of influences and states.

8. Solve Numerically

Don't use calculus. Very likely the differential equation will have nonlinear terms, and conventional analytical procedures will direct you to locally linearize the terms, distorting the phenomena you wish to reveal. Further, conventional analytical procedures presume that all influences are constant in time while the process settles, which probably will not match your situation.

If you have the model equation in an ODE format, expand the derivative to a finite difference, multiply both sides by Δt , and add the prior state variable to obtain a function that can be solved as an executable line of computer code.

9. Example

This example will be a very simple level in a tank responding to inflow rate and the position of the valve stem on the exit line.

Since level is of interest, the inventory is the mass of liquid in the tank. There is no internal generation. The mass that flows in during a small time-interval is $F_{in}\rho\Delta t$, what flows out is $F_{out}\rho\Delta t$, and the mass that accumulates is $M_{t+\Delta t} - M_t$. The IOGA balance is

$$F_{in}\rho\Delta t - F_{out}\rho\Delta t = M_{t+\Delta t} - M_t$$

Add constitutive relations. Relate inventory to level. For a tank that is a right cylinder of uniform area, $M = \rho hA$. And relate outflow rate to level. For a flow control valve with a linear characteristic, $F_{out} = C_v x \sqrt{\frac{\Delta P_v}{G\xi}}$. ξ , which has the numerical value of 1 with the units that match ΔP_v , is usually not explicitly shown but is required for dimensional consistency. If the discharge pressure is the same as the tank over-pressure then ΔP_v is just due to the hydrostatic head, $\Delta P_v = \rho gh/g_c$.

Substituting constitutive relations in the IOGA equation:

$$F_{in}\rho\Delta t - C_v x \sqrt{\frac{\rho gh}{G\xi g_c}} \rho\Delta t = \rho Ah_{t+\Delta t} - \rho Ah_t$$

Considering that fluid density is a constant, divide by Δt , switch RHS and LHS, and use the explicit notation:

$$A \frac{h_{t+\Delta t} - h_t}{\Delta t} = F_{in,t} - C_v x_t \sqrt{\frac{\rho gh_t}{G\xi g_c}}$$

Note: In the limit as $\Delta t \rightarrow 0$, $\frac{h_{t+\Delta t} - h_t}{\Delta t} = \frac{dh}{dt}$, which would reveal the nonlinear ODE. $A \frac{dh}{dt} = F(t)_{in} - C_v x(t) \sqrt{\frac{\rho gh(t)}{G\xi g_c}}$. But we don't need the differential equation to solve for the response.

Rearranging to solve for the response, $h_{t+\Delta t}$, obtains the finite difference (numerical solution procedure) to the differential equation.

$$h_{t+\Delta t} = h_t + \frac{\Delta t}{A} \left(F_{in,t} - C_v x_t \sqrt{\frac{\rho gh_t}{G\xi g_c}} \right)$$

This model is to be solved as an assignment statement for computer code. At any point in time, use values for h_t , x_t , and $F_{in,t}$ at time t , the beginning of the time increment Δt , on the RHS of the equation to determine the value for $h_{t+\Delta t}$, tank level at the end of the time increment. Assign $h_{t+\Delta t}$ that value. This value becomes h_t for the next iteration.

The subscripts, and array variables, are not necessary in a computer assignment statement.

$$h := h + \frac{\Delta t}{A} \left(F_{in} - C_v x \sqrt{\frac{\rho gh}{G\xi g_c}} \right)$$

Here the $:=$ represents an assignment statement: Go to the storage locations to find the values of variables on the RHS, do the RHS calculation, and store the new value in the variable named on the LHS. The new h -value will be updated from the prior h -value.

Note: The model is nonlinear. The new h -value depends on the square root of the prior h -value.

Note: It is also interacting. The gain for how valve stem position affects the rate of change of level, is partly dependent on the h -value.

Note: The model also mechanistically includes the disturbance, F_{in} .

Note: The time interval, Δt , should be small relative to the rate that the state variable, h , will change. Roughly, Δt should be about $1/50^{\text{th}}$ of the open loop settling time. If Δt is too large, the solution will tend to zig-zag. If you observe that, halve the Δt value. Repeat until you get a smooth h curve that does not change with new Δt values. Alternately, if Δt is too small, the procedure will take excessive iterations. If you suspect that, double the Δt value until you detect a change in the solution.

Note: Do not learn this by memorizing it. There will be no test question like “What is the third step in developing a dynamic model?” Learn by using the guide to develop your own dynamic models. Your test will be in creating a model. I often opened my college classes by telling the students I will reveal the secret to success, then writing on the board, a sentence that seems strange in school: “Do not learn.” I’d talk for a few seconds about why this was important, then look at the board, pretended to see an error, and say, “Oops. I missed the comma.” Then added the comma, so the secret read, “Do, not learn.”

Practice creating first-principles models on your own process. Feel free to ask me to check your results. My email is russ@r3eda.com.

In subsequent Pods, I’ll introduce how to calibrate and validate models, how to integrate models into a unit, how to simulate environmental vagaries, and how to use the models to evaluate the various economic indicators of transient events. I hope to visit with you later. Meanwhile, visit my web site www.r3eda.com to access information about modeling, control, optimization, and statistical analysis.