Since January 2020 Elsevier has created a COVID-19 resource centre with free information in English and Mandarin on the novel coronavirus COVID-19. The COVID-19 resource centre is hosted on Elsevier Connect, the company's public news and information website.

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Using SIR Epidemic Modeling and Control to Teach Process Dynamics and Control to Chemical Engineers

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Abstract: The COVID-19 pandemic has brought about unprecedented opportunities to introduce control systems topics in the undergraduate engineering curriculum. This paper describes two computer modeling assignments based on MATLAB with Simulink developed for CHE 461: Process Dynamics and Control taught at Arizona State University during the fall 2020 semester. A myriad of important concepts, among these dynamic modeling using conservation and accounting principles, linearization, state-space system and transfer function model representations, PID feedback control and Internal Model Control design can be applied to the problem and explained to students in the context of a significant world event representing a unique "process" system, notably the COVID-19 pandemic.

Keywords: Process control applications, epidemic modeling and control, model-based control, computer-based control education.

1. INTRODUCTION

The COVID-19 pandemic is a significant world event that is still among us, and has touched literally every individual in the planet in some way. It is difficult to find anyone with family or loved ones who have not been affected or impacted. The pandemic has brought about unexpected opportunities for education and research, which includes the field of process control. Meaningful learning opportunities exist on a problem for which students are bound to have a personal perspective.

The paper describes the experience of using an epidemic model, namely, a Susceptible-Infectious-Recovered (SIR) model, to teach process dynamics and control to chemical engineering undergraduates taking CHE 461: Process Dynamics and Control, a required course in the chemical engineering curriculum at Arizona State University. Students normally enroll in CHE 461 during the first semester of their senior year. The excellent paper by Simon (2020) provided the background upon which these assignments were conceived. We describe the computer modeling and Exam Preparation Assignments (EPAs, aka "homework") in support of the modeling work, and present representative results. We conclude with a description of extensions and current and future efforts on the problem.

2. SIR MODEL FOR DISEASE TRANSMISSION

The first of the two computer modeling assignments (CMA) involves building a MATLAB with Simulink implementation of the analysis in the paper by Simon (2020), which is preceded by two homework assignments (or EPAs). Compartmental models used in epidemiology to model infectious disease can be understood using a chemical reactor analogy, where disease transmission and remission correspond to an autocatalytic reaction with catalyst deactivation. In particular, we are interested in developing a dynamical model for a variation of the classical Susceptible-Infectious-Recovered (SIR) problem (Kermack and McKendrick, 1927) that considers births, deaths and time-varying transmission $\beta(t)$ and recovery $\gamma(t)$ rates. A problem schematic is shown in Figure 1, illustrating the problem in terms of a continuously-stirred tank reactor (Levenspiel, 1998; Fogler, 2016).

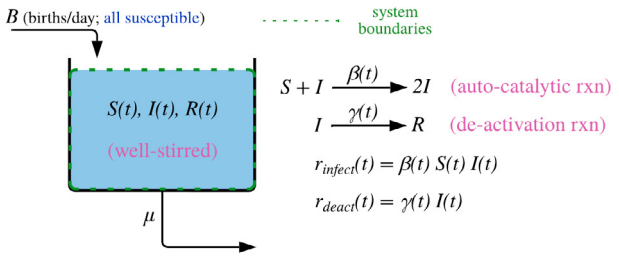

Fig. 1. SIR disease modeling as a continuously-stirred tank reactor (CSTR) featuring autocatalytic and deactivation reactions.

The goal of the model is to determine how the populations of Susceptible ($S(t)$), Infectious ($I(t)$), and Recovered/Removed ($R(t)$)) individuals, as well as the rates of infection and deactivation, change over time during an epidemic. For simplicity, the inflow to the reactor B, the number of births/day, is considered constant, as well as mortality rates per day for each of the populations ($\mu = \mu_S = \mu_I = \mu_R$, respectively). Correspondingly, the total

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population $N = S(t) + I(t) + R(t)$ remains constant, with the population of Removed individuals $R(t)$ computed from the solutions to $S(t)$ and $I(t)$. The incidence rate, i.e., the number of new infections per day, is determined by the autocatalytic reaction with constitutive expression,

$$S + I \overset{\beta(t)}{\rightarrow} 2I \qquad r_{infect} = \beta(t) S(t) I(t) \tag{1}$$

The time-varying transmission rate $\beta(t)$ is influenced by government mandates for social distancing and hygienic procedures (e.g., mask wearing) and hence it is a variable that could be considered to be "adjustable" by society and thus falls as manipulated. A lower value for β results in a decrease in the infection rate, and would result in a decrease in the number of infected individuals. Deactivation of infected individuals per day is described by a first-order reaction

$$I \overset{\gamma(t)}{\rightarrow} R \qquad r_{deact} = \gamma(t) I(t) \tag{2}$$

The recovery rate $\gamma(t)$ is time-varying, with γ^{-1} corresponding to the average duration of infectiousness. Increasing γ implies that infected individuals remain infectious for a shorter amount of time, which would ultimately result in a decrease in the infected population. Actions such as the availability of more effective treatments and therapeutics can influence γ. In the assignment, students are asked to consider $\gamma(t)$ as an exogeneous variable that is external to the process, and can thus be treated as a disturbance.

With this information in hand, students are able to then write species accounting equations that describe the dynamics of this system; these equations can then be expressed as a nonlinear lumped parameter system model amenable to integration in MATLAB w/Simulink.

$$\frac{dx}{dt} = f(x, u, d) \tag{3}$$

$$y = g(x, u, d) \tag{4}$$

The nonlinear lumped parameter system consistent with the problem statement can be found in Fig. 2. Linearization (which the students accomplish as a homework exercise) then leads to a dynamical system in state-space form,

$$\frac{d\Delta x}{dt} = A\,\Delta x + B\,\Delta u + \Gamma\,\Delta d \tag{5}$$
$$\Delta y = C\,\Delta x + D_u\,\Delta u + D_d\,\Delta d$$

where A, B, Γ, C, D_u and D_d are constant-valued matrices, while Δ denotes deviation variables. $\bar{x}$, $\bar{u}$, $\bar{d}$, and $\bar{y}$ represent initial steady-state conditions obtained by solving $f(\bar{x}, \bar{u}, \bar{d}) = 0$. For the problem at hand there are two steady-state conditions, with the most interesting case (denoting endemic conditions) consisting of

$$\bar{S} = \frac{\mu + \bar{\gamma}}{\bar{\beta}} \qquad \bar{I} = \left(\frac{B}{\mu + \bar{\gamma}} - \frac{\mu}{\bar{\beta}} \right) \tag{6}$$

The other steady-state condition consists of a disease-free state ($\bar{S} = B/\mu$, $\bar{I} = 0$). The steady-state according to (6) results in non-zero $\bar{I}$ from which an informative linearized model useful for control design can be obtained. The computer model (consisting of a MATLAB `.mlx` livescript and one Simulink `.slx` file) built by students must meet the following functional requirements:

(1) The nonlinear and linearized state-space equations must be solved using MATLAB with Simulink R2019a (or higher). Non-MATLAB or MATLAB-only solution (that do not integrate the differential equations using Simulink) are not accepted.
(2) The `.mlx` file should allow the user to specify initial conditions for the two input variables (β and γ) and use sliders for maximum effect. The programs should also use sliders to specific the initial step times (separate for each input) and final simulation time. Multiple figure windows and properly labeled transfer functions (in symbolic and gain-time constant forms), corresponding to the linearized model should appear following proper execution of the `.mlx` files.

$$\frac{dS(t)}{dt} = \underbrace{B}_{\substack{\text{birthrate}\\(\text{inflow})}} - \underbrace{\beta(t)\,S(t)\,I(t)}_{\substack{\text{infection rate}\\(\text{consumption})}} - \underbrace{\mu\,S(t)}_{\substack{\text{mortality rate}\\(\text{outflow})}} = f_1(x,u,d)$$

$$\frac{dI(t)}{dt} = \underbrace{\beta(t)\,S(t)\,I(t)}_{\substack{\text{infection rate}\\(\text{generation})}} - \underbrace{\gamma(t)\,I(t)}_{\substack{\text{deactivation rate}\\(\text{consumption})}} - \underbrace{\mu\,I(t)}_{\substack{\text{mortality rate}\\(\text{outflow})}} = f_2(x,u,d)$$

$$x = \begin{bmatrix} S(t) \\ I(t) \end{bmatrix},\ u = [\beta(t)],\ d = [\gamma(t)],\ f(x,u,d) = \begin{bmatrix} f_1(x,u,d) \\ f_2(x,u,d) \end{bmatrix}$$

$$y = \begin{bmatrix} S(t) \\ I(t) \\ r_{infect}(t) \\ r_{deact}(t) \end{bmatrix},\ g(x,u,d) = \begin{bmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \end{bmatrix} = \begin{bmatrix} S(t) \\ I(t) \\ \beta(t)\,I(t)\,S(t) \\ \gamma(t)\,I(t) \end{bmatrix}$$

Fig. 2. Nonlinear lumped parameter model equations representing SIR disease modeling dynamics.

A Canvas quiz randomly assigns parameters for $\bar{\beta}$ and $\bar{\gamma}$ individually to students. Students are asked to generate illustrative step responses for *independent* changes in *each* input variable (β and γ) for the base parameters ($B = 500$, $\mu = 0.1$). For each input, they are asked to produce a *nontrivial* change that shows when the linear model is a valid approximation for this system, and a second change that highlights process nonlinearity. To illustrate some desired simulation results, a set of model responses (linear and nonlinear) to a β change of 0.0012 (occurring at time $t = 1$) and a γ change of +0.3 (occurring at time $t = 20$ days) for parameters $\bar{\beta} = 0.0008$ and $\bar{\gamma} = 0.25$ is shown in Figure 3. The numerical transfer function generated by MATLAB (in gain-time constant form) is shown (for β changes only) in Figure 4, while a symbolic transfer function (from MATLAB's `Symbolic Math Toolbox`) is shown in Figure 5. The following are among the questions that students are asked to answer in the discussion section:

(1) How well do the responses obtained agree with physical intuition?
(2) How do the linearized and nonlinear model responses compare with each other?
(3) How useful are the transfer function expressions in predicting the *intrinsic* dynamic behavior of this system (e.g., shape, speed, direction, and final values of the response)?

From this computer modeling assignment (and the homework assignments that support it), students discover the following:

(1) When demographics (i.e., births and deaths) are considered, the SIR model (henceforth referred to as the "plant") will display an endemic steady-state that

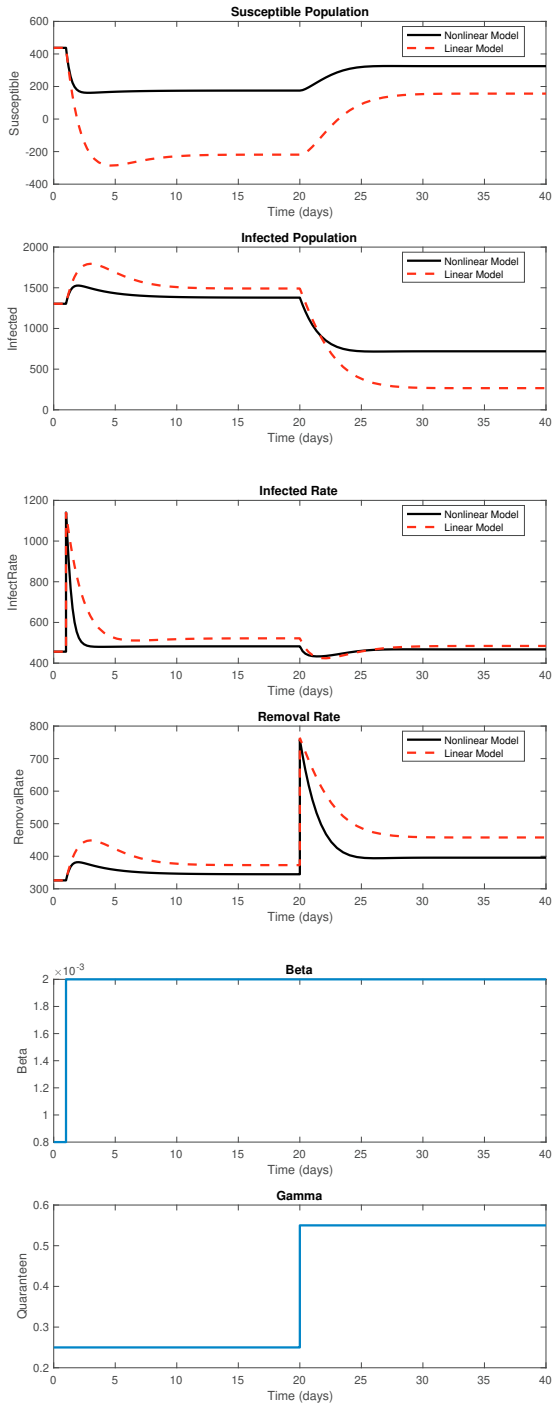

Fig. 3. Susceptible, infected population responses (top), infection and removal rates (middle), for linear and nonlinear models to a β change of 0.00012 (occurring at time $t = 1$) and a γ change of +0.3 (occurring at time $t = 20$ days) for parameters $B = 500$, $\mu = 0.1$, $\bar{\beta} = 0.0008$ and $\bar{\gamma} = 0.25$.

will serve as the initial conditions for infected ($I(t)$) and susceptible ($S(t)$) populations in our problem.

(2) The plant dynamics can be very nonlinear, based on the magnitude of changes in β and γ,

(3) Nonetheless, the linearized model from the endemic steady-state can be very informative (and useful).

```
From input "Beta" to output...

                    -5.4688e05 (1+2.857s)
 Susceptible:  ---------------------------------
               (1 + 1.892(1.655s) + (1.655s)^2)

                    1.5625e05 (1+10s)
 Infected:  ------------------------------------
            (1 + 1.892(1.655s) + (1.655s)^2)

                     54687 (1+2.857s) (1+10s)
 InfectedRate:  --------------------------------
                (1 + 1.892(1.655s) + (1.655s)^2

                     39063 (1+10s)
 RemovalRate:  ---------------------------------
               (1 + 1.892(1.655s) + (1.655s)^2)
```

Fig. 4. MATLAB-generated numerical transfer functions in gain-time constant form (for β changes only) resulting from steady-state conditions obtained from parameters $B = 500$, $\mu = 0.1$, $\bar{\beta} = 0.0008$ and $\bar{\gamma} = 0.25$. Under these conditions, the system is slightly underdamped in the open-loop.

$$\begin{pmatrix} -\frac{\text{Infec Suscpt}\ (\gamma+\mu+s)}{\sigma_1} & \frac{\text{Infec Suscpt}\ \beta}{\sigma_1} \\ \frac{\text{Infec Suscpt}\ (\mu+s)}{\sigma_1} & -\frac{\text{Infec}\ (\mu+s+\text{Infec}\ \beta)}{\sigma_1} \\ \frac{\text{Infec Suscpt}\ (\mu+s)\ (\gamma+\mu+s)}{\sigma_1} & -\frac{\text{Infec Suscpt}\ \beta\ (\mu+s)}{\sigma_1} \\ \frac{\text{Infec Suscpt}\ \gamma\ (\mu+s)}{\sigma_1} & \frac{\text{Infec}\ (\mu+s)\ (\mu+s+\text{Infec}\ \beta-\text{Suscpt}\ \beta)}{\sigma_1} \end{pmatrix}$$

where

$$\sigma_1 = \gamma\,\mu + \gamma\,s + 2\,\mu\,s + \mu^2 + s^2 + \text{Infec}\,\beta\,\gamma + \text{Infec}\,\beta\,\mu + \text{Infec}\,\beta\,s - \text{Suscpt}\,\beta\,\mu - \text{Suscpt}\,\beta\,s$$

Fig. 5. Symbolic transfer functions for the linearized model, obtained from the `Symbolic Math Toolbox` in MATLAB. The absence of RHP zeros in the (2,1) element (i.e., the transfer function between $\Delta\beta(s)$ and $\Delta I(s)$) over all practical operating conditions has significant impact on control design.

Lessons learned in the computer assignment regarding the linearized plant model include the following:

- The plant response characteristics can range from underdamped to overdamped, based on operating conditions.
- The nominal linearized transfer function model describing the dynamics between $\beta(t)$ and $I(t)$ conforms to a second-order transfer function according to:

$$\tilde{p}(s) = \frac{b_1 s + b_2}{s^2 + a_1 s + a_2} \tag{7}$$

- The symbolic transfer function model from Fig. 5 shows that, over all operating conditions, 1) the steady-state gain for (7) is always greater than zero, which implies that lowering β will always reduce

the infected population, and 2) the plant zero in the transfer function (7) will always lie in the Left-Half Plane (LHP). This latter characteristic greatly simplifies the application of the IMC design procedure to obtain a feedback control law in this case, as the IMC controller $\tilde{q} = \tilde{p}^{-1}$ will always be stable and causal (only requiring a first-order filter to be made semiproper.

Having put the MATLAB w/Simulink model through its paces, students are encouraged in their report to discuss its usefulness (or lack thereof) of the modeling exercise. Although the proposed model is very simple, students are asked to consider and discuss:

- How could the model be helpful to public health officials? to the general public?
- Assumptions made in the model, and list the major deficiencies that come to mind.
- Modifications and enhancements to make this model much more useful.

3. CONTROLLER DESIGN COMPUTER ASSIGNMENT

The control strategy to be evaluated in the second assignment relies on the transmission rate constant $\beta(t)$ as a manipulated variable ($u(t)$) to reduce the infected population $I(t)$ (the controlled variable $y(t)$) to a desired setpoint, all while in the presence of "disturbances" arising from changes in the removal/recovery rate constant $\gamma(t)$. Design requirements for the control system are as follows:

(1) The control system must not differentiate step setpoint changes;
(2) Controlled variable responses should be smooth with little or no oscillation; preferably no more than 10% overshoot (or undershoot) for a step setpoint change,
(3) The closed-loop speed of response should be comparable (and preferably faster) than the open-loop speed-of-response,
(4) While an abrupt change may initially be necessary in the manipulated variable response, the controller should avoid taking $\beta(t)$ to 0 (i.e., full lockdown), and avoid oscillations and significant variations (e.g., imagine what this response might imply for society).
(5) The control system must demonstrate *robustness* to nonlinearity; that is, the ability to maintain the system under control in spite of changes in operating conditions.

Students have been taught in class the Internal Model Control design procedure (Rivera et al., 1986; Morari and Zafiriou, 1989) which can be applied to the linearized model. For the second-order model with zero shown in (7) and a first-order filter with adjustable parameter λ_d, the corresponding feedback controller conforms to an ideal PID with filter structure according to:

$$c(s) = K_c \left(1 + \frac{1}{\tau_I s} + \tau_D s\right)\left(\frac{1}{\tau_F s + 1}\right) \tag{8}$$

with tuning rules for this control system determined on the basis of the model coefficients in (7) and an adjustable parameter λ_d.

$$K_c = \frac{a_1}{\lambda_d\, b_2} \quad \tau_I = \frac{a_1}{a_2} \quad \tau_D = \frac{1}{a_1} \quad \tau_F = \frac{b_1}{b_2} \tag{9}$$

A further enhancement to the control strategy is to implement the IMC design as a two-degree of freedom (2DoF) classical feedback controller according to Figure 6. Such a controller will have individual adjustable parameters (e.g., λ_r, λ_d) to allow the user to independently adjust the speed of response for each degree-of-freedom (i.e., setpoint tracking versus disturbance rejection). The setpoint shaping prefilter resulting from a 2DoF design is

$$h(s) = \frac{\lambda_d s + 1}{\lambda_r s + 1} \tag{10}$$

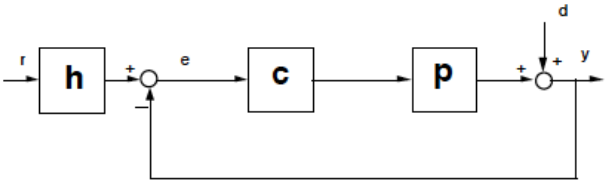

Fig. 6. Two degree-of-freedom structure for classical feedback control. A setpoint shaping prefilter $h(s)$ allows for decoupling the setpoint tracking response from disturbance rejection.

As before, a working MATLAB livescript with Simulink model and report describing the SIR closed-loop simulation is required from each student. A representative Simulink window for the problem is shown in Figure 7. The closed-loop system is set up to evaluate deterministic (step) changes in γ, as well as *stochastic* changes according to the equation:

$$\Delta\gamma(k) = \alpha\, \Delta\gamma(k-1) + n_d(k) \tag{11}$$

where $\alpha = 0.7$ is an autoregressive model parameter, $\Delta\gamma$ is the change in γ, k is the sampling instant, and $n_d(k)$ is a zero-mean, white noise signal. A switch variable (`cl_ask`) which can be set by a menu item will determine if the deterministic or stochastic case is evaluated. For the deterministic scenario, the Integral Square Error (only) is computed for both the nonlinear and linear models, for setpoint tracking separately from disturbance rejection. In the stochastic case, the variance of $y(t)$ and $u(t)$ (using the MATLAB command `var`) are calculated, after the setpoint response has settled. This is done only for the nonlinear plant and help illustrate the fundamental concept of *transfer of variance*.

Some representative scenarios that students are asked to evaluate are presented. Consider the closed-loop responses to a setpoint change corresponding to a 50% reduction in the endemic infected population (occurring at time $t = 1$) and a γ change of $+0.3$ (occurring at time $t = 40$ days) for a single DoF controller ($\lambda_r = \lambda_d = 1$) and model parameters $B = 500$, $\mu = 0.1$, $\bar{\beta} = 0.0008$ and $\bar{\gamma} = 0.25$, as shown in Figure 8. This controller fails the desired specifications through an underdamped with significant undershoot in $I(t)$, resulting from $\beta(t) = 0$ (i.e., complete lockdown) during the initial part of the simulation. Figure 9, in contrast, uses a 2DoF design with $\lambda_r = 3$ and $\lambda_d = 1$ that maintains an overdamped response in $I(t)$, avoids undershoot, and keeps β from ever reaching 0. In both single DOF and 2DoF cases, the reduction in infectiousness resulting from the γ change of $+0.3$ leads

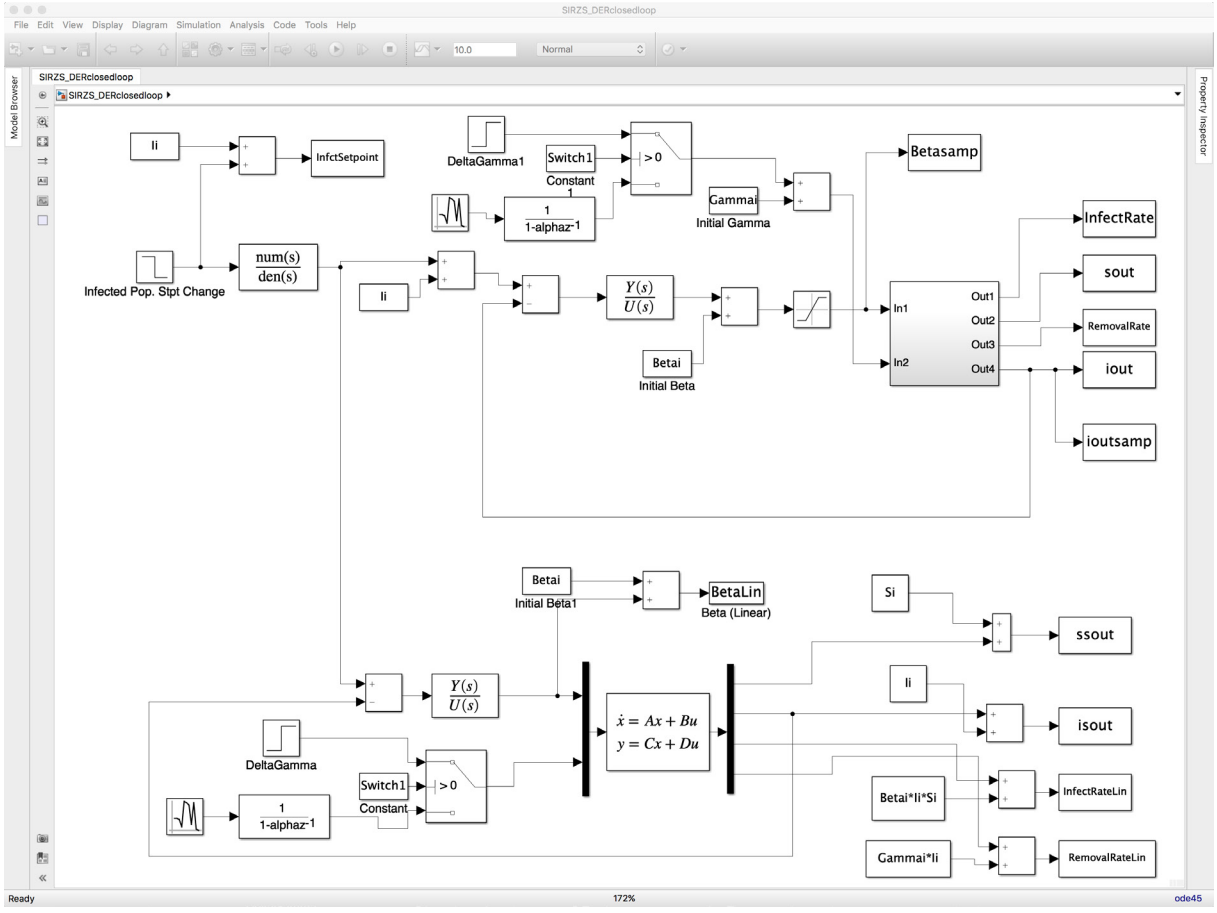

Fig. 7. Illustrative Simulink window for the closed-loop system evaluated in the control design modeling assignment.

to maintaining the setpoint while allowing β to increase substantially (implying a return to normalcy and pre-pandemic conditions).

In their written report, students are asked to compare their responses relative to the closed-loop performance criteria noted previously. The questions that they must answer in the discussion section include:

(1) How do the linearized and nonlinear closed-loop responses compare with each other?
(2) What performance criteria are satisfied (and particularly, not satisfied) by the closed-loop system as currently tuned? What may be viewed as problematic regarding your controller's current performance?
(3) How is controller robustness to nonlinearity reflected in the responses from your design? What conclusions can you make regarding the adequacy of a linearized model for controlling a highly nonlinear system (such as the epidemic SIR model)?

The same set of questions posed to students during the first modeling assignment are repeated in controller design: *Now that you have put your closed-loop simulation through its paces, discuss its usefulness (or lack thereof). This is clearly a very simplified evaluation of infectious disease control, but please discuss way(s) (illuminated by your closed-loop results) in which it can still be useful. How could it be helpful to public health officials? the general public? What modifications/enhancements would you propose to make this model much more useful?*

4. EXTENSIONS AND FUTURE WORK

A natural extension of the problem is to consider the effect of vaccination rates. Vaccines, which are now a present reality of the pandemic, were reaching final stages of testing and development in fall 2020. The effect of vaccines is to take susceptible individuals directly to the removed category. Vaccination of susceptible individuals per day can be described by a first-order reaction

$$S \overset{k_v(t)}{\rightarrow} R \qquad r_{vacc} = k_v(t)S(t) \tag{12}$$

with the rate of vaccination $k_v(t)$ now serving as an additional disturbance to the problem. Incorporating this problem feature in the nonlinear model and step testing this additional disturbance (from $k_v = 0$ to some value) will have a significant positive influence the problem. This was provided as an extra credit opportunity in fall 2020, but is part of the assignment that is currently being solved by students in CHE 561: Advanced Process Control. Students in 561 will also consider the use of Model Predictive Control as an alternative to IMC.

Enhancements to the SIR model through the inclusion of additional compartments have been proposed by many; evaluating these would represent interesting extensions. However, additional compartments would lead to higher-order systems and consequently, (from applying IMC) to controller structures beyond PID.

We have also had the opportunity to supervise masters students in applied projects who have examined (or are

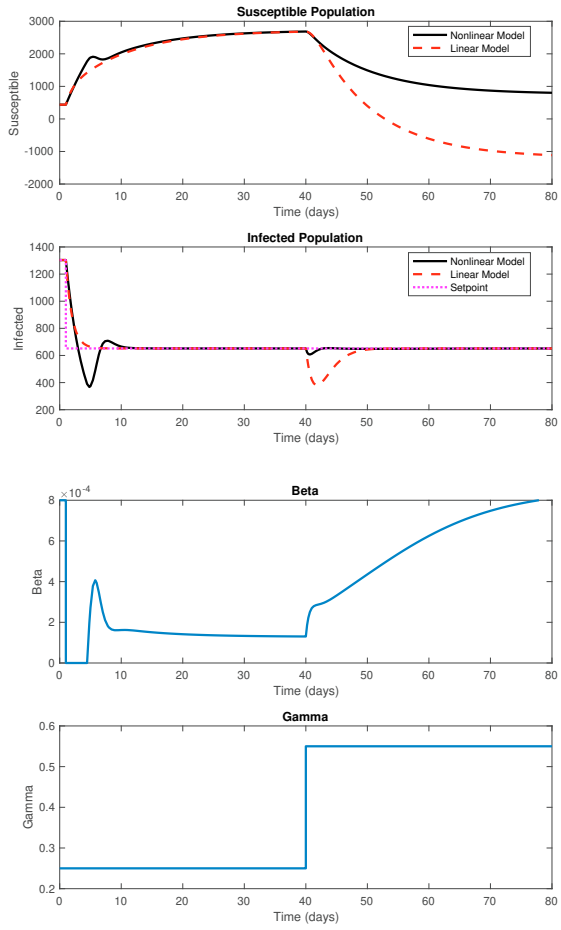

Fig. 8. Closed-loop responses (for susceptible and infected populations, linear and nonlinear) to a setpoint change corresponding to a 50% reduction in the endemic infected population (occurring at time $t = 1$) and a γ change of $+0.3$ (occurring at time $t = 40$ days) for a single DoF IMC-PID with filter controller ($\lambda_r = \lambda_d = 1$) and model parameters $B = 500$, $\mu = 0.1$, $\bar{\beta} = 0.0008$ and $\bar{\gamma} = 0.25$.

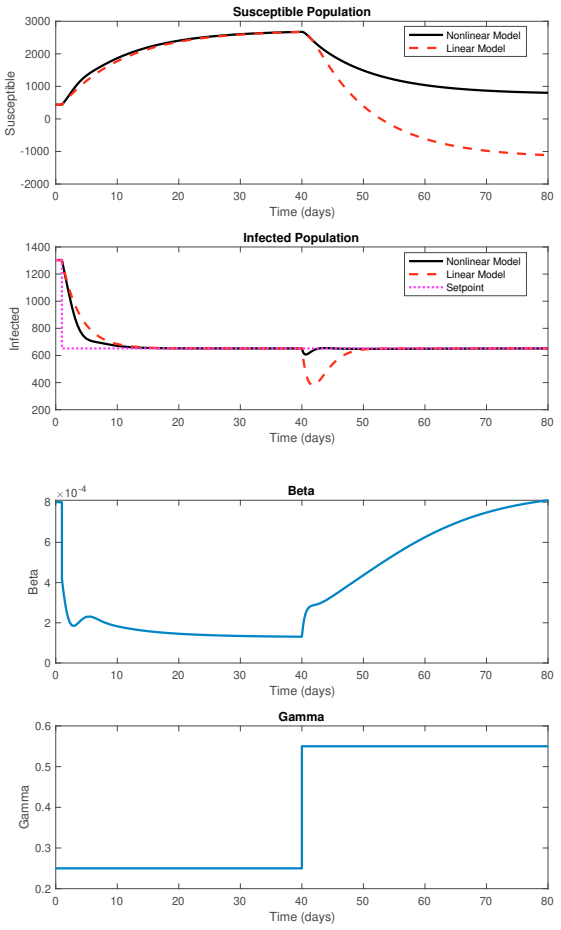

Fig. 9. Closed-loop responses (for susceptible and infected populations, linear and nonlinear) to a setpoint change corresponding to a 50% reduction in the endemic infected population (occurring at time $t = 1$) and a γ change of $+0.3$ (occurring at time $t = 40$ days) for a 2DoF IMC-PID with filter controller ($\lambda_r = 3$, $\lambda_d = 1$) and model parameters $B = 500$, $\mu = 0.1$, $\bar{\beta} = 0.0008$ and $\bar{\gamma} = 0.25$.

contemplating) working on extensions of the project. Particular interest has been in applying both nonlinear IMC and MPC controller formulations. Dynamic theories of behavior change such as Social Cognitive Theory (Martín et al., 2020) can be incorporated in the model to address how $\beta(t)$ and $\gamma(t)$ are affected by behavioral constructs.

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