3 Mathematical Modeling

In this chapter, representative lumped-parameter nonlinear ODE models, involving mixing with chemical reaction, phase change, interaction of different capacities, closed loop system with dead time, and interacting and coupled systems are considered. Two examples of inherent linear second-order systems with derivative of the input are included in Section 3.8. For convenience in comparison of alternative initializations in subsequent chapters, the native models rather than the dimensionless forms are used. These models are different in their physical structure, analysis for the effect of initial discontinuities and the effect of linearization.

The models considered contain coupled ODEs, which on simultaneous solution for one of the output variables yields ODEs with terms containing differentials of the input function. Upon linearization, such models yield second-order numerator-dynamics transfer functions, which exhibit initial discontinuities in their profiles. To explore the general range of their behavior, conditions are worked out for their assorted solution profiles to identify characteristic parameters, which unfold interesting cases of maximum, minimum, inflection, input multiplicity, pole-zero cancellation, reduction to standard systems, etc., as the value of one such parameter changes relative to that of the others on the real axis. These profiles would be discussed later in this chapter. The profiles exhibiting maximum and minimum in step and impulse responses respectively are not observed in the standard over-damped systems, and become important even from the point of view of design of the system. During the dynamic changes, the operating variables can attain maximum/minimum values that are significantly beyond the steady state range of values. The design is certainly influenced due to these dynamic changes and must be based on the maximum/minimum values as the design based on steady state values would be unsatisfactory.
3.1 Non-isothermal CSTR

A benchmark model that has been used to study nonlinear dynamics in the literature, i.e., a non-isothermal CSTR, is considered first (Inamdar et al., 2011; Lemoine-Nava et al., 2006; Moudgalya and Jaguste, 2001; Prasad and Bequette, 2003; Prasad et al., 2002; Ray, 1995; Salehi and Shahrokhi, 2008). With changes in the inlet flow rate, material and thermal capacities are interacting. This model is considered in Sections 5.3 and 5.4 to study inconsistencies from singularities and illustrate the framework of methodology for the analysis of discontinuities and initialization for the numerical solution for the impulse inputs.

The constant density, jacketed, non-isothermal CSTR is carrying out a liquid-phase, first-order reaction \( A \rightarrow R \) with rate constant \( k \) and enthalpy \( -\Delta H_R \). The feed contains only \( A \). Assuming that the jacket fluid is at saturated condition, thus, its temperature \( T_j \) is constant and uniform throughout. Heat capacity of the reaction mass \( C_p \) also stays constant throughout. \( C_A \) and \( C_R \) are concentrations of \( A \) and \( R \). \( v_o, v, T_o \) and \( T \) are respectively flow rates and temperatures of feed and exit. \( k_o \) and \( E \) are Arrhenius parameters, \( R \) is the universal gas constant. Writing material and energy balances give (Coughanowr and LeBlanc, 2009):

\[
\frac{dV}{dt} = v_o - v
\]  
(3.1)

\[
\frac{d(VC_A)}{dt} = v_o C_{A_o} - v C_A - k C_A V
\]  
(3.2)

\[
\rho C_p \frac{d(VT)}{dt} = \rho C_p (v_o T_o - v T) + (-\Delta H_R)k C_A V + U h A_h (T_j - T)
\]  
(3.3)

\[
k = k_o \exp \left( -\frac{E}{RT} \right)
\]  
(3.4)

3.1.1 Linearized model

The tank is now assumed closed and always fully filled, so that, its hold-up volume \( V \) can be taken constant. Linearizing the above model (using Taylor’s series expansion of the nonlinear terms in the neighborhood of initial steady state and ignoring the terms of order
greater than or equal to two), taking the Laplace transforms of the linearized equations, and solving these simultaneously, the following transfer functions are obtained (valid for step perturbations in jacket temperature):

\[
\frac{\tilde{T}}{\tilde{T}_j} = K \frac{s + l}{s^2 + (l + d)s + ld - e} \quad \text{and} \quad \frac{\tilde{C}_A}{\tilde{T}_j} = K' \frac{1}{s^2 + (l + d)s + ld - e} \tag{3.5}
\]

where

\[
K = \frac{U_h A_h}{\rho V C_p}, \quad l = \frac{v}{V} + k_s, \quad d = \frac{v}{V} + K + \frac{\Delta H_R}{\rho C_p} C_{A_0} k_s \frac{E}{RT_s^2}, \quad e = \frac{\Delta H_R}{\rho C_p} C_{A_0} k_s^2 \frac{E}{RT_i^2} \tag{3.6}
\]

Subscript \(s\) and over bar represent initial steady state and the deviations of variables from their initial steady states, respectively.

### 3.2 Isothermal CSTR

It is a constant hold-up volume tank carrying out a liquid-phase constant-density reaction \(A \rightarrow R\) having first-order rate constant \(k\). Assume that the system is closed and is always fully filled, so that, the hold-up volume of the tank remains unchanged. Only reactant \(A\) is in the feed and is dissolved in an inert solvent \(I\). The component material balance for \(R\) and \(A\) respectively are:

\[
\frac{dC_R}{dt} = -\frac{v_o}{V} C_R + k C_A \tag{3.7}
\]

\[
\frac{dC_A}{dt} = \frac{v_o}{V} C_{A_0} - \left(\frac{v_o}{V} + k\right) C_A \tag{3.8}
\]

If the volumetric flow rate of feed \(v_o\) is perturbed at zero time. The differential equation for \(C_R\) is derived from Eqs. (3.7) and (3.8), and is given below.

\[
\frac{d^2C_R}{dt^2} + \left(2\frac{v_o}{V} + k\right) \frac{dC_R}{dt} + \left(\frac{v_o^2}{V^2} + k \frac{v_o}{V}\right) C_R = \left(k C_{A_0} / V\right) v_o - \left(C_R / V\right) \frac{dv_o}{dt} \tag{3.9}
\]

This is a nonlinear ODE with a term containing differential of the input function \(v_o\).

Eqs. (3.7) and (3.8) are derived as follows. The first term in the transient material balance (3.7) is the rate accumulation of \(R\) in tank; the inflow rate of \(R\) is zero; the second
term is the rate of out-flow of $R$ and the third term is the rate of formation of $R$. In Eq. (3.8), the first term is the rate accumulation of $A$; the second term is the inflow rate of $A$; the third term is the rate of out-flow of $A$ plus the rate of disappearance of $A$. All these terms are in moles per unit time and volume. Where, $C_A$, $C_R$ and $C_I$ are concentrations of $A$, $R$ and $I$ respectively in the tank and in the exit stream; $C_{A_0}$ is the feed stream concentration; $v$ is the volumetric feed rate and $V$ is holdup volume.

### 3.2.1 Linearized model

The system is assumed to be at steady state at time $t \rightarrow 0^-$. For a perturbation in volumetric flow rate of feed $v_o$, linearizing Eqs. (3.7) and (3.8) and converting to deviation variables, gives:

$$
\frac{d\overline{C_R}}{dt} = -\frac{C_R}{V} - \frac{v}{V} \overline{C_R} + k \overline{C_A} \tag{3.10}
$$

$$
\frac{d\overline{C_A}}{dt} = \left( \frac{C_A - C_{A_0}}{V} \right) \frac{v}{V} - \left( \frac{v}{V} + k \right) \overline{C_A} \tag{3.11}
$$

For impulse perturbation in $C_{A_0}$, the system of Eqs. (3.8) and (3.7) behaves as standard first and second order respectively for $A$ and $R$. However, considering the effect of initial discontinuity (discussed in Section 4.2.4 for the linear systems) would yield a second-order numerator-dynamics form for $R$ as it would lead to an un-accounted discontinuity in $C_R(0)$. This gives the following Eq. (3.12), where $(s)$ denotes Laplace parameter, over-bar denotes deviation of a variable from its initial steady state value and subscript $s$ denotes the initial steady state value:

$$
\frac{\overline{C_R}}{\overline{C_{A_0}}} = \frac{\overline{C_R}(0^+)}{\overline{C_{A_0}}} \left( \frac{(s + (v_o / V + k)) / M + kv_o / V}{(s + (v_o / V + k))(s + v_o / V)} \right) \tag{3.12}
$$

Thus, this transfer function would have reduced to the standard second-order transfer function, if $\overline{C_R}(0^+)$ was zero, i.e., the discontinuity was ignored.
3.3 Semi-batch Reactor

Consider a variable holdup semi-batch reactor, in which, $A$ was already in the reactor and $B$ was being fed continuously at constant rate $v_o$ for time $t \leq 0^-$. No outlet stream is there. $M$ (m$^3$) of reactant $B$ is fed suddenly at $t \to 0^+$. This is equivalent to an impulse perturbation (in $B$) volumetric flow rate of feed $v_o$ at $t \to 0^+$. For the elementary reaction $A + B \rightarrow R$, the component molar balance for $B$ and $A$ respectively are (Fogler, 2005):

$$\frac{d(VC_b)}{dt} = v_o C_{B_0} - kA C_b V$$  \hspace{1cm} (3.13)

$$\frac{d(VC_A)}{dt} = -kA C_B V$$  \hspace{1cm} (3.14)

3.4 Single-component Condenser

This model is also used in literature (Chowdhary et al., 2004; Kröner et al., 1997; Majer et al., 1995; Pantelides et al., 1988; Unger et al., 1995; Vieira and Biscaia Jr., 2001). The symbols were defined in the last chapter.

$$\frac{dN}{dt} = F - L$$  \hspace{1cm} (3.15)

$$NC_p \frac{dT}{dt} = FC_p (T_o - T) + L\Delta H + U_h A_h (T_j - T)$$  \hspace{1cm} (3.16)

$$P^* = A \exp \left( -\frac{B}{T+C} \right)$$  \hspace{1cm} (3.17)

$$V = \frac{NRT}{P^*}$$  \hspace{1cm} (3.18)

3.4.1 Revised model

In the above literature model of Section 3.4, Eq. (3.16) is obtained by applying differentiation rule of the product of variables $N$ and $T$ in the accumulation term of the original energy balance equation, and substituting material balance Eq. (3.15) for the
differential of $N$. This model might work for the step input. However, the *impulse* input causes initial discontinuities in $N$ and $T$ that make these variables non-differentiable, and, so, the symbolic manipulations and differentiations are bound to lead to errors. Hence, for the impulse input, the first principles energy balance must replace Eq. (3.16).

The original energy balance equation for the vapor phase is re-formulated as:

$$C_p \frac{d(NT)}{dt} = FC_pT_o + U_sA_k(T_j - T) - L(C_pT - \Delta H)$$  \hspace{1cm} (3.19)

The first term is the accumulation of energy, the second term is enthalpy of inlet vapors, the third term is heat transfer to the cooling jacket, and the fourth term is the enthalpy of outlet condensed liquid.

The comparisons of this model with others are made in Sections 5.13 and 5.14.

### 3.4.2 Model obtained through symbolic manipulations

If $V$ is a variable, the above model has one degree of freedom for perturbation in $F$, and, so, $V$ has been assumed constant in the above literature model. Assuming constant volume, the model has zero degree of freedom. For solution, the model can be converted to a different form after symbolic differentiations and manipulations. Limitations of the symbolic manipulations were outlined in Section 2.3.1 of the last chapter. The model formulated here will be used to illustrate the inconsistencies arising out of symbolic manipulations and differentiations in Section 5.13. Consider a step disturbance in the molar feed rate $F$ introduced into the single component condenser model with volume $V$ held constant at $V_o$. The above model is converted to explicit ODE system in order to use the standard explicit ODE solvers. To obtain $L$ explicitly from the above equations, the model is converted to the following form after symbolic differentiations and manipulations. Eq. (3.18) is first written as:

$$N = \frac{P^*V_o}{RT}$$  \hspace{1cm} (3.20)

Then, an explicit equation for $L$ is obtained by cumbersome manipulations: differentiating Eqs. (3.17) and (3.20), and combining them together to give Eq. (3.21).
Substituting Eq. (3.21) and the value of \( \frac{dT}{dt} \) obtained from Eq. (3.16) into Eq. (3.15), finally gives the following Eq. (3.23) for \( L \).

\[
\frac{dN}{dt} = Z \frac{dT}{dt} \tag{3.21}
\]

where

\[
Z = \frac{BV_o P^*}{RT(T + C)} - \frac{V_o P^*}{RT^2} \tag{3.22}
\]

\[
L = \frac{FNC_p - Z\{FC_o(T_o - T) + U_h A_h(T_j - T)\}}{NCp + Z\Delta H} \tag{3.23}
\]

Hence, an alternative system consisting of Eqs. (3.15), (3.16), (3.17), (3.22), and (3.23) is obtained.

However, for \( N \), there is a choice of including either the differential Eq. (3.15) or the algebraic Eq. (3.20). These alternative systems are solved using explicit ODE solvers for a step and impulse perturbation in \( F \), and many unsatisfactory results are exhibited. The analysis of discontinuities and the numerical results of these alternative systems, exposing their inconsistencies are presented in Section 5.13.

### 3.4.3 Linearized model

The system is assumed to be at steady state at time \( t \to 0^- \). Linearizing Eq. (3.19) and using Eq. (3.15), for no change in the jacket temperature, the following equation is obtained:

\[
C_p N_s \frac{d\bar{T}}{dt} = C_p (T_o - T_j) T - (U_h A_h + L_s C_p) \bar{T} + (\Delta H) \bar{L} \tag{3.24}
\]

Subscript \( s \) and over bar represent initial steady state and the deviations of variables from their initial steady states, respectively.

Various tank models are considered next. The flow-level tanks and their draining times are used in the next chapter to validate the initialization effects as these are clearly
observed in the level responses. Coupled and interacting flow-level tanks, stirred-tank heaters, reactors, etc. have been reported quite often in the literature studies (Engin et al., 2004; Gatzke et al., 2000; Oh and Yeo, 1996; Roy, 2003; Sundaram and Radhakrishnan, 2003; Thakkar and Gaikwad, 2005; Watt et al., 2010).

3.5 Gravity-flow Tank

A gravity-flow tank consists of a tank with an inflow stream and a straight, horizontal outflow pipe at the bottom exit (Fig. 3.1). It is unique in the respect that it has interacting material (tank) and mechanical energy (pipe) capacities. This results in coupled differential equations. Plug flow is assumed in the pipe and, hence, the velocity profile is flat. This facilitates the application of momentum balance on the pipe fluid as it can be considered as a lumped free body. Writing transient material and momentum balances (Luyben, 1990) gives the following two Eqs. (3.25) and (3.26). These equations may be solved for \( h \) to yield a cumbersome nonlinear ordinary differential equation that contains a term with a differential of the input function \( q \) (see Eq. (3.27)). \( A_T \) is x-sectional area of the tank, \( h \) is level, \( q \) is volumetric feed rate, \( u_p \) is efflux velocity in the pipe, \( f \) is friction factor \( A_p, L, D_p \) are respectively x-sectional area, length and diameter of the pipe.

\[
\frac{dh}{dt} = - \frac{A_p}{A_T} u_p + \frac{q}{A_T} \tag{3.25}
\]

\[
\frac{du_p}{dt} = \frac{g}{L} h - \frac{2f}{D_p} u_p^2 \tag{3.26}
\]
3.5.1 Linearized model

The system is assumed to be at steady state at time \( t \to 0^- \). Linearizing, combining and taking Laplace transforms of these equations, give:

\[
\begin{align*}
    s^2 H(s) - sH(0) - H'(0) &+ \frac{B}{A} [sH(s) - H(0)] + \frac{C}{A} H(s) = K [sQ(s) - Q(0)] + \frac{B}{A} Q(s) \\
\end{align*}
\]

where \( K = 1/A_r, \ A = A_p L, \ B = (4fLQ_s)/(D_p), \ C = gA_p^2 / A_r \)

Capitals \( H, U \) and \( Q \) are deviation variables corresponding to variables of lower case. These deviations are from their initial steady states. Subscript \( s \) represents initial steady state and superscript (') represents derivative. The corresponding transfer function form (valid for step inputs, see next chapter, Section 4.2.2) becomes:

\[
\begin{align*}
    H(s) & = \frac{1}{A_r} \frac{(\rho A_p L)s + \left(4fL\rho Q_s\right)/D_p}{(\rho A_p L)s^2 + \left[\left(4fL\rho Q_s\right)/D_p\right]s + \left(\rho gA_p^2\right)/A_r} \\
\end{align*}
\]

It is rewritten in a different version as:

\[
\begin{align*}
    \frac{Y(s)}{X(s)} & = K' \frac{s + l}{A s^2 + Bs + C} \\
\end{align*}
\]

where \( K' = \rho A_p L / A_r, \ l = \left(4fQ_s\right)/(A_p D_p), \ A = A_p L, \ B = \left(4fLQ_s\right)/(D_p), \ C = gA_p^2 / A_r \)

3.6 Interacting Tanks System

The first tank of the two interacting liquid-level tanks-in-series is considered (Fig. 3.2). Writing transient material balances gives the following two Eqs. (3.30) and (3.31). These equations may be solved for the level of the first tank \( h_1 \) to yield a cumbersome ordinary differential equation that contains a term with differential of input function \( q \). Here, \( q \) stands for volumetric inflow rate to the first tank; \( A_1 \) and \( h_1 \) are cross-sectional area and level rate of the first tank, respectively; \( q_21, h_2 \) and \( q_2 \) are the input flow, level and output flow of the second tank.
\[
\frac{dh_1}{dt} = -\frac{q_{21}}{A_1} + \frac{1}{A_1} q \quad (3.30(a)) ; \quad \frac{dh_2}{dt} = -\frac{q_2}{A_2} + \frac{1}{A_2} q_{21} \quad (3.30(b))
\]

For non-linear resistances the flow-head relationships with constants \(k_1\) and \(k_2\) are:

\[
q_{21} = k_1\sqrt{h_1 - h_2} ; \quad q_2 = k_2\sqrt{h_2} \quad (3.31)
\]

![Schematic of the two interacting tanks system](image)

**Fig. 3.2** Schematic of the two interacting tanks system

### 3.6.1 Linearized model

The system is assumed to be at steady state at time \(t \to 0^-\). Assuming the outflows from tanks 1 and 2 are related to the liquid levels with constant linear resistances \(R_1\) and \(R_2\):

\[
Q_{21} = \frac{H_1 - H_2}{R_1} \quad (3.32(a)) ; \quad Q_2 = \frac{H_2}{R_2} \quad (3.32(b))
\]

Combining Eqs. (3.30) and (3.32), and solving for \(H_1\) gives:

\[
\tau_1 \tau_2 \frac{d^2H_1}{dt^2} + (\tau_1 + \tau_2 + A_1R_2) \frac{dH_1}{dt} + H_1 = (R_1 + R_2)Q + \tau_2R_1 \frac{dQ}{dt} \quad (3.33)
\]

Capitals \(Q_{21}\), \(H_1\), \(Q_2\), \(H_2\) are deviation variables corresponding to variables of lower case.

\[
\tau_1 = A_1R_1 \text{ and } \tau_2 = A_2R_2.
\]

The above system Eq. (3.33) is written in the following useful Laplace transform version:

\[
\tau_1 \tau_2 [s^2H_1(s) - sH_1(0) - H_1'(0)] + [(\tau_1 + \tau_2 + A_1R_2)\times[sH_1(s) - H_1(0)] + H_1(s)] = (R_1 + R_2)Q(s) + \tau_2R_1[sQ(s) - Q(0)] \quad (3.34)
\]
The transfer function form for the first tank is (see next chapter, Section 4.2.2):

\[
\frac{H_1}{Q} = \frac{(\tau_2 R_1) s + (R_1 + R_2)}{(\tau_1 \tau_2) s^2 + (\tau_1 + \tau_2 + A_1 R_1) s + 1}
\] (3.35)

It is rewritten in a different version as:

\[
\frac{Y(s)}{X(s)} = K' \frac{s + l}{As^2 + Bs + C}
\] (3.36)

where \( K' = \tau_2 R_1, l = (R_1 + R_2) / (\tau_2 R_1), A = \tau_1 \tau_2, B = \tau_1 + \tau_2 + A_1 R_2, C = 1 \)

### 3.7 Closed-loop Stirred Tank Heater with Dead Time

This model is selected to illustrate the effect of initial conditions on the closed-loop systems in the presence of dynamic lags in Chapter 5. Consider a stirred tank heater system that consists of a constant holdup tank of volume \( V \) and a horizontal pipe at the bottom exit. Liquid of density \( \rho \) and specific heat \( C_p \) enters at a flow rate \( v_o \) and temperature \( T_o \), and it is heated in the tank to a temperature \( T \) with a thyristor controlled electric heater. Temperature transmitter senses the temperature \( T_m \) at the pipe exit, and transmits the signals to the control module. The process temperature is controlled through a proportional controller of gain \( K_c \) by manipulating heat input to the process \( Q \). A tank heater is rigorously modeled as a distributed-parameter system, or a lumped-parameter system with dead time (Goswami et al., 1997; Jotshi et al., 2001). Here, it is modeled as a first-order system with dead time \( \tau_d \) (FOPDT). There is no lag in any other component of the control loop. Writing energy balance and using the controller equation, the following delay differential equation (DDE) of the regulator system perturbed by inflow rate \( v_o \) is obtained (Coughanowr and LeBlanc, 2009):

\[
\frac{dT_m}{dt} = K_1 Q(0^-) - K_1 K_c T_m(t - \tau_d) + K_1 K_c T_m(0^-) + K_3 v_o(t - \tau_d) - K_2 v_o(t - \tau_d) T_m
\]

where \( K_1 = 1 / (\rho C_p v_o) \), \( K_2 = 1 / V \), and \( K_3 = T_o / V \) (3.37)

An FOPDT model has been a prevalent model of process plant dynamics, and has been of considerable research interest (Arbogast et al., 2007, Banu and Uma, 2008;
Juneja et al., 2009; Kanagaraj et al., 2009; Kaya, 2004; Skogestad 2004; Toscano, 2005; Vilanova and Pedret, 2010), as the presence of a significant dead time makes the closed system oscillatory, unstable and difficult to design and control. This DDE can’t be solved through ordinary means; hence, a numerical algorithm based on fourth order Runge-Kutta method is developed for the solution (refer to Appendix II).

3.7.1 A degenerate system – linearized jacketed stirred tank heater

In a stirred-tank heater, material and thermal energy capacities are interacting. It consists of a perfectly stirred tank of variable hold up \( V \), which heats the incoming liquid stream of flow rate \( v_o \), using a jacket fluid of temperature \( T_j \). The leaving stream is thus at a higher temperature \( T \). Let the incoming temperature \( T_o \) be a constant. The jacket fluid is saturated. The input variable considered here is the inflow rate \( v_o \). The material and energy balance equations respectively are (Coughanowr and LeBlanc, 2009):

\[
\frac{dV}{dt} = v_o - v \tag{3.38}
\]

\[
\rho C_p \frac{d(VT)}{dt} = v_o \rho C_p T_o + U_h A_h (T_j - T) - v \rho C_p T \tag{3.39}
\]

Assume constant linear resistance \( R \), i.e., \( v = V / R \). The system is assumed to be at steady state at time \( t \rightarrow 0^+ \). Introducing deviation variables, linearizing the non-linear terms and solving simultaneously, gives:

\[
\frac{\bar{T}}{\bar{v}_o} = -\frac{(T_s - T_o)(Rs + 1)}{V_s(Rs + 1)(s + v_s / V_s + U_h A_h / \rho C_p)} = -\frac{(T_s - T_o)}{V_s(s + v_s / V_s + U_h A_h / \rho C_p)} \tag{3.40}
\]

Hence, this linear system behaves as a first-order negative gain system due to pole-zero cancellation.
3.8 Inherent Second-order Systems with Derivative of the Input

3.8.1 U-tube manometer

Such systems are the linear systems with terms containing derivative of the input function, i.e., inherent numerator-dynamics. Consider a simple U-tube manometer that measures a pressure difference $\Delta P$ imposed on its two legs. It contains a liquid of density $\rho$ and viscosity $\mu$. The mass of the liquid column is $m$, total length of the column is $L$, and its cross sectional area is $A$, $g$ is acceleration due to gravity, $u$ is the velocity of the liquid column, and $y$ is the deviation of liquid level from the initial rest position if the levels in the two legs were equal. $U$, $Y$, & $\Delta P$ are the corresponding deviations from the pre-initial state. Assuming laminar flow in the tube but ignoring radial variations in velocity so that the system can be modeled through the lumped-parameter approach. This facilitates application of momentum balance on the column as a whole as it can be considered a free body; this gives the following equations for $Y$ and $U$ (Coughanowr & LeBlanc, 2009):

\[
m\ddot{y} = -a\dot{y} - by + A(\Delta P) \quad \text{or} \quad m\ddot{Y} = -a\dot{Y} - bY + A(\Delta P) \quad (3.41)
\]

\[
m\ddot{u} = -a\dot{u} - bu + A(\Delta P) \quad \text{or} \quad m\ddot{U} = -a\dot{U} - bU + A(\Delta P) \quad (3.42)
\]

where \( a = 8\pi\mu LA, \quad b = 2\rho g A \)

The last equation is derived by noting that $u = \dot{y}$

3.8.2 Car wheel suspension example

This system described in the last chapter (Fig. 2.3) consists of a spring and damper in parallel and is described by Eq. (2.24) of the last chapter, i.e., a second-order ODE containing a derivative of the input term (Lundberg et al., 2007).

3.8.3 Model for car-body subjected to applied force

This system described in the last chapter (Fig. 2.3) again consists of a spring and damper in parallel and is described by Eq. (2.28) of the last chapter, i.e., a second-order ODE containing a derivative of the input term. The above three systems shall be used in the treatment of inconsistencies in the Laplace transforms in Chapter 6.
As can be seen in the above models, the governing equations, in general, yield second-order ODEs with terms containing differentials of the input function. In particular, Eqs. (3.5), (3.9), (3.12), (3.28), (3.33), (3.36), (3.40), and (3.42) exhibit this fact. These systems are called second-order numerator-dynamics systems in their linearized, transfer function adaptations, because their transfer functions contain a variable term in the numerator. These systems contain singular terms of differentials of the input function even for the step perturbation, and, thus, exhibit initial discontinuities in initial values and/or slopes of the step and impulse responses. To explore the range of behavior of these systems in general, their comprehensive treatment is provided in the next section (Ahuja, 2010). Their general profiles are derived and their characteristic parameters are identified. The solution profiles of these systems depend upon the value of one such parameter relative to that of the others on the real axis. These conditions unfold different types of profiles exhibiting initial discontinuity, maximum, minimum, inflection, input multiplicity, etc., when applied to the models presented above. Negative real part poles are considered, deviation variable are used and the magnitudes of the inputs are taken as positive throughout.

### 3.9 Second-order Numerator-dynamics Transfer Functions

The second-order numerator-dynamics systems represented by Eq. (2.2) exhibit an assortment of behavior. For such systems, the same three types of step and impulse responses viz. over-damped, under-damped and critically-damped as encountered in the standard second order systems are exhibited. However, there are some differences, which can be observed from response profiles shown in the figures in the following sections. There are discontinuities in initial values and/or initial slopes, and the over-damped case exhibits maximum and minimum in step and impulse responses respectively, which are not there in the standard second-order systems, i.e., not containing the derivative of the input terms. In general, the responses are faster than that of standard counterparts because the relative order is one. Relative order: (order of denominator – order of numerator) of the transfer function. The speed of the response is not given only by the parameters $\tau$ (time constant) and $\zeta$ (damping coefficient), but also by the relative magnitudes of the constants in the numerator of their transfer functions. Eq. (2.2) is repeated below:
\[
A \frac{d^2 Y}{dt^2} + B \frac{dY}{dt} + CY = D \frac{dX}{dt} + EX \tag{2.2}
\]

### 3.9.1 Over-damped response

The over-damped step response of these systems, unlike the standard second-order systems, is found to exhibit a range of behavior: (a) a response similar to first-order systems, (b) a curve containing a maximum with a point of inflection, and (c) a curve containing a point of inflection at origin as a limiting case (this limiting case will be shown to be valid for the gravity-flow tank system). They are shown in Figs. 3.3(a) through 3.3(d) below.

![Fig. 3.3(a)](image)

![Fig. 3.3(b)](image)

![Fig. 3.3(c)](image)

![Fig. 3.3(d)](image)

**Fig. 3.3** Step responses of non-oscillatory numerator-dynamics systems, (a) for Cases (A) and (D); (b) for Cases (B.1) and (E); (c) for Case (B.2); (d) for Cases (B.3) and (F) discussed later in this section and represented on the real axis.
Note that the initial slope is not zero for any of these cases, unlike the standard second-order systems. The impulse response is found to exhibit even more number of cases, viz. (a) one like a first-order system, (b) a curve containing a point of inflection at zero time, (c) a curve containing a maximum near zero time with a point of inflection, and finally (d) one like a standard second-order impulse as a limiting case. These curves are shown in the Figs. 3.4(a) through 3.4(e). The conditions of the respective profiles can be found. Since the roots of the characteristic equation for the over-damped case are real and unequal, Eq. (2.2) can be written in a different form:

\[
\frac{Y(s)}{X(s)} = K \frac{s + l}{(s + m)(s + n)}
\]  

(3.43)

where constants \( K, l, m, n \geq 0 \) and \( l \neq m, n \)

The solution for unit step input, obtained through inverse Laplace transforms, is:

\[
Y_{st}(t) = K \left( \frac{l}{mn} \right) \left[ 1 + \frac{n}{l} \left( \frac{m-l}{n-m} \right) e^{-mt} - \frac{m}{l} \left( \frac{n-l}{n-m} \right) e^{-nt} \right]
\]

For \( m \neq n \)  

(3.44)

One of the two roots of the quadratic characteristic equation is smaller (say \( m \)) than the other (say \( n \)) for the over-damped case. The derivative of Eq. (3.44) is the following equation, which also represents the unit impulse response:

\[
Y_{st}'(t) = Y_{imp}(t) = K \left[ \frac{l-m}{n-m} e^{-mt} + \frac{n-l}{n-m} e^{-nt} \right]
\]

For \( m \neq n \)  

(3.45)

**Maximum for the step response and zero for the impulse response** Differentiating the step response and equating it to zero finds the condition for the step response curve containing a maximum. Equating Eq. (3.45) to zero gives:

\[
t_{\text{max}} = \frac{1}{n-m} \ln \frac{n-l}{m-l} \quad \text{For} \ m \neq n
\]

(3.46)
Fig. 3.4 Impulse responses of non-oscillatory numerator-dynamics systems, (a) for Cases (A) and (D); (b) for Cases (B.1) and (E); (c) for Case (B.2); (d) for Cases (B.3.a) and (F); (e) for Case (B.3.b) discussed later in this section and represented on the real axis.
For a feasible value of $t_{\text{max}}$, the quantity within the logarithm term should be positive. This is possible under two conditions (namely Case (A) and Case (B)): Case (A) $l$ should be less than both $m$ and $n$; Case (B) $l$ should be more than both $m$ and $n$. The condition (B) gives a negative value of time, whereas (A) gives a positive value of time, which corresponds to Fig. 3.3 (a), note that this curve depicts a point of infection. This time also corresponds to the zero value of the impulse response in Fig. 3.4 (a). The feasibility condition for Eq. (3.46) corresponding to the Case (A) is reiterated mathematically as:

**Case (A): $l < \min (m, n)$** \hspace{1cm} (3.47)

**Minimum/maximum for the impulse response and inflection for the step response** The impulse response corresponding to Case (A) depicts a minimum in Fig. 3.4 (a) at the time when the step response depicts a point of inflection in Fig. 3.3 (a). Differentiating Eq. (3.45) and equating it to zero gives this time. The derivative of Eq. (3.45) is as follows:

$$Y_{st}''(t) = Y_{imp}'(t) = -K \left[ \left( \frac{l-m}{n-m} \right) me^{-mt} + \left( \frac{n-l}{n-m} \right) ne^{-mt} \right] \text{ For } m \neq n$$ \hspace{1cm} (3.48)

Equating it to zero gives:

$$t_m = \frac{1}{n-m} \ln \left[ \left( \frac{n-l}{m-l} \right) \frac{n}{m} \right] \text{ For } m \neq n$$ \hspace{1cm} (3.49)

From this Eq. (3.49), the condition for a positive value of this time for the Case (A) is:

$$l < m + n$$ \hspace{1cm} (3.50)

It may be noted that Eq. (3.50) is always true for Case (A) and, hence, gives a minimum for impulse because the further derivative of Eq. (3.48) results in a negative value at $t_m$.

And from Eq. (3.49) again, the following condition for a positive value of this time under **Case (B)** is obtained:

$$l \geq m + n$$ \hspace{1cm} (3.51)
Subdivisions of Case (B) The feasibility condition for Case (B) is reiterated as:

\[
\text{Case (B): } l > \max(m, n) \quad (3.52)
\]

Combining Eqs. (3.51) and (3.52), lead to three subdivisions of Case (B). These are discussed below as (B.1), (B.2) and (B.3):

Sub-case (B.1): \( l > m + n \). This corresponds to Figs. 3.3 (b) for the step response and 3.4 (b) for the impulse response. They show an inflection for the step response and a maximum for the impulse response, respectively. Note that for the impulse input, the same Eq. (3.49) corresponds to the time of minimum for Case (A) but to the time of maximum for Case (B).

Sub-case (B.2): \( l = m + n \). This corresponds to Figs. 3.3 (c) for the step response and 3.4 (c) for the impulse response. Note that in this case the point of inflection in the step response and the maximum in the impulse response are occurring at the zero value of time.

Sub-case (B.3): \( l < m + n \). This corresponds to Figs. 3.3 (d) and 3.3 (c) for the step response, and 3.4 (d) and 3.4 (e) for the impulse response. There is no maximum/minimum for step or impulse responses.

Inflection for the impulse response The above Sub-case (B.3) is further bifurcated into following two cases on the basis of inflection for impulse:

Case (B.3.a): \( l < (n^2 + m^2 + nm) / (n + m) \) \quad (3.53)

Case (B.3.b): \( l > (n^2 + m^2 + nm) / (n + m) \) \quad (3.54)

The former of the two correspond to no point of inflection for the impulse response as shown in Fig. 3.4 (d) but the latter yields to a point of inflection for the impulse response as shown in Fig. 3.4 (e). Other cases and sub-cases do not yield this bifurcation because of the following reasons (inflection is either present or absent throughout their domain).

For Case (A), the condition for impulse showing an inflection is reversed, i.e., Eq. (3.53) is valid for inflection and not Eq. (3.54). But Eq. (3.53) always holds for Case (A). This is shown below.
Since \( n > m \), the condition given by Eq. (3.47) reduces to \( l < m \). Combining it with Eq. (3.53) gives the following condition:

\[
m < \frac{(n^2 + m^2 + nm)}{(n + m)}
\]  \hspace{1cm} (3.55)

This yields \( n^2 > 0 \), which is always true. Thus, Case (A) always depicts an inflection in the impulse response as depicted in Fig. 3.4 (d). The time of inflection is given by:

\[
t_i = \frac{1}{n-m} \ln \left[ \left( \frac{n-l}{m-l} \right) \frac{n^2}{m^2} \right] \quad \text{For } m \neq n
\]  \hspace{1cm} (3.56)

Likewise, for Case (B) the governing equation becomes \( l > n \). For Case (B.1), combining this with Eqs. (3.51) and (3.54) gives:

\[
m + n > \frac{(n^2 + m^2 + nm)}{(n + m)}
\]  \hspace{1cm} (3.57)

This yields \( 2 > 1 \), that again is always true and, thus, Case (B.1) always shows inflection throughout its domain, the time of inflection is given by the same Eq. (3.56). Whereas, for the Case (B.2), the time for inflection in the impulse response is given by placing:

\[l = n + m\]

in Eq. (3.56), one gets:

\[
t_i = \frac{1}{n-m} \ln \frac{n}{m} \quad \text{For } m \neq n
\]  \hspace{1cm} (3.58)

Eq. (3.58) is always feasible because \( n > m \). Thus, the Case (B.2) also, always shows inflection for the impulse response, throughout its domain.

The only condition that still remains uncovered is the Case (C), it is given below:

**Case (C):** \( m < l < n \), for which there is neither a maximum/minimum, nor any inflections. Its response curves are shown in Figs. 3.3 (d) and 3.4 (d).
The above inequalities are comprehensively represented on the real axis:

\[
\begin{array}{cccccc}
0 & m & n & z & w \\
\text{I} & \text{(A)} & \text{I} & \text{(C)} & \text{I} (B.3.a) & \text{I} (B.3.b) & \text{I} (B.2) & \text{I} (B.1)
\end{array}
\]

where \( w = m + n \quad z = (n^2 + m^2 + nm) / (n + m) \)

To summarize, \( l \) can lie in any of the regions shown: Region (A) corresponds to maximum and inflection for the step response and minimum for the impulse response, (B.1) to inflection for the step response and maximum for the impulse response. (B.2) is the limiting Case of (B.1) in which the inflection and the maximum are at zero time, (B.3) and (C) depict no extremes. The response curves corresponding to all these regions are shown in this order in Figs. 3.3 (a), 3.3 (b), 3.3 (c) and 3.3 (d) respectively for the step response, and 3.4 (a), 3.4 (b), 3.4 (c), and 3.4 (d) respectively for the impulse response.

Finally, initial slopes for the impulse response curves of all the cases are given by:

\[
Y_{imp}'(0) = K (l - n - m) \quad (3.59)
\]

**3.9.2 Critically damped response** This case can be worked out similarly. Let \( m = n \) in Eq. (3.43) for this case yields the following Regions D, E, and F on the real axis.

\[
\begin{array}{cccc}
0 & m & 2m \\
\text{I} & \text{(D)} & \text{I} (F) & \text{I} (E)
\end{array}
\]

**Case (D):** This depicts maximum for the step response and minimum for the impulse response in Figs. 3.3 (a) and 3.4 (a), respectively.

**Case (E):** This gives a maximum for the impulse response similar to Fig. 3.4 (b).

**Case (F):** This case can again be bifurcated at the mid-point on the basis of inflection for impulse: The left half shows no maximum/ minimum or inflection but the right half depicts inflection for impulse at the time given by:

\[
t_i = (3m - 2l) / (m - l) \quad (3.60)
\]
3.9.3 **Under-damped response** For oscillatory response, better use $\zeta$ and $\tau$ of second-order systems and the transfer function becomes:

$$\frac{Y(s)}{X(s)} = P \frac{s + l}{\tau^2 s^2 + 2\zeta \tau s + 1} \quad (3.61)$$

Unit impulse response for this case is:

$$Y_{\text{imp}}(t) = \frac{P}{\tau^2} e^{-\zeta \tau t} \left[ \cos \left( \frac{t}{\tau} \sqrt{1 - \zeta^2} \right) + \frac{\tau l - \zeta}{\sqrt{1 - \zeta^2}} \sin \left( \frac{t}{\tau} \sqrt{1 - \zeta^2} \right) \right] \quad (3.62)$$

The initial slope of the impulse response is given by:

$$Y_{\text{imp}}'(0) = Y_{\text{imp}}''(0) = \frac{P}{\tau^3} \left( \tau l - \zeta \right) / \tau - \frac{P}{\zeta \tau} \quad (3.63)$$

The impulse response curves are similar to those for the standard second-order systems, except that they are faster and with initial value non-zero. Depending upon whether the initial slope is positive, negative or zero, they are of different shapes. These are shown in Figs. 3.5 (a), 3.5 (b) and 3.5 (c), respectively. Step response is also similar to its standard counterpart, except that its initial slope is a non-zero positive, is faster, has more overshoot and higher final value.

3.9.4 **Applications of the results**

It is further illustrated how the conditions of Sections 3.9 unfold for different numerator-dynamics cases.

**Input multiplicity** If $l = 0$ and gain is positive, the step response undergoes a maximum and eventually returns to the same initial value irrespective of the magnitude of the input as shown in Fig. 3.6. The impulse response undergoes a minimum and goes below zero as shown in Fig. 3.4 (a) irrespective of the magnitude of the input. Velocity transfer function of a damped vibrator under perturbation in applied force (Fig. 2.3 and Section 2.2.3.), velocity of the liquid manometer column under applied pressure or current in the RLC circuit under applied electro motive force (voltage) exhibit such a behavior.
Fig. 3.5 Impulse responses for oscillatory numerator-dynamics systems with (a) positive, (b) negative, and (c) zero initial slopes discussed in Section 3.9.3
**Pole-zero cancellation** In case, $l = (m \text{ or } n)$ in the system transfer function Eq. 3.43, the system reduces to first order as shown in the stirred tank heater example in Sections 3.7.1 and non-isothermal CSTR example in Eq. (3.77) below. These systems, thus, do not show numerator-dynamics form.

**Two interacting-tanks system** For Region (A) on the real axis for this system, i.e., the condition given by Eq. (3.36) requires the following two conditions to be met simultaneously:

$$A_l < B/2 \text{ and } A_l > B - C/l$$

(3.64)

And for Region (B) on the real axis (condition given by Eq. (3.51)):

$$A_l > B/2 \text{ and } A_l > B - C/l$$

(3.65)

$$A_l > B - C/l, \text{ gives } \tau_2 R_2 < 0$$

(3.66)

which is not possible. Hence, Regions (A) and (B) are non-feasible regions. The only feasible Region is (C), the curves for which neither show any maximum/minimum nor any point of inflection.

**Coupled CSTRs** Consider coupled constant flow isothermal CSTRs having a recirculation loop given in Figs. 3.7 (a) and 3.7 (b). They are carrying out an incompressible liquid phase, first-order reaction $A \rightarrow R$. 
For the first of the two coupled tanks, the numerator-dynamics transfer functions $C_{A}/C_{Ao}$ are found out corresponding to Figs. 3.7 (a) and 3.7 (b). The transfer functions are found by applying unsteady material balance of $A$. On comparison of the transfer function of Fig. 3.7 (a) with the equation of type (3.36), one gets:

\[
I = \frac{(kV_s + v_s)}{v_s} A = VV_s, B = kV_sV + v_sV + vV_s + \frac{V_s}{V}V
\]

\[
C = kV_s + k^2VV_s + kV_sV + vV_s + kV_s
\]

(3.67)

Cases (A) and (B) on the real axis are not feasible because for $AI > B - C/I$:

\[
v_s^2 < 0
\]

(3.68)

For the second Fig. 3.7 (b); finding $I$, $A$, $B$, and $C$ and applying, $AI > B - C/I$:

\[
v_r^2/v + v_r^2kV_s / (v + v_r) < 0
\]

(3.69)
which is again not possible. So, such systems fall only in Region (C) on the real axis. Thus, they are never under-damped. Also, note that the value of the damping factor $\zeta > 0$.

It can also be checked that $l < (m + n)$ (the equality never holds), and the initial slope of their impulse response obtained from Eq. (3.59) is non-zero and negative due to this. These findings apply across all the interacting systems discussed above.

All interacting and coupled systems composed of first-order systems, in general, come under Case (C) on the real axis.

**Gravity-flow tank** From Eq. (3.28) for this system, the sum $(m + n)$ is equal to $B/A$, and this gives:

$$l = m + n$$

Eq. (3.70) implies that the system coincides with point $w$ or (B.2) on the real axis, and Eq. (3.51) and (3.57) are valid. The response thus shows a point of inflection at the origin for the step input and corresponds to that shown in Fig. 3.3 (c). For the impulse input it shows a maximum at zero time and an inflection near zero time and shown in Fig. 3.4 (c).

**Jacketed non-isothermal CSTR**

From Eqs. (3.5) and (3.6) for this system, $K$ and $l$ are always positive. But $d$ and $e$ can be negative or positive. To detect that, following two cases are taken: (1) If the reaction is exothermic, $\Delta H_R$ is negative and, (2) if the reaction is endothermic, $\Delta H_R$ is positive. Note that the first case can give unstable poles. Also, recall that only stable cases are being dealt with for which $(l + d)$ and $(ld - e)$ are positive. The exothermic case is treated first.

**Exothermic reaction** This system can exhibit maximum for impulse too. For this case, $e$ is negative but $d$ can either be positive, negative or zero. The over-damped domain is first considered.

For Case (A) to be valid $l < m$. Applying this condition and using the roots of the quadratic gives, $e < 0$ and $l < d$. 

$$\text{(3.71)}$$
For Case (B) to be valid $l > n$. Applying this condition and using the roots of the quadratic gives, $l > d$ and $e < 0$.  \( (3.72) \)

For Sub-case (B.1) to be valid, $l > (m + n)$, that gives, $d < 0$.  \( (3.73) \)

For Sub-case (B.3) to be valid, $l < (m + n)$, that gives, $d > 0$.  \( (3.74) \)

For Sub-case (B.2), $d = 0$.  \( (3.75) \)

So, it is found that all the above cases are feasible and even the conditions of stability do not make them non-feasible.

The Case (C) is, however, not feasible.

The results are analogous for critically-damped case too. This system is over-, critical- and under-damped depending on the following conditions, respectively.

\[
(l - d)^2 + 4e > 0, \quad (l - d)^2 + 4e = 0, \quad (l - d)^2 + 4e < 0
\]

Thus, if $l = d$ this system is oscillatory.

**Endothermic reaction** For this case $K, l, d, e$ are all positive and non-zero. Only feasible region in this Case is (C). Also, this case can only be over-damped. This is, therefore, one of the kinds of the first-order interacting and coupled systems in series.

**Reaction enthalpy zero ($\Delta H_R = 0$)**

For this case of no heat effect, the system Eqs. (3.5) and (3.6) reduce to first-order as shown:

since, $e = 0$  

\[
\frac{T}{T_j} = K \frac{s + l}{s^2 + (l + d)s + ld - 0} = K \frac{s + l}{(s + l)(s + d)} = \frac{K}{s + d}
\]

Another numerator-dynamics case, i.e., a stirred tank heater too, invariably turned out to be standard first-order in Section 3.7.1.
3.9.5 Discussion

Figs. 3.3 through 3.5 reveal the variation in the nature and speed of the response profiles as \( l \) changes on the real axis. The impulse response of the over-damped case of second-order numerator-dynamics system derived in Section 3.9 is given by Eq. (3.45) with parameters \( K, l, m, n \geq 0 \). Observe the effect of parameter \( l \) on the response from Eq. (3.45). Initial discontinuity, initial value and final value of the response don’t depend on \( l \). Eq. (3.45) contains two terms involving \( l \), namely, \( le^{-mt} (n - m) \), and \( -le^{-rt} / (n - m) \). If \( l \) is decreased (keeping all other parameters constant), the first term increases but the second one decreases, however, since \( m < n \) the first term dominates and there is a net decrease in the magnitude of impulse response. Thus, the response for a lower value of \( l \) always lies below the one with a higher value of \( l \). Hence, the decrease of the response is faster on decreasing \( l \). Looking at the curves of Figs. 3.3(b), 3.3(c), 3.3(e), 3.3(d) and finally 3.3(a) serially in this order, it is seen that as \( l \) decreases, the response decreases faster. In Fig. (2.a), it even goes below the initial value and exhibits minimum.

However, as \( l \to \infty \), the impulse response of the numerator-dynamics system approaches the impulse response of a standard second-order system. Thus, the impulse response increases initially, rather than decreasing, and has positive initial slope and has no initial discontinuity, i.e., the one corresponding to a standard second-order system. On comparing the transfer function of the second-order numerator-dynamics with the standard second-order transfer function, the limiting case is obtained:

\[
\text{Standard second-order response} = \lim_{l \to \infty} \left\{ \frac{\text{Second-order numerator-dynamics response}}{l} \right\}
\]

The above facts are equally true of critically-damped and oscillatory responses. For the step response of Eq. 3.44, the same pattern is observed, the speed of the rise in the response increases with decrease in \( l \), and is maximum at \( l = 0 \) that exhibits input multiplicity (Fig. 3.6). However, as \( l \to \infty \), the system approaches a standard second-order one exhibiting no initial discontinuity.
So, it is seen that the lumped-parameter models presented in this chapter can be represented by second-order ODE with terms containing differential of the input function. These systems are called second-order systems with numerator-dynamics in their linear, transfer form adaptation. These systems present themselves with an initial discontinuous behavior for initially discontinuous inputs like step and impulse, unlike the standard second-order system. Numerator-dynamic behavior is different and has more classified branches than its standard counterpart. Different behaviors and their characteristic conditions are obtained in various Sub-sections of Section 3.9, for negative real part poles, and represented concisely on the real axis in the same section.

Second-order numerator-dynamics systems of relative order one, such as, gravity-flow tank, isothermal/non-isothermal CSTR, interacting tanks system, RLC circuit, single-component condenser, damped vibrator, etc. show an assortment of behaviors viz. maximum, minimum, inflection, input multiplicity and oscillations depending upon the characteristic system parameters and the conditions identified, these behaviors shall also be encountered in the corresponding nonlinear cases in next chapters, particularly in Chapter 5, where their numerical solutions will be carried out. It can also be observed that the magnitude, speed and nature of these response profiles changes as a result of the effect of initial discontinuities. This happens because the parameter $l$ undergoes changes with initial discontinuities and the systems change their positions on the real axis and switch over the regions on the real axis, or could result in the appearance of numerator-dynamics behavior for standard systems (see Eq. (3.22), Section 3.3.1 above).

ODE models representing lumped-parameter systems were considered in this chapter and the treatment in the following chapters applies to them. Distributed-parameter systems in two dimensions, however, lead to partial differential equations. Nevertheless, ODEs are also generally obtained by the reduction of partial differential equations through separation of variables to give an accurate analytical treatment (e.g., Kumar et al., 2000; 2008).