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Control Using First-Principles Models

By R. Russell Rhinehart

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Abstract

Some model-based controllers are nonlinear, such as those based on neural networks. But for empirical models to capture the range of process behaviors, they must be calibrated with extensive process testing throughout all operating conditions. In contrast, first-principles models express process nonlinearity. These models could be considered digital twins, as the same model that is useful for control would support many other analysis and forecasting applications. This excerpt from Russ Rhinehart's new book, **Nonlinear Model-Based Control: Using First-Principles Models In Process Control**, explains first-principles models, while the book provides illustrations and set-up examples.

Introduction

First-principles models are the simple mechanistic (phenomenological) models used by engineers for process design and on-line analysis of material and energy efficiency. These are not rigorous, high-fidelity models that seek to perfectly model nuances such as fugacity coefficients and equations of state. First-principles models use simple representations like the Ideal Gas Law and constant liquid density. Here is why you should consider using them in control:

PID control is useful, but the controller imagines that the process gain and dynamics do not change in time. But gain, delay, and time constants usually change with operating conditions such as set point, throughput, tank level, or closeness to a constraint. Continual retuning of controllers is one solution, but it is an aggravation to operators. Gain scheduling is another solution. But it means that the controller must be pre-tuned for disparate operating conditions, and then it selects those tuning values when the situation arises and is identified.

Most model-based controllers are linear. These include Internal Model Control, Dhalin's Algorithm, and Dynamic Matrix Control. When models are based on Laplace or z-transforms, finite impulse response vectors, ABCDmatrices, Laguerre polynomials, or ARMA structures, not only do the models retain the issues of imagining that process behavior does not change in time; but also, use of the models requires the control engineer to learn such modeling techniques. Wouldn't it be preferred if implementing the controller required the engineer to understand the mechanisms of the process, not expend effort to understand the diverse techniques of linear modeling approximation methods?

Some model-based controllers are nonlinear, such as those based on neural networks. But for empirical models to capture the range of process behaviors, they must be calibrated with extensive process testing throughout all operating conditions. The magnitude and cost of experimental work is expensive. And again, to implement such controllers the engineer is distracted by learning the modeling method.

By contrast, first-principles models express the process nonlinearity, and usually have a few coefficients that are easily adjusted from normal operating data to match the process and to adapt when the process changes. The models could be considered as digital twins, and the same model that is useful for control would support many other analysis and forecasting applications, and they would be functional throughout the entire operating range.

A vision is to have one model that is used for training, control, supervisory optimization, constraint prediction, process analysis, and process design. Development of the model will also reinforce fundamental engineering knowledge of the process. "The One Model to replace them all".

The idea to test using first-principles model for automatic control was an outcome of the 70's digital revolution in control systems, and independently several folks throughout the world developed several practicable control approaches. The challenges were to determine how to remove steady state off-set, what to use for the control objective, how to tune the controllers, how to compute the model inverse, how to ensure bumpless transfer, how to handle constraints and multiple variables, and how to comply with the K.I.S.S. principle. Today, process computers are fast enough to implement model-based control, and the techniques using first-principles models have established credibility through substantial testing on industrial scale and pilot scale processes.

Methods that seem to have found success range from the simple Generic Model Control using steady-state models (which is equivalent to output characterization on a PI controller) to Process-Model Based Control using first-order dynamic models with on-line model adjustment, to Predictive Functional Control which can use more complicated dynamic models (including inverse acting), to imbedding nonlinear dynamic models within a Horizon-Predictive Constraint-Avoiding Control structure.

The recently released ISA book, Process Control Using First-Principles Models describes and illustrates the many approaches. This article will introduce one approach, Simple Model Based Control.

Application and controller model

For this illustration, a simple nonlinear process is the titration of a wild flow to meet a composition set point. Figure 1 is a P&ID for the process. Wild flow enters the mixing tank on the left, with flow rate Fw and composition zw. Titrant fluid enters from the right, with flow rate Ft and composition zt. The liquid level in the tank, measured by LT, and the outlet composition, measured by AT, need to be controlled. The model-based controller (not shown in the P&ID) will decide values for the titrant and outlet flow rates and send them as set points to the PI

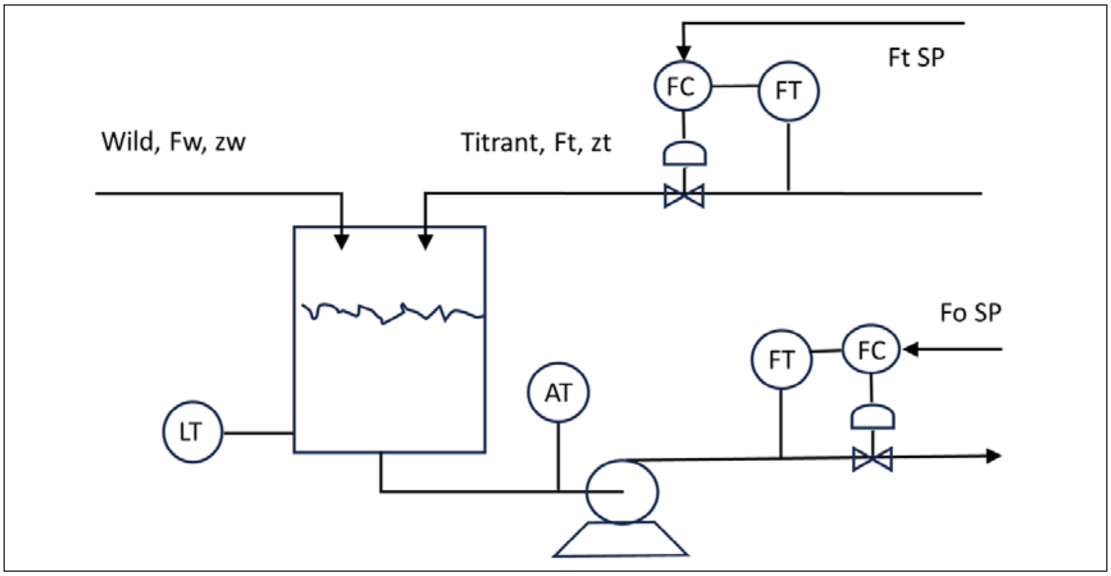

Figure 1 – Process Illustration

secondary flow controllers. Certainly, the model-based controller can send signals directly to the titrant and outlet flow control valves, but that requires an extra step of modeling flow rate as a function of valve position. The cascade arrangement comfortably reverts to classic control if the model-based controller is taken off line, and since the secondary PI controllers contain all of the desired auxiliary features such as communication protocol, data validity checks, etc., the process engineer does not need to code those in the supervisory model-based controller.

The simple first-principles models representing the tank level, h, and outlet concentration, z_o, are developed from material balances around the tank. This effort may take a reader back to college skills. Hopefully, this calculus-free trip will be enjoyable. The mass that flows in, less what flows out, is the mass that accumulates in the tank. In a time-interval, Δt, the equation for the material balance is:

$$F_w \rho_w \Delta t + F_t \rho_t \Delta t - F_o \rho_o \Delta t = hA\rho_{in}|_{t+\Delta t} - hA\rho_{in}|_t \qquad (1)$$

Here, F represents flow rate, and ρ density. The subscripts w, t, and o refer to the wild flow, the titrant, and the out-flow. h represents the height of the fluid in the tank, of cross-sectional area A. The notation $x|_t$ means the value at the beginning of the time-interval, Δt, and $x|_{t+\Delta t}$ means at the end of the time-interval. Classic model simplifications are that there is no density change due to mixing, and that the tank is perfectly mixed so that the fluid composition flowing out of the tank, z_o, is the same as that in the tank, z_{in}, and that the cross-sectional tank area, A, does not change with time or liquid level. Divide by density, divide by Δt, and take the limit as Δt becomes very small, and rearrange to the conventional differential equation form.

$$A\frac{dh}{dt} = F_w + F_t - F_o \qquad (2)$$

However, since the flow rates change over time in nonanalytical manners, Eq. 2 cannot be solved analytically. Instead of using the differential equation to solve for how h changes in time, do not divide Eq. 1 by Δt, divide by A, to obtain a classic numerical solution method for the differential equation (which is termed Eulers explicit, or a forward finite difference method).

$$h|_{t+\Delta t} = h|_t + \Delta t[(F_w + F_t - F_o)/A]|_t \tag{3}$$

Eq. (3) is the first principles dynamic model for the tank level. The reader may be very pleased that neither calculus nor analytical solutions of a differential equation are involved with control or control modeling. Nor are Laplace transforms!

The differential equation representing how concentration in the tank changes in time is similarly developed from a component mass balance. The component mass that flows in, less what flows out is the component mass that accumulates in the tank in a time interval, Δt. The equation is:

$$F_w z_w \Delta t + F_t z_t \Delta t - F_o z_o \Delta t = hAz_{in}|_{t+\Delta t} - hAz_{in}|_t \tag{4}$$

With the same classic simplifications, rearrange to a differential equation form.

$$\frac{dhz_o}{dt} = [F_w z_w + F_t z_t - F_o z_o]/A \tag{5}$$

Since both h and z_o change in time, $\frac{dhz_o}{dt}$ becomes $h\frac{dz_o}{dt} + z_o\frac{dh}{dt}$. Using $\frac{dh}{dt}$ from Eq. 2, Eq. 5 becomes

$$\frac{dz_o}{dt} = [F_w(z_w - z_o) + F_t(z_t - z_o)]/hA \tag{6}$$

Again, although Eq. 6 would be a conventional calculus presentation of the model, it cannot be solved analytically. Instead, use a classical numerical solution method.

$$z_o|_{t+\Delta t} = z_o|_t + \Delta t\{[F_w(z_w - z_o) + F_t(z_t - z_o)]/Ah\}|_t \tag{7}$$

Eqs. 3 & 7 represent the model that would be in the MBC algorithm.

The model in the controller is not the same as the process, which has many confounding features. The simulated process in this article has dead zones in the mixer and composition measurement lag. The simulated process has density change in the mixing, and the true value of the tank cross-sectional area is affected by insertions, baffles, the mixing impeller, and ridges in the tank. The measured flow rates and level have noise and drifting calibration error. The wild flow rate and composition both vary in time, and the composition is not measured. There are small evaporative losses. The "known" titrant composition has error. Dynamics of the secondary flow controllers are not included in the controller model.

Figure 2 illustrates the process-to-model mismatch as well as process nonlinearities. In the figure, the supervisory controller is in MAN and makes equal magnitude steps in the flow rate set point to the titrant flow controller. The two solid lines in the lower part of the figure are the set point to the outlet flow controller (held constant) and to the titrant flow controller (making step changes). The process and controller model responses are the four upper traces. Dashed lines represent the true (but unknowable) process values of the simulator. These would not be known in a real application but could be measured. The trapezoidal trends represent the integrating aspect of the tank level, and the first-order like trends represent composition.

Note, although the steps in the set points from the supervisory controller have identical magnitudes, the rate of change for the tank level shows about a 5:1 change. Note the fast response of the composition to the first step up in the influence and the slower response of the equivalent but opposite second step. Also note the longer yet time constant and larger gain change of the third step

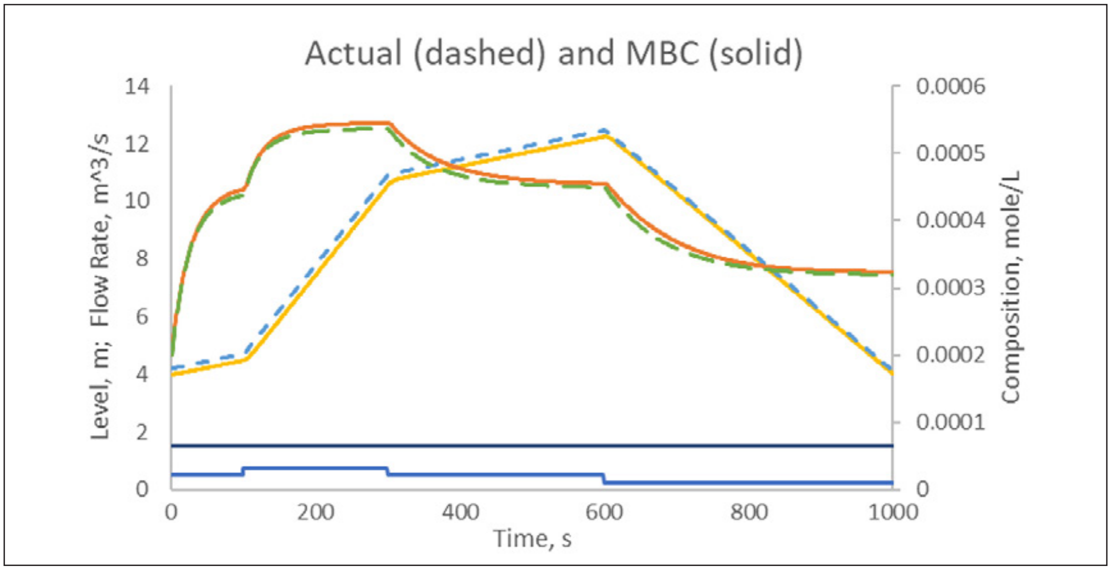

Figure 2 – Supervisory MBC in MAN with Steps in Titrant Flow Rate SP

down of equal magnitude. The effective settling time for the response also has about a 5:1 change, and the gain change has about a 2:1 ratio.

The modeled CV values are not the same as the process. This is more evident for the composition but the modeled level lags behind by about 5 s. It would be "cheating" to test a controller with the same model in the simulator as in the controller, and no measurement error. The mismatch in the modeled and true process indicates process-to-model mismatch. The mismatch is somewhat greater between the controller model and the measured CV values, which is all that the controller can know.

As well as being nonlinear, with variable time constants, the process is interactive. As illustrated in Figure 2, changing one controller output affects both CVs.

The process is nonlinear, non-stationary and interactive.

A Model-Based Control Strategy

Figure 3 presents a block diagram of the controller strategy. The block in the upper right represents the process. It receives the inputs from the controller, MV, and responds. Labeled as $y_{process}$ are the measured CVs and auxiliary variable values. Below it, and processing data in parallel to the process block, is the block representing the controller model of the process. It executes Eqs. (3) & (7) and predicts the current values of the process from the prior model predictions. The

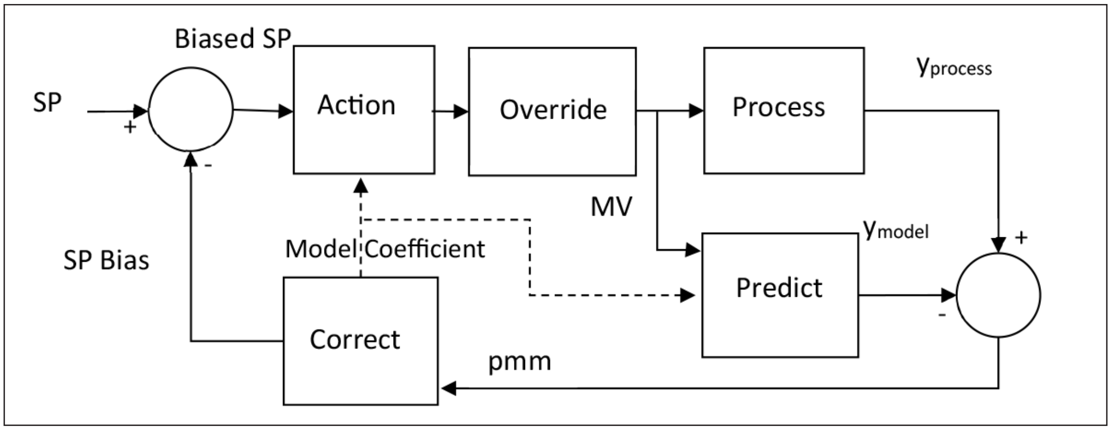

Figure 3 – Simple Model-Based Control Strategy

difference between the modeled and measured values are the process-to-model mismatch, pmm, values. Not shown, the process will also have many other inputs, such as a wild flow and environmental effects, and model will have those wild inputs that are measured.

The pmm values are used in the block labeled "Correct" to generate a bias to adjust the set points for the model. Since the model is not the same as the process, if the controller finds MV values that make the model hit the set point, the process will have a steady state offset. This simple model-based control adjustment to remove offset is analogous to an archer seeking to hit the center of a target. If the arrow falls 3 cm below the bull's eye, next time aim 3 cm above.

The Correct function might also adjust a model coefficient to improve the model match to the process, or it could perform data reconciliation. Either procedure would improve the model prediction. The Correct function could filter the pmm value to temper process noise or dynamic mismatch when there are large changes.

In this simulation, the measured flow rate values include calibration bias, which makes the modeled mass balance continually integrate up or down. The correct function uses a simple material balance data reconciliation to determine a fictitious outlet flow rate F_{error}.

The block labeled Action uses the controller model, biased set point, and desired rate for the model to move the modeled CV to the biased SP to calculate MV values. When the models are first-order, as Eqs. (2) & (6) are, then desire that the modeled CVs move to the biased SPs in a first-order manner. For the composition, this desired rate of change is

$$\left.\frac{dz_m}{dt}\right|_{desired} = \frac{z'_{SP} - z_m}{\tau_{desired\ for\ z}} \tag{8}$$

For the height, this is

$$\left.\frac{dh_m}{dt}\right|_{desired} = \frac{h'_{SP} - h_m}{\tau_{desired\ for\ h}} \tag{9}$$

When substituted in the models (Eqs 2 & 6) and rearranged to solve for the MV values:

$$F_t = \left[F_w(z_w - z_o) - hA\frac{z_{SP}' - z_m}{\tau_{desired\ for\ z}}\right] / (z_t - z_o) \tag{10}$$

$$F_o = F_w + F_t - F_{error} - A\frac{h_{SP}' - h_m}{\tau_{desired\ for\ h}} \tag{11}$$

First use Eq. 10 to determine F_t, the set point for the titrant flow controller, then Eq. 10 to determine F_o, the set point for the outlet flow controller.

Although this is a 2X2 control strategy the one-way coupling permits sequential solutions. In other situations, the two equations must be solved simultaneously, and nonlinearities in the model or auxiliary variable constraints could require an optimization procedure.

Finally, the block labeled Override would impose rate of change or limits on the MV, or it could be a safety override to keep an auxiliary from violating a constraint, or operator imposed override for maintenance or testing. What ever the reason, the MV value that goes to the process also needs to be an input for the prediction model.

Control Results

Figure 4 simulates control with bumpless transfer and two set point changes. The controller starts in MAN mode. Because the outlet flow rate is initially higher than the combined inlet flow rates, the level ramps down. And because the titrant flow rate is higher than necessary, the tank composition rises in a first-order like manner. At a time of 100 s the controller is switched to AUTO. Prior to that, in MAN mode, the set points follow the CV. There is no bump in CVs when the controller is switched to AUTO, but the controller makes a small correction in the titrant flow rate set point to hold the measured composition at the set point.

At a time of 400 s the composition SP changes. Note the coupled MV action minimizes the disruption upset to the level. At a time of 700 s the level SP changes.

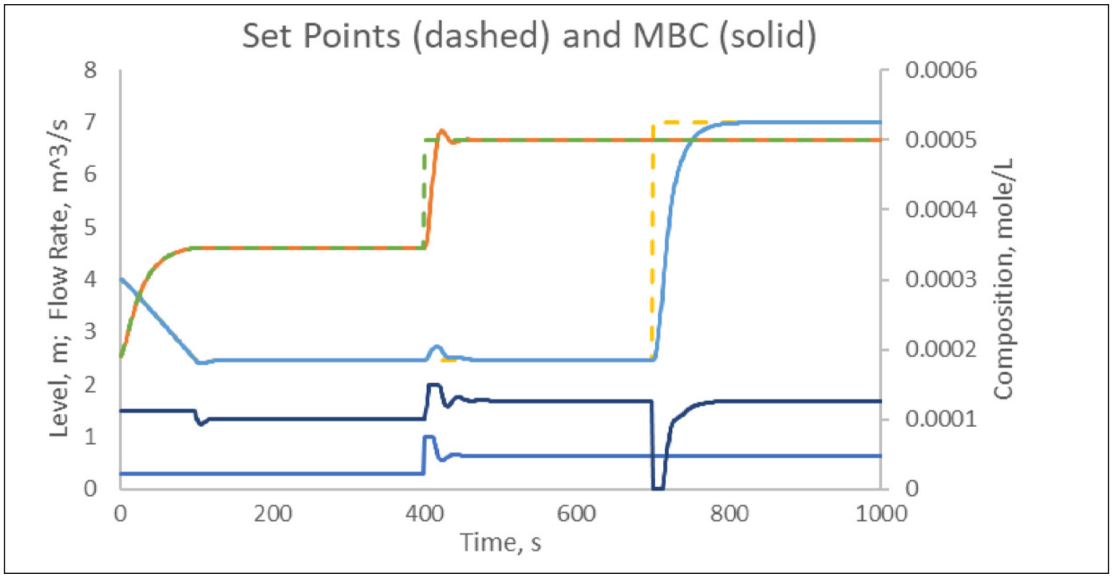

Figure 4 – Controlled Process

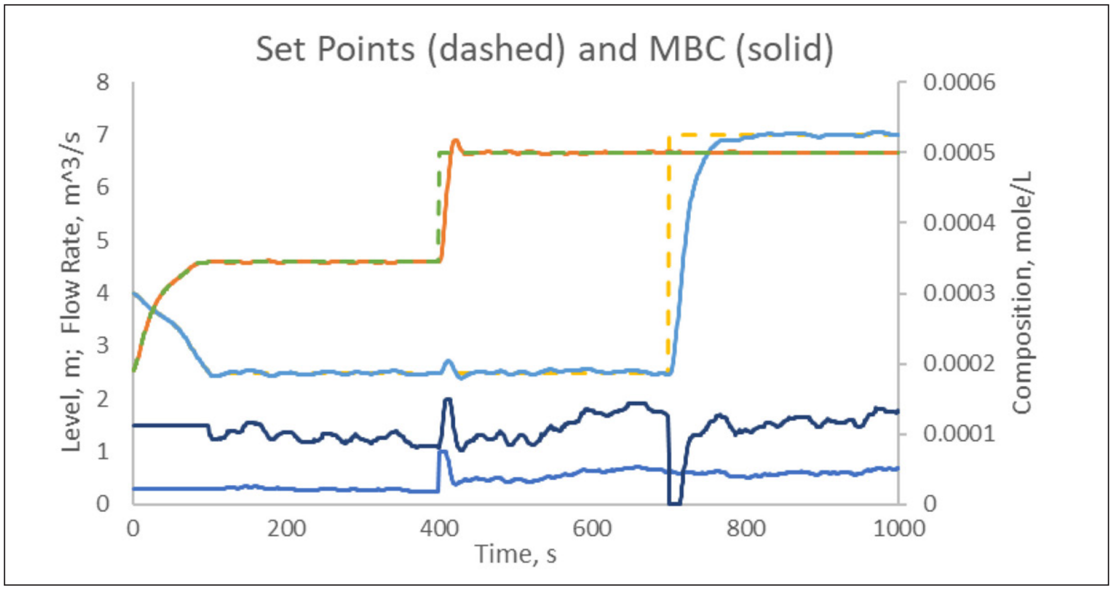

Figure 5 – Controlled Process with Disturbances

Figure 5 illustrates the same sequence of events, but with continually changing values of the wild flow, the wild composition, and measurement calibration drifts. Also, there is measurement noise on the level and three flow rates. The magnitude of the influent drifts is evident in the continually changing flow rate SPs during the extended periods where the level and composition SPs are held constant.

Conclusions

The first principles modeling supports other engineering activities, such as process analysis, identification of constraints, using supervisory RTO SS models that are consistent with those used by the controller, and operator and engineer training.

- The MBC approach has one tuning factor per CV, which relates the desired rate of return to the set point. This is a tuning advantage.
- If valve and pump models are included, the controller could calculate desired valve positions, which could go direct to the valves. But the cascade strategy illustrated here is preferred for flexibility and to make use of safety and communication features already embedded in traditional PID controllers.
- For bumpless transfer, in MAN mode the set points should follow their CVs, and after initialization of the model states at the process measurements, the models need to be incrementally calculated at each time-interval.
- The required skill requires time domain modeling, elementary numerical methods, coding, and possibly optimization.
- The approach does not divert engineer or operator attention to understanding transformed or linear modeling mathematics, or to empirical linear or nonlinear modeling principles.

About R. Russell Rhinehart

Dr. R. Russell Rhinehart, professor emeritus in the School of Chemical Engineering at Oklahoma State University, has experience in both industry (13 years) and academia (31 years) and was head of the school for 13 years. Russ is a past president of the American Automatic Control Council, was editor-in-chief of ISA Transactions from 1998 to 2012, and Director of the ISA Automatic Control Systems Division (now Control and Robotics). He is a Fellow of both ISA and AIChE and a Process Automation Hall of Fame inductee. He received the 2009 ISA Distinguished Service Award and the 2013 Fray International Sustainability Award.Inspired by his industrial experience, his mission has been to bridge the gap between industry and academia. Russ was the codirector of two industrial consortia (one at Texas Tech and a second at Oklahoma State) and built pilot-scale laboratories for dual use in undergraduate education and graduate research. He left industry in 1982 with a vision to use engineers' process models in control and pursued many aspects of doing so in his academic research career. This book is his collection of practicable methods. His goal is for it to be a useful guide to others seeking to use nonlinear models in control.

His 1968 BS in chemical engineering and subsequent MS in nuclear engineering are both from the University of Maryland. His 1985 PhD in chemical engineering is from North Carolina State University.

He maintains a website (www.r3eda.com) to provide open access to software (including simulators to support this text) and technique monographs. He also offers consulting services related to engineering analysis, and serves on several ISA, American Automatic Control Council (AACC), and International Federation of Automatic Control (IFAC) committees.

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