5 General Framework for Analysis and Initialization

The last chapter strongly indicated the significance of putting the theoretical analysis consistent with the physical principles, i.e., of material, energy, and momentum balances. These effects of initial discontinuities were revealed for systems essentially by matching the coefficients of input and output terms in the models. Having established these qualitative effects of initial discontinuities on the calculated solution profiles of the nonlinear systems, a simple, direct, and comprehensive framework in the time domain is now proposed. The framework is meant for the analysis and initialization of the lumped-parameter chemical engineering systems containing a set of first-order ODEs. The aim is to quantitatively describe their response to a singular (step or impulse), initial or input condition.

Effects of linearization will be discussed in the subsequent Section 5.12. Limitations of the symbolically transformed models shall be discussed in Section 5.13. The framework shall be applied to the linear time-invariant systems in Chapter 6 to address, reveal, and resolve the inconsistency in the Laplace transform treatment.

5.1 Framework of Discontinuity Analysis and Initialization

The analysis of initial discontinuities is carried out to expose the inconsistency in initial conditions, and to estimate the initial values of the discontinuous output variables. Mathematical models are used in conjunction with the physical principles of material, energy, and momentum balances. A schematic of the proposed methodological framework for singular inputs is presented in Fig. 5.1. The methodology is based on the fact that a physical balance must maintain equality at all times, and, in particular, must be balanced at the initial time that includes the singularity.
Include singularities in the effects and find initial conditions through mass, energy, and momentum balances on the physical system (Initialization B)

Include singularities in the cause, i.e., input function and find initial conditions through initial integrations of the models (Initialization A)

Solve the ODE models numerically with the initial conditions obtained from the two initialization methods and setting the singular terms zero

Compare solutions obtained through alternative initialization methods and through smoothened impulse (Initialization C) to check for mutual inconsistency, convergence and error deviations

Decide the appropriate initialization alternative

Fig. 5.1 Framework of the proposed analysis and initialization methodology for the systems with singular inputs
Furthermore, since the derivatives of discontinuous functions contain singularity at the origin, the resultant magnitudes of the initial discontinuities can also be worked out by integrating the ODE at the initial time. These are explained further in the strategy that is adopted to address singularity and the inconsistency thus emanating. The analysis is carried out in two steps by including impulse first in the cause, and then, in the effect.

In the first step (Initialization A), impulse is included in the cause, i.e., the input function, and the magnitude of the initial discontinuities in the outputs is estimated from the time integration of the model within the limits of 0− to 0+, and the sifting property of the impulse (δ-Dirac) function is used to evaluate the singular terms. This integration is carried out, using its physical interpretation as the area under a curve within the limits of integration without following the generalized functions treatment. The applicability of this procedure is suggested in this study by its comparison with other approaches.

Consider a general physical process represented by the following set of first-order nonlinear ODE system, which has an input variable suffering a singular perturbation.

\[ \dot{z}(t) = F(t, z(t), m(t)) \]  \hspace{1cm} (5.1)

where \( t \) is the independent variable (time), \( m(t) \) is the input forcing function, and \( z(t) \in \mathbb{R}^n \) are the dependent variables. As is remarked in the following sections, the original models, rather than the models obtained from symbolic differentiations and manipulations, must be used.

As described in Fig. 5.1, the discontinuity analysis for the system Eq. (5.1) is first carried out by including impulse in the input function. The system is initially at a particular state at time \( t \to 0^- \). For impulse input at \( t \to 0^+ \), the forcing function \( m \) changes from its pre-initial value \( m(0^-) \) (steady or unsteady) to:

\[ m(t) = m(0^-) + M \delta(t - t_o) \text{ with } t_o = 0^+ \]  \hspace{1cm} (5.2)

where \( M \) represents the magnitude of the impulse and \( \delta \) represents the unit-impulse function. Since Eq. (5.1) must maintain equality at all times, each equation in (5.1) can be integrated at \( 0^+ \) time by placing this value of the input function. This gives:
\[ \int_{0^-}^{0^+} \dot{z}(t) \, dt = \int_{0^-}^{0^+} F(t, z(t), m(t)) \, dt \]  \hspace{1cm} (5.3)

The right side of this Eq. (5.3) is evaluated in the following way. The integrals of the terms with limited integrands vanish, i.e.:

\[ \int_{0^-}^{0^+} m(0^-) \, dt = 0; \quad \int_{0^-}^{0^+} z(t) \, dt = 0; \quad \int_{0^-}^{0^+} m(0^-)z(t) \, dt = 0 \]  \hspace{1cm} (5.4)

The integral of the term involving impulse function of magnitude \( M \), equals \( M \), as the integral of unit impulse equals one.

\[ \int_{0^-}^{0^+} M \delta(t-t_o) \, dt = M \int_{0^-}^{0^+} \delta(t-t_o) \, dt = M \]  \hspace{1cm} (5.5)

The integral of the terms involving the product of the dependent variable(s) with the impulse function are evaluated as:

\[ \int_{0^-}^{0^+} z(t)M \delta(t-t_o) \, dt = Mz(t_o) = Mz(0^+) \]  \hspace{1cm} (5.6)

The last Eq. (5.6) follows from the sifting property of \( \delta \)-Dirac function. This property is applicable for continuous functions at \( t_o \). Though \( z \) may have a discontinuity at \( t_o \), it can be considered continuous from the right of \( t_o \), i.e., \( 0^+ \); thus, interpreting the integral as the area under the curve, which is 0 everywhere except at the point \( t = t_o \), and at \( t = t_o \), the area under the impulse, \( M \), is scaled by the value of the function \( z \), i.e., \( Mz(t_o) \), this leads to Eq. (5.6).

Evaluation of left side of Eq. (5.3) gives:

\[ \int_{0^-}^{0^+} \dot{z}(t) \, dt = z(0^+) - z(0^-) \]  \hspace{1cm} (5.7)

Using Eqs. (5.2), (5.4), (5.5), (5.6), and (5.7), the set of Eq. (5.3) can be solved simultaneously to get the initial discontinuity in each variable of \( z \), i.e., \( z(0^+) - z(0^-) \).
The procedure can be easily extended to a second-order linear time-invariant system containing a derivative of the input term, as illustrated in the next chapter. The proposed framework is also applicable to systems initially at steady or unsteady state, and, so, it is equally applicable to systems perturbed by an impulse train with impulses occurring at non-zero times.

In the second step of the analysis (Initialization B), the impulse is included in the effect, i.e., the effect of the introduction of impulse on the initial conditions of the system is quantified by the application of physical balances. Thus, the magnitudes of the initial discontinuities are obtained by applying the principles of mass, energy, and momentum balances on the physical system at the initial instant of the introduction of the input.

The applicability of the initialization A procedure is suggested in the next section. Its resultant initial values are identical with the definitely and apparently known initial values of several cases. Also, the initial values of initialization A are, invariably, identical with that of the elementary Laplace analysis of the linear cases (see Chapter 6).

As seen in the following sections, the initial values obtained from even the well established Laplace analysis may or mayn’t be consistent with that obtained from initialization B. For many linear and nonlinear cases studied, it is found that the initialization A can be either consistent or inconsistent with initialization B. The initial discontinuities calculated from the physical principles, i.e., initialization B are found to be more accurate as compared to that calculated from a mathematical model of the physical system, i.e., initialization A, because of the inability of a model to completely represent the physical system affected by singularity at the origin. It can be shown that initializations A and B respectively reduce to routes (a) and (b) for the cases of Chapter 4.

The analysis carried out in Chapter 4 for linear and nonlinear systems also showed that for some chemical engineering systems, an initial discontinuity in the output variable of the impulse response, identified on applying the physical principles, couldn’t be accounted for on theoretical analysis of the model (Ahuja, 2010; 2011). This effect was corroborated by the finding that, the numerical solution profiles were closer to the experimental results, when this discontinuity was taken into account.

For carrying out the solution through initialization C, the unit impulse function is approximated with a continuous function of area equal to one, i.e., a Gauss pulse function.
of a parameter $a$, that becomes sharper as the parameter $a$ decreases and approaches an impulse function as $a \to 0$. So, the input function, in general, is approximated as:

$$m(t) = m(0^-) + \frac{M}{a\sqrt{\pi}} e^{-t^2/a^2}$$

(5.8)

This equation is substituted in the system Eq. (5.1), which is solved numerically for each dependent variables $z$. Several numerical computations for decreasing value of the parameter $a$ should reveal the correct asymptotic behavior of the solution profiles. The sharpened Gauss pulse functions for several decreasing values of $a$ applied in the numerical integrations are plotted in Fig. 5.2. The plots for still lower applied values of $a$ couldn’t be shown because of extreme sharpening.

Numerical results are discussed in the next section. To quantify the degree of accuracy of initialization A, the numerical solutions obtained through it are compared with that obtained through initialization B and the resulting error margins are noted. The models are then solved by interpreting an impulse function as the limit of Gaussian pulse (Initialization C), and the above error margins for initialization A are compared with the corresponding error margins for initialization C.

The error deviations of the solution profiles obtained through alternative initialization approaches A and C are presented as normalized root mean square deviations (NRMSD), and are expressed as percentage of the range of values of the dependent variable obtained through initialization B:

$$\text{NRMSD} = \frac{100}{b_{\text{max}} - b_{\text{min}}} \sqrt{\frac{\sum_{i=1}^{m} (b_i - y_i)^2}{m}}$$

(5.9)

where $b_{\text{max}}$ and $b_{\text{min}}$ represent the maximum and the minimum of $m$ values of the dependent variable $b_i$ obtained through initialization B, and $y_i$ represent the corresponding values obtained through an alternative approach.
Gauss pulse function for decreasing value of $a$

Fig. 5.2 Approximation of unit impulse function ($\delta(t)$) with a continuous Gauss pulse function ($\delta_a(t)$) sharpened with decreasing value of parameter $a$

5.2 Applications

The proposed framework is illustrated in the following sections by using some examples from chemical engineering. Initial conditions were first evaluated from the direct methods proposed above, and the corresponding numerical results were computed. For the numerical integration of the systems using initializations A and B, the values of singular input terms in the equations were substituted equal to their initial values, since the effect of the impulse was already included in the model while calculating the initial conditions. The working of the proposed methodology is, in no way, limited to the establishment of an initial steady state, $a$ priori, at $t \to 0^-$, still the pre-initial values were arbitrarily taken equal to the initial steady state values for the numerical solution and the convergence of the solution to these values was examined. The numerical integrations of the models were carried out using RKF45 from Polymath.
For convenience in comparison of alternative initializations A and B, the native models of Chapter 3 rather than the dimensionless forms were used. Nonlinear models involving mixing with chemical reaction, phase change, interaction of different capacities, and closed loop system with dead time, were considered, viz., non-isothermal CSTR, single component condenser, closed loop stirred tank heater with dead time, gravity-flow tank, and semi-batch reactor with a II order reaction. The cases discussed here are different in their physical and model structure, analysis, and effects of initial discontinuities. Relatively simple cases are treated first, followed by the intricate ones. The cumulative results and corresponding discussion follow each example sequentially.

5.3 Example 1

The non-isothermal CSTR model of Chapter 3 that has been used extensively to study nonlinear dynamics in the literature is first considered in this section. With changes in flow rate, material and thermal capacities are interacting. The constant density, jacketed, non-isothermal CSTR is carrying out a liquid-phase, first-order reaction \( A \rightarrow R \). The feed contains only \( A \). The symbols were defined in Chapter 3.

\[
\frac{dV}{dt} = v_o - v \tag{5.10}
\]

\[
\frac{d(VC_A)}{dt} = v_o C_{A_o} - v C_A - k C_A V \tag{5.11}
\]

\[
\rho C_p \frac{d(\rho V T)}{dt} = \rho C_p (v_o T_o - v T) + (-\Delta H) k C_A V + U A_b (T_j - T) \tag{5.12}
\]

\[
k = k_o e^{-E/RT} \tag{5.13}
\]

For estimating exit flow rate \( v \), various equations have been assumed in the literature, i.e., depending upon that based on linear resistance, weir or valve characteristics, controller equations, etc. (Coughanowr and LeBlanc, 2009; Luyben, 1996). It is worth noting that the magnitudes of the initial discontinuities obtained through the application of the above framework, and hence, the effects to be studied are independent of the choice of this equation because any selected equation—as can be seen in the treatment that follows—
would yield a limited integrand, whose integral would be zero according to Eq. (5.4) of the framework.

Two simple flow head relationships were assumed (and the head is proportional to the holdup volume), i.e.:

\[ v = c_1 V \quad (5.14); \quad v = c_2 \sqrt{V} \quad (5.14') \]

These are applicable respectively to the cases of laminar and turbulent flow through pipes and valves. The constants of proportionality are based on the pre-initial conditions.

An impulse perturbation in exit flow rate \( v \) is, first, considered. The variable holdup non-isothermal CSTR, which was at a particular state at the pre-initial time instant \( t \rightarrow 0^- \), is perturbed at the post-initial time instant \( t \rightarrow 0^+ \) by an impulse in the exit volumetric flow rate \( v \). This impulse input at \( t \rightarrow 0^+ \) in the exit flow can be realized by suddenly withdrawing \( M \) (m\(^3\)) of the liquid directly from the tank suddenly, all in one go.

**Initialization A**

Following the initialization A procedure, let the impulse be included in the cause, first. So, \( v \) has two components: one due to the perturbation, and the other due to the change in \( V \) (since, \( v = c_1 V \)). So, \( v \) becomes \( v = c_1 V + M \delta(t-t_o) \) with \( t_o = 0^+ \) (Note that \( c_1 V \) already includes \( v(0^-) \)). Placing this in Eqs. (5.10) through (5.14) gives the discontinuities in \( V \), \( C_A \), and \( T \). For the case of laminar flow through the exit line, Eqs. (5.10) and (5.14) give:

\[
\frac{dV}{dt} = v_o - (c_1 V + M \delta(t-t_o)) \quad (5.15)
\]

Upon time integration with in the limits \( 0^- \) to \( 0^+ \), gives:

\[
\int_{0^-}^{0^+} \frac{dV}{dt} dt = \int_{0^-}^{0^+} v_o dt - \int_{0^-}^{0^+} c_1 V dt - M \int_{0^-}^{0^+} \delta(t-t_o) dt \quad (5.16)
\]

The last term is evaluated by Eq. (5.5). The integrands in the second and the third terms are limited (though \( V \) is discontinuous), and their integrals vanish (Eq. (5.4)). This gives:

\[
V(0^+) - V(0^-) = -M \quad (5.17)
\]
Now, for evaluating the discontinuities in $C_A$ and $T$, integrating Eq. (5.11) gives:

$$\int_{0^-}^{0^+} \frac{d}{dt}(VC_A)dt = \int_{0^-}^{0^+} v_o C_A dt - \int_{0^-}^{0^+} (c_1 V + M \delta(t-t_o))C_A dt - \int_{0^-}^{0^+} k_o e^{-E_{RT}/C_A} dt$$

(5.18)

The third term in this equation is evaluated according to the sifting property of $\delta$-Dirac function, Eq. (5.6), and, thus, the integral evaluated at $t_o = 0^+$ is: $MC_A(t_o) = MC_A(0^+)$. Eq. (5.18) yields an implicit equation:

$$V(0^+)C_A(0^+) - V(0^-)C_A(0^-) = -MC_A(0^+)$$

(5.19)

Combining this with Eq. (5.17) and solving, gives the initial discontinuities in $C_A$ (and similarly $T$, see also Example 2):

$$C_A(0^+) - C_A(0^-) = 0; \quad T(0^+) - T(0^-) = 0$$

(5.20)

Thus, initialization A yields these initial discontinuities to be zero. Similarly, all these discontinuities in $V, C_A$, and $T$ are the same as well for the case of exit flow following the square-root relation Eq. (5.14'), these are used in the numerical solutions below.

**Remark 1** A linear case: It may be noted that Eq. (5.15) is linear, and its solution can be obtained by using the following elementary Laplace analysis. Eq. (5.15) is first subtracted from the same equation at $t \to 0^-$. This equation upon Laplace transformation and inverse transformation ($v_o$ is constant), gives ($s$ is the Laplace parameter):

$$s(V - V(0^-))(s) = (v_o - v_o(0^-))(s) - c_1 (V - V(0^-))(s) - M;$$

(5.21)

$$s(V - V(0^-))(s) = \frac{M}{s + c_1}; \quad V(t) - V(0^-) = -Me^{-ct}$$

(5.22)

The initial discontinuity evaluated from this equation at $t \to 0^+$ turns out to be $(-M)$, i.e., the same as given by Eq. (5.17). This also turns out to be the same from the physical balances (initialization B below).
**Initialization B**

Impulse is now included in the effect. Application of material and energy balances to the initial effect of impulse on conditions of the system also gives the same extent of the above initial discontinuities. The impulse in \( v \) is realized by suddenly withdrawing \( M \) (m\(^3\)) of liquid from the tank, all in one go. Thus, the holdup volume of tank decreases by an amount \( M \), which is same as in Eq. (5.17) above.

Next, applying the component material balance on \( A \) and energy balance lead to zero initial discontinuities in \( C_A \) and \( T \) respectively, since withdrawing \( M \) (m\(^3\)) of liquid at the exit conditions \( C_A(0^-) \) and \( T(0^-) \) from the tank that is already at this state, will cause no initial change in the state of the tank. These definitely known results through initialization B conform to the results obtained through initialization A above.

**Remark 2 A transformed model case:** However, in the above model, if Eq. (5.11) was transformed by applying differentiation rule of the product of variables \( V \) and \( C_A \) on the left hand side, and substituting material balance Eq. (5.10) for the differential of \( V \), one would obtain (some studies use such an equation as in Example 2 below):

\[
\frac{dC_A}{dt} = \frac{V}{V}(C_{A_0} - C_A) - kC_A
\]

Finding the initial discontinuities from this equation (and similarly for \( T \)) through initialization A, as is done above, would yield:

\[
C_A(0^+) - C_A(0^-) \neq 0; \quad T(0^+) - T(0^-) \neq 0 \tag{5.23}
\]

which are obviously wrong. Hence, the original, mathematically non-transformed models must be used to obtain correct results from the procedure. Its relevance comes across further in later discussion.

**Perturbation in \( T_j \)**

Let \( M \) (K)(s) be the magnitude of the impulse perturbation in the jacket temperature. The initial discontinuity in the tank temperature \( T \) through initialization A on Eq. 5.12 comes out to be \( U_bA_bM / V\rho C_p \) (K). This is same through initialization B as shown below.
**Initialization B** The impulse perturbation of magnitude $M \, \text{(K)(s)}$ in $T_j$ is equivalent to introducing $U_h A_h M$ (Joules) of enthalpy directly into the tank, all in one go. This causes the same increase in the tank temperature $T$ of $U_h A_h M / V \rho C_p$ (K) through the application of energy balance at the initial instant as:

Initial change in temperature in tank \quad = \quad \text{Enthalpy change of } U_h A_h M \, \text{(J)} \text{ per unit thermal capacity of the tank liquid (J/K)}

$$T(0^+) - T(0^-) = U_h A_h M / V \rho C_p$$  \hspace{1cm} (5.24)

**Perturbation in $C_{A_o}$**: A perturbation in $C_{A_o}$ makes Eq. (5.11) *linear*, it can also be verified that it would result in identical initial conditions for $C_A$ through initializations A, B, and the Laplace analysis. This case was considered in Section 4.2.4, wherein it was shown that the system exhibits same results for $C_A$ but different ones for the product concentration $C_R$ through the two alternative initialization routes (see also Chapter 6).

**Perturbation in $v_o$**: Similarly, it can be shown that a perturbation in the volumetric feed rate $v_o$ results in the same initial discontinuities through initializations A & B, again if the original non-transformed models are used (as is shown in Example 2).

**Initialization C**: For perturbation in $v$, the system was solved numerically with the Dirac function $\delta(t - t_o)$ in Eq. (5.15) replaced with the Gauss pulse term $\frac{1}{a \sqrt{\pi}} e^{-t^2/a^2}$.

### 5.3.1 Numerical results

To quantify the resultant effects of the initial conditions, the numerical solution of this model for impulse perturbation in exit flow rate $v$ was carried out using the above initializations A & B and the results were compared with the approach of smoothening of impulse (initialization C). For the numerical solution, Eqs. (5.10) and (5.12) were numerically integrated and the results of $V$ and the product $(V \times T)$ were obtained with
respect to time, respectively; the values of $T$ were obtained as: $T = (V \times T) / V$. The parameter values used are presented in Table 5.1. The magnitude of impulse input, $M = 3.40 \times 10^{-1} \text{ m}^3$ (25% of the initial holdup volume) was used.

**Table 5.1  Parameters for Non-isothermal CSTR**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V$</td>
<td>$1.359 \text{ m}^3$</td>
</tr>
<tr>
<td>$C_{Ao}$</td>
<td>$8.0 \text{ kg mol/m}^3$</td>
</tr>
<tr>
<td>$R$</td>
<td>$8.314 \times 10^3 \text{ J/kg mol-K}$</td>
</tr>
<tr>
<td>$A_h$</td>
<td>$23.225 \text{ m}^2$</td>
</tr>
<tr>
<td>$\rho$</td>
<td>$800.848 \text{ kg/m}^3$</td>
</tr>
<tr>
<td>$\Delta H_R$</td>
<td>$-6.978 \times 10^7 \text{ J/kg mol}$</td>
</tr>
<tr>
<td>$T_j$</td>
<td>$330.33 \text{ K}$</td>
</tr>
<tr>
<td>$k_o$</td>
<td>$1.967 \times 10^7 /\text{s}$</td>
</tr>
<tr>
<td>$E$</td>
<td>$6.978 \times 10^7 \text{ J/kg mol}$</td>
</tr>
<tr>
<td>$T_o$</td>
<td>$294.44 \text{ K}$</td>
</tr>
<tr>
<td>$v_o(0^-)$</td>
<td>$3.147 \times 10^{-4} \text{ m}^3/\text{s}$</td>
</tr>
<tr>
<td>$U$</td>
<td>$851.721 \text{ W/m}^2 \cdot \text{K}$</td>
</tr>
<tr>
<td>$T(0^-)$</td>
<td>$333.33 \text{ K}$</td>
</tr>
<tr>
<td>$C_A(0^-)$</td>
<td>$3.924 \text{ kg mol/m}^3$</td>
</tr>
<tr>
<td>$C_p$</td>
<td>$3.140 \times 10^3 \text{ J/kg-K}$</td>
</tr>
</tbody>
</table>

The results for $V$ are presented in Fig. 5.3 for the square-root resistance, where the curves corresponding to initializations A, B, and C are plotted together. The results converge to the consistent steady state values. Initializations A and B yield identical curve, give the correct quantitative results, and exhibit the correct initial discontinuity of $3.40 \times 10^{-1} \text{ m}^3$. This value must be achieved as is seen even from the elementary Laplace analysis in Remark 1. However, it is observed that the smoothening approach yield highly inaccurate results, since it can’t reveal the actual asymptotic behavior despite several decreasing value of the parameter $a$, as the curve for initialization C exhibit an initial discontinuity of only $1.59 \times 10^{-1} \text{ m}^3$, i.e., an error of 53%, and shows large deviations (NRMSD = 21%) from the correct curve obtained through initializations A & B.
The curves for $C_A$ and $T$ are plotted in Figs. 5.4 and 5.5. The response curves plotted through initialization C show large error deviations of 26% for $C_A$, and 12% for $T$, from the corresponding correct curves obtained using initializations A & B. For decreasing value of $a$, viz. $a = 10^{-4}$, $a = 10^{-5}$, and $a = 10^{-6}$, there is no improvement in the behavior of the curves for initialization C as these curves overlap. Exactly the same was observed for the linear resistance when the value of $a$ was decreased, as the curves practically overlapped even until the value of $a$, as low as $a = 10^{-150}$. Simulations failed below the respective lowest values mentioned for the square-root and the linear resistances.
**Figs. 5.4 and 5.5** Comparison of alternative initialization approaches for impulse response of concentration and temperature, respectively in variable holdup CSTR, to a perturbation in exit volumetric flow rate
To observe these effects minutely and more accurately, the simulations for initializations C were repeated by focusing on the initial time duration of only 0.9 s. These curves are plotted together for $V$ in Fig. 5.6, for the square-root resistance, for several decreasing value of $a$, viz. $a = 10^{-4}$, $a = 0.5 \times 10^{-4}$, $a = 0.25 \times 10^{-4}$, $a = 10^{-5}$, $a = 10^{-6}$, and $a = 0.25 \times 10^{-6}$ below which the simulation failed. It can be observed from this figure that as the value of $a$ decreases, the value of the initial discontinuity in $V$ (occurring at $t \sim 0.02$ s) is the same of $1.70 \times 10^{-1}$ m$^3$ (against the correct value of $3.40 \times 10^{-1}$ m$^3$), thus, exhibiting a very high error of 50%. This value of initial discontinuity is the same in all these cases, and there is no improvement upon decreasing the value of $a$ below $a = 10^{-6}$, as the curves for $a = 10^{-6}$ and $a = 0.25 \times 10^{-6}$ practically overlap. The behavior couldn’t be improved even on increasing the accuracy further by decreasing the focus of the time duration.

![Fig. 5.6 Comparison of the impulse response of holdup volume of variable holdup CSTR, to a perturbation in exit volumetric flow rate, for decreasing value of parameter $a$ of smoothened impulse function](image-url)
5.3.2 Discussion

The above treatment of Example 1 substantiates the applicability of the proposed methodology as it predicts the correct and the same initial conditions as are obtained from an elementary physical balance or Laplace analysis. The initial discontinuities and solution profiles computed through initialization A exactly conform to the definitely known values of initial discontinuities and solution profiles for several cases, and these are computed equally well through Laplace analysis for the linear cases. Initialization A is, thus, adequate and found to be consistent with initialization B for the above cases.

However, despite extreme sharpening, the smoothened impulse (Gauss pulse) in initialization C is not able to catch up with the initial discontinuity. The solution profiles obtained through initialization C exhibit high magnitudes of error deviations from the correct solution profiles.

This indicates that the Gaussian pulse approximation can’t reliably model the singularity of the $\delta$-Dirac function, which is accurately done through initialization A. The limitations of initialization procedure C further come across in the following cases.

5.4 Constant Holdup CSTR

The tank is, then, assumed closed and fully filled, so that, the holdup volume $V$ is taken constant. The constant density CSTR, which was at a particular state initially at $t \to 0^-$, is perturbed by an impulse in the volumetric flow rate of the feed $v_o$.

**Initialization A:** Applying this procedure gives the following discontinuities in $C_A$ and $T$:

$$C_A(0^+) - C_A(0^-) = M\{C_{Ao} - C_A(0^-)\}/(M + V) \quad (5.25)$$

$$T(0^+) - T(0^-) = M\{T_o - T(0^-)\}/(M + V) \quad (5.26)$$

**Initialization B**

The impulse in $v_o$ is realized by plunging $M$ (m$^3$) of liquid feed into the tank, all in one go. Since the tank is closed and fully-filled, and the liquid is incompressible; this sudden introduction will cause a sudden ejection (of an equal volume) of the already present tank
fluid at concentration $C_A(0^-)$ and temperature $T(0^-)$. Applying material balance on $A$, to these effects of the impulse, gives:

Initial change in moles of $A$ in tank  =  \((\text{Moles of } A \text{ in the inserted } M (\text{m}^3) \text{ of liquid that is at concentration } C_{A_0} \text{ (mol/m}^3)) - (\text{Moles of } A \text{ in the ejected } M (\text{m}^3) \text{ of liquid that is at concentration } C_A(0^-) \text{ (mol/m}^3))\), or:

$$VC_A(0^+) - VC_A(0^-) = MC_{A_0} - MC_A(0^-)$$

$$C_A(0^+) - C_A(0^-) = M \{C_{A_0} - C_A(0^-)\} / V \tag{5.27}$$

So, the corresponding discontinuities calculated from material balance on the effects are not the same as in the cause (Eq. (5.25)). On exactly same lines, energy balance gives:

Initial change in enthalpy in tank  =  \((\text{Enthalpy of the inserted } M (\text{m}^3) \text{ of liquid that is at temperature } T_o) - (\text{Enthalpy of the ejected } M (\text{m}^3) \text{ of liquid that is at temperature } T(0^-))\), or:

$$V \rho c_p T(0^+) - V \rho c_p T(0^-) = M \rho c_p T_o - M \rho c_p T(0^-)$$

$$T(0^+) - T(0^-) = M \{T_o - T(0^-)\} / V \tag{5.28}$$

Hence, unlike the previous case, the initial discontinuities calculated from model’s considerations (initialization A) are not consistent with that calculated from the consideration of physical balances (initialization B).

### 5.4.1 Numerical results

The numerical results for the above impulse perturbation in feed rate $v_o$ are discussed. The parameter values are the same as presented in Table 5.1. A magnitude of perturbation, $-3.40 \times 10^{-1} \text{ m}^3$ (25% of the initial value), was, first, used for the three initializations A, B, and C. For initialization C, an extremely low value of $a$, i.e.,
\( a = 10^{-150} \) was used. The results for \( C_A \) and \( T \) are presented in Figs. 5.7 and 5.8, respectively. In all Figs. henceforth, the darkened segments along the y-axis mark the magnitude of initial discontinuities. The results converge to the consistent steady state values. For \( C_A \) and \( T \) respectively, the profiles for initialization C show significant deviations of 20% and 10% from the solution profile for initialization B; whereas, the corresponding deviations in the solution profiles for initialization A are of much smaller magnitudes of 11% and 4%.

A lower magnitude of perturbation, \(-1.13 \times 10^{-1} \) m\(^3\) (8% of the initial value), was, then, used, and the above runs were repeated. The above deviations for initialization C remained nearly the same of 19% for \( C_A \) (Fig. 5.9), and 10% for \( T \) (Fig. 5.10). Thus, the deviations are significant as in the previous case, which reaffirm the non-applicability of the smoothening of impulse approach, irrespective of the magnitude of perturbation.

However, for initialization A, the deviations reduce to as low as 6% for \( C_A \) (Fig. 5.9), and 2% for \( T \) as the curves for initializations A and B practically overlap (Fig. 5.10), for this reduced magnitude of perturbation, \(-1.13 \times 10^{-1} \) m\(^3\). So, as the magnitude of the initial discontinuities decrease, the deviations become further smaller.
**Fig. 5.7** Comparison of alternative initialization approaches for concentration response of constant holdup CSTR to an impulse perturbation in volumetric feed rate
Fig. 5.8 Comparison of alternative initialization approaches for temperature response of constant holdup CSTR to an impulse perturbation in volumetric feed rate
Fig. 5.9 Comparison of alternative initialization approaches for concentration response of constant holdup CSTR to a lower magnitude of impulse perturbation in volumetric feed rate
Fig. 5.10 Comparison of alternative initialization approaches for temperature response of constant holdup CSTR to a lower magnitude of impulse perturbation in volumetric feed rate

5.4.2 Outcomes revisit

Initialization A can be adequately used for moderate magnitudes of perturbation, i.e., for the system not being operated very far away from its normal operating conditions, whereas, initialization C is found to be inadequate.

5.5 Example 2

Consider the vapor-phase dynamics, single component condenser system described in Sections 3.4, and 3.4.1. It assumes quasi-static conditions, so that, the specific rate of condensation is small and, thus, at any moment, the amount of vapor condensed is small in comparison to the amount of vapor present in the condenser. Hence, the time rate of accumulation of the material and energy in the liquid phase can be neglected. Therefore, this model neglects the dynamics of the liquid phase. It also assumes that vapor and
liquid are in equilibrium throughout and any sub-cooling of the liquid is, thus, neglected. So, the pressure of the vapor is replaced by the vapor pressure of the liquid.

\[
\frac{dT}{dt} = \frac{F}{N} (T_o - T) + \frac{L \Delta H}{NC_p} + \frac{U A_{h}}{NC_p} (T_j - T) \tag{5.29}
\]

\[
C_p \frac{d(NT)}{dt} = FC_p T_o + UA_{h} (T_j - T) - L (C_p T - \Delta H) \tag{5.29'}
\]

\[
\frac{dN}{dt} = F - L \tag{5.30}
\]

\[
P^* = A \exp \left( -\frac{B}{T + C} \right) \tag{5.31}
\]

\[
V = \frac{NRT}{P^*} \tag{5.32}
\]

Eq. (5.29) is energy balance on the vapor phase, Eq. (5.30) is the molar balance on the vapor phase, Eq. (5.31) is the Antoine’s equation and Eq. (5.32) is the equation of state for vapor. For \( L \), various equations have been assumed in the literature, i.e., the equations based on valve or weir characteristics, controller equations, etc. (Luyben, 1996; Unger et al., 1995). In the following treatment, the molar rate of condensation of vapors (also equal to exit molar flow rate of liquid \( L \) as there is no accumulation of liquid as per the vapor-phase dynamics assumptions) is taken proportional to the moles of vapor \( N \) at any time, this gives:

\[
L = c' N \tag{5.33}
\]

The constant of proportionality \( c' \) is based on the pre-initial conditions. As remarked in Example 1, it re-emphasized here that the magnitudes of the initial discontinuities resulting through the framework, and hence, the effects to be studied are independent of the choice of this equation because any selected equation—as can be seen in the treatment that follows—would yield a limited integrand, whose integral would be zero according to Eq. (5.4) of the framework.
As noted in Section 3.4.1 of Chapter 3, Eq. (5.29) has been used in the literature and is obtained through symbolic manipulations and differentiation of the original energy balance Eq. (5.29'). This model works for the step input only, and not for the impulse input (as is also seen through Eqs. (5.23) and (5.24) in the CSTR case).

The original energy balance Eq. (5.29') was formulated in section 3.1.1. In this section, explicit model containing Eqs. (5.29') through (5.33) is considered. The numerical results obtained from this model are also plotted along with the corresponding results of mathematically transformed models approaches in Section 5.13, where several limitations of mathematical transformations are discussed.

**Perturbation in \( F \)**

For impulse perturbation in \( F \), the initial discontinuity in \( T \) is given by the following Eq. (5.34), obtained through initialization A.

**Initialization A:** It is applied (presented in brief) on Eqs. (5.30) and (5.29'), respectively:

\[
\int_{0^-}^{0^+} \frac{dN}{dt} dt = \int_{0^-}^{0^+} F(0^-)dt + M \int_{0^-}^{0^+} \delta(t-t_o)dt - \int_{0^-}^{0^+} Ldt \tag{5.34.a}
\]

\[N(0^+) - N(0^-) = M \tag{5.34.b}\]

\[C_p \int_{0^-}^{0^+} \frac{d}{dt}(NT)dt = \int_{0^-}^{0^+} FC_p T_o dt + \int_{0^-}^{0^+} UA(T_c - T)dt - \int_{0^-}^{0^+} L(C_pT - \Delta H)dt \tag{5.34.c}\]

\[C_pN(0^+)T(0^+) - C_pN(0^-)T(0^-) = C_pMT_o \tag{5.34.d}\]

\[T(0^+) - T(0^-) = \frac{MT_o - T(0^-)}{N(0^+)} \tag{5.34.e}\]

**Initialization B:** Physical balances on the conditions of the system at the time of introduction of the input also give the same extent of discontinuities in both \( N \) and \( T \). The impulse in \( F \) is introduced by plunging \( M \) moles of vapor into the condenser at the feed temperature \( T_o \), all in one go. So, the sudden rise in the energy of the vapor in the condenser (same as the left side of Eq. (5.34.d)), is equal to the enthalpy of \( M \) moles of vapor added at temperature \( T_o \) (same as the right side of Eq. (5.34.d)). Eq. (5.34) yields
mutually consistent results for the initialization procedures A and B of the framework, and the system, thus, remains unaffected by the initial discontinuities.

**Perturbation in L.**

Consider, now, a perturbation in the exit liquid molar flow rate $L$. The condenser, which was at a particular state initially at $t \to 0^-$, suffers an impulse perturbation of magnitude $M$ (moles) at $t \to 0^+$. Now, $L$ has two components: one of the perturbation and the other of the initial discontinuity caused by the change in $N$ (since, $L = c'N$). Therefore, the value of $L$ is placed as: $L = c'N + M \delta(t-t_o)$ with $t_o = 0^+$ in the model (Note that $c'N$ already includes $L(0^-)$).

**Initialization A:** Initialization A on Eqs. (5.30) and (5.29') as in Example 1 gives:

\[
N(0^+) - N(0^-) = -M \tag{5.35}
\]

\[
T(0^+) - T(0^-) = \frac{M \Delta H / C_p}{N(0^-)} \tag{5.36}
\]

**Initialization B**

The discontinuity for $N$, calculated from material balance is the same as that given by Eq. (5.35). However, the discontinuity for $T$, calculated from energy balance, is not equal to the discontinuity given by Eq. (5.36). As $M$ moles of liquid are removed from the condenser, the initial change in the energy of the vapors in the condenser is equal to the enthalpy of $M$ moles of condensed liquid leaving the condenser (including the enthalpy of condensation). And, the rate of condensation is equal to the rate of exit of liquid, as per the assumptions of the model. So:

\[
N(0^+)C_pT(0^+) - N(0^-)C_pT(0^-) = -M (C_pT(0^-) - \Delta H) \tag{5.37}
\]

Combining Eq. (5.37) with Eq. (5.35), and solving for the initial discontinuity in $T$, gives:

\[
T(0^+) - T(0^-) = \frac{M \Delta H / C_p}{N(0^+)} \tag{5.38}
\]
Hence, in this case, the initial discontinuity calculated from initialization A is not consistent with that calculated from initialization B. Therefore, the impulse response is affected by the discontinuities as seen from the following results of numerical solutions.

### 5.5.1 Numerical results

The parameter values used for the numerical solution are presented in Table 5.2. An impulse perturbation in \( L \) is considered for the three initializations A, B, and C. For initialization C, an extremely low value of \( a \), i.e., \( a = 10^{-150} \) was used. The variables \( P \) and \( T \) exhibited high sensitivity to the initialization effects. Other variables exhibited little sensitivity. The results converge to the consistent steady state values. The results for \( N \) are presented in Fig. 5.11 for a magnitude of impulse of 100 mol (27% of the initial mol of vapor).

**Table 5.2 Parameters for the Condenser Example**

<table>
<thead>
<tr>
<th>For Example 2</th>
<th>( \Delta H ) = ( 5.0 \times 10^3 ) J/mol</th>
<th>( F(0^-) ) = 50 mol/s</th>
<th>( L(0^-) ) = 50 mol/s</th>
<th>( A = 1.2 \times 10^{10} ) Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>( UA_h ) = 2.0 \times 10^3 W/K</td>
<td>( M ) = 100 mol</td>
<td>( T(0^-) ) = 376.73 K</td>
<td>( B = 3816 ) K</td>
<td></td>
</tr>
<tr>
<td>( C_p ) = 3.35( \times 10^3 ) J/mol-K</td>
<td>( V(0^-) ) = 10 m( ^3 )</td>
<td>( N(0^-) ) = 373.63 mol</td>
<td>( C = -46 ) K</td>
<td></td>
</tr>
<tr>
<td>( R = 8.314 ) J/mol-K</td>
<td>( T_o = 373 ) K</td>
<td>( T_j = 283 ) K</td>
<td>( k = 1.338 \times 10^{-1} ) (mol/s)/mol</td>
<td></td>
</tr>
</tbody>
</table>

Initializations A and B yield identical curve, give the correct quantitative results, and exhibit the correct initial discontinuity of 100 mol. Whereas, the initialization C curve exhibit an initial discontinuity of only 44.33 mol, and shows large deviations from the correct curve, thus, exhibiting the inadequacy of initialization C once again. The error deviation in the two curves is of 17%.

The results for \( T \) are presented in Fig. 5.12. The initializations A and C curves respectively exhibit initial discontinuity values of 1.617 K and 3.99 K, against the value of 5.452 K exhibited by the initialization B curve based on the considerations of physical
balances. The deviation of the initialization C curve vis-à-vis the initialization B curve is a significant value of 13%; whereas, the corresponding deviation of the initialization A curve is only of 5%.

Fig. 5.11 Comparison of alternative initialization approaches for impulse response of moles of vapor in condenser, to a perturbation in exit liquid molar flow rate

These runs were, then, repeated for a lower magnitude of impulse of magnitude, 30 mol (8% of the initial mol of vapor). The initialization C curve for $N$, presented in Fig. 5.13, shows the same magnitude of deviation, i.e., of 17%. The results for $T$ are shown in Fig. 5.14, where again it is clearly seen that the initialization C curve still shows an error of 12%, thus, confirming our earlier observations of inadequacy of initialization C, in spite of the decreased magnitude of perturbation.

However, in same Fig. 5.14, the initialization A curve comes even closer to the initialization B curve, and the corresponding deviations become insignificant (2%) for this small magnitude of perturbation of 30 mol.
Fig. 5.12 Comparison of alternative initialization approaches for impulse response of temperature in condenser to a perturbation in exit liquid molar flow rate
Fig. 5.13 Comparison of alternative initialization approaches for impulse response of moles of vapor in condenser, to a lower magnitude of perturbation in exit liquid molar flow rate.
Fig. 5.14 Comparison of alternative initialization approaches for impulse response of temperature in condenser, to a lower magnitude of perturbation in exit liquid molar flow

5.6 Discussion

Cumulative results are now discussed. For linear and nonlinear cases studied throughout this chapter (Examples 1 through 5), it is found that initialization A (or alternatively the Laplace analysis) is consistent with initialization B for many cases. However, it can also be inconsistent with initialization B for many other cases, which indicates the inherent inability of a model to exactly represent the physical system affected by singularity at the origin. Thus, the techniques of Laplace transformation of a model, and initialization A of integration of a model (interpreted as area under a curve) have inherent limitations of mathematical representation of singularity. The machinery of generalized functions also involves many complications and ad hoc interpretations when the Dirac function is multiplied with a discontinuous function, and, hence, some studies prefer to use the basic integral notion rather than the generalized integral notion (Grizzle, 2004; Makila, 2006). These remarks are more appropriate for the nonlinear systems for which the machinery
involves further mathematical technicalities (Pilipchuk, 1999). Thus, the model’s considerations would inherently lead to less than exact solution profiles for some cases, which are, therefore, affected by the discontinuities.

Nevertheless, the numerical results exhibit that initialization A attains exact or close to exact initial values, while initialization C—despite extreme sharpening of the smoothened impulse—is far off from the correct initial values calculated from the application of the physical balances (initialization B) or Laplace analysis. Also, initialization A exhibits small deviations, while initialization C exhibits large deviations in their solution profiles. Furthermore, on decreasing the magnitudes of perturbation, the errors for initialization A decrease sharply and become negligible, while the percentage errors for initialization C remain nearly the same (though actual errors decreased marginally).

The outcomes of these examples, thus, show that the initialization procedure A that involves including the impulse in the cause, can be safely used for the systems operated not very far away from their normal operating conditions. Operations fairly close to the normal operating conditions are of significant practical importance if the plant variables are well controlled to remain close to the steady state. Hence, initialization A, based on ready-to-use initial integration of the model, can be a good substitute to the procedure of initialization B that requires additional effort of applying physical balances on the effects of singularity at the origin.

However, the same is not true for initialization C, based on the smoothening of impulse function, which is found to be highly inadequate in all the cases of above examples, and, so, is not discussed further. Nevertheless, the trajectories for initializations A, B, and C of all the cases studied exhibited the same trend and so the plausibility of our results.

5.7 Example 3

This example is selected to illustrate the effect of initial conditions on the closed-loop systems in the presence of dynamic lags. This is done by the comparison of the solution profiles of an open and closed loop system with dead time obtained through initializations A and B. Consider the stirred tank heater system of Section 3.7, Chapter 3:
\[
\frac{dT_m}{dt} = K_i Q(0^-) - K_i K_c T_m (t - \tau_d) + K_i K_c T_m (0^-) + K_3 v_o (t - \tau_d) - K_2 v_o (t - \tau_d) T_m
\]

where \( K_i = 1/(\rho \cdot C_p \cdot v_o) \), \( K_2 = 1/V \), and \( K_3 = T_o / V \) \hspace{1cm} (5.39)

This DDE couldn’t be solved through ordinary means; hence, an independent program was developed (algorithm is presented in Appendix II).

**Initialization A:** If the impulse is included in the cause, \( v_o = v_o (0^-) + M \delta(t - t_o) \), with \( t_o = 0^+ \). Thus, \( v_o (t - \tau_d) = v_o (0^-) + M \delta(t - \tau_d) \). The discontinuities now occur at \( t = \tau_d^+ \) because of the dead time. Carrying out the initial integration procedure on Eq. (5.39), the discontinuity in this constant volume system becomes:

\[
\int_{\tau_d^+}^{\tau_d^-} \frac{dT_m}{dt} dt = 0 - K_i K_c \int_{\tau_d^+}^{\tau_d^-} T_m (t - \tau_d) dt + 0 + K_3 \int_{\tau_d^+}^{\tau_d^-} M \delta(t - \tau_d) dt - K_2 \int_{\tau_d^-}^{\tau_d^+} M \delta(t - \tau_d) T_m dt
\]

\( T_m (\tau_d^+^-) - T_m (\tau_d^-^-) = \frac{M \{ T_o - T_m (\tau_d^-^-) \}}{V + M} \hspace{1cm} (5.40) \)

**Initialization B:** However, the corresponding discontinuities calculated from energy balance on the effect are not the same as these. Since the tank is closed and fully-filled, and, the liquid is incompressible; an introduction of \( M \) (m\(^3\)) of liquid at temperature \( T_o \) in the tank will cause an equal amount of the additional ejection of tank fluid at temperature \( T_m (\tau_d^-^-) \). Carrying out initial energy accounting in the tank, gives:

\[ V \rho C_p T_m (\tau_d^-)^+ - V \rho C_p T_m (\tau_d^-^-) = M \rho C_p T_o - M \rho C_p T_m (\tau_d^-^-); \]

\[ T_m (\tau_d^-)^+ - T_m (\tau_d^-^-) = \frac{M \{ T_o - T_m (\tau_d^-^-) \}}{V} \hspace{1cm} (5.41) \]

### 5.7.1 Numerical results

To see the effect of buildup of errors in the closed loop systems in the presence of dynamic lags in the loop, numerical solution of the above model was carried out. The parameter values used for the numerical solution of this model are presented in Table 5.3. Open and closed loop cases were solved almost immediately by the program.
Table 5.3 Parameters for Closed Loop Stirred Tank Heater

\[ \rho C_p = 9.87 \times 10^3 \text{kJ/m}^3\text{°C} \quad T_o = 34 \text{°C} \quad V = 5.0 \times 10^{-4} \text{m}^3 \]
\[ v_o(0^-) = 1.262 \times 10^{-5} \text{m}^3/\text{s} \quad \tau_d = 21.4 \text{s} \quad M = 4.0 \times 10^{-4} \text{m}^3 \]
\[ K_3 = 6.8 \times 10^4 \text{°C/m}^3 \quad T(0^-) = 45 \text{°C} \quad K_2 = 2.0 \times 10^3/\text{m}^3 \]
\[ K_1 = 2.027 \times 10^{-1} \text{°C/kJ} \quad Q(0^-) = 1.37 \text{kW} \quad K_c = 0.35 \text{kW/°C} \]

---

**Fig. 5.15** Comparison of open loop (1) and closed loop (2) cases—Impulse responses of stirred tank heater with dead time (\(\tau_d = 21.4 \text{s}\) ) through alternative initialization approaches

The results are presented in Fig. 5.15 for both the open and the closed loop cases. The systems remain at the steady state until the dead time (\(\tau_d = 21.4 \text{s}\). The profiles start at one dead time and the discontinuities occur at this time, rather than at zero time. It is interesting to note that the corresponding solution profiles for the open and the closed loop cases are the same for the initial period until a further lapse of one more dead time. This is so, because the controller action signal takes one more dead time to reach the
output end. The solutions converge to the consistent steady state values. The deviation between the solution profiles of the two initialization procedures A and B is of 7\% for the open loop case, and increases to 10\% for the closed loop case. Thus, there are moderate errors involved in the initial integration procedure A for a high magnitude of perturbation of 0.0004 m$^3$.

5.8 Outcomes Revisit

The above Examples 1, 2, and 3 show that for relatively high magnitudes of perturbation there are moderate errors in the solution profiles obtained through initialization A, and, so, initialization B may be used in case a high degree of accuracy is the need. Nevertheless, for the systems, in which, initialization B doesn’t seem handy, the initial conditions calculated through the initial integration, i.e., initialization A satisfactorily predict the system behavior with an error not more than 10\% for moderate magnitudes of perturbations in the cases studied.

5.9 Example 4

The framework is applied to the gravity-flow tank system of Section 3.5 consisting of a tank with an inflow stream and a straight, horizontal outflow pipe at the bottom exit. It is unique in the respect that it has interacting material (tank) and mechanical energy (pipe) capacities. The system is at steady state at time $t \rightarrow 0^-$. Volumetric flow rate is perturbed by impulse at $t \rightarrow 0^+$. This is realized by plunging a measured amount of liquid into the tank, all in one go (with no change in inflow rate $q$); the magnitude of disturbance $M$ (m$^3$) equals the volume of liquid added. So, $q(t) = q(0^-) + M \delta(t-t_\delta)$ with $t_\delta = 0^+$.

Application of initialization A to the model equations respectively yields the following initial discontinuities:

\begin{align*}
h(0^+) - h(0^-) &= M / A_t \\
\dot{h}(0^+) - \dot{h}(0^-) &= M \delta(t-t_\delta) / A_t \\
u_p(0^+) - u_p(0^-) &= 0
\end{align*}
Eq. (5.43) exhibits singularity because of the initial jump discontinuity in the initial level in Eq. (5.42). From the initialization B approach, i.e., applying material balance on the effects of singularity, it is found that Eq. (5.42) is valid because the sudden level rise in the tank is equal to the $M \text{ (m}^3\text{)}$ of the volume of liquid inserted per unit area of the tank. However, the last Eq. (5.44) is not true, as the impulse perturbation causes a sudden change in the initial level, and simultaneously in the initial velocity $u_p$ because of the instantaneous head change. Hence, the level impulse response exhibits inconsistency in the initialization A approach. A better value of this discontinuity can be evaluated by assuming quasi-static process and zeroing differentials, valid if $A_T$ is quite large compared to $A_p$ (or further approximate Bernoulli’s Eq. be used):

$$
 u_p(0^+) - u_p(0^-) = \left( \frac{gD_o}{2fL} \right)^{1/2} \left( h^{1/2}(0^+) - h^{1/2}(0^-) \right) \tag{5.45}
$$

This equation can be combined with the material balance Eq. (5.42) above and the two solved simultaneously to yield the initial discontinuity in velocity $u_p$.

5.10 Example 5

The model of semi-batch reactor presented in Section 3.3 is considered. It is carrying out a liquid-phase constant-density reaction $A + B \rightarrow R + S$ having second-order rate constant $k$. No outlet stream is there. $A$ is already in the reactor, and $B$ is being fed continuously at constant rate $v_o$. $M$ (m$^3$) of reactant $B$ is fed suddenly at $t \rightarrow 0^+$. This is equivalent to an impulse perturbation (in $B$) volumetric flow rate of feed $v_o$ at $t \rightarrow 0^+$.

Holdup volume $V$ is not constant.

Following initialization A to the model, gives the discontinuities in $C_B$ and $C_A$.

$$
 C_B(0^+) - C_B(0^-) = M \left[ C_{Bo} - C_B(0^-) \right] / \left[ V(0^-) + M \right] \tag{5.46}
$$

$$
 C_A(0^+) - C_A(0^-) = -MC_A(0^-) / \left[ V(0^-) + M \right] \tag{5.47}
$$

Here, these initial discontinuities are consistent with that obtained from initialization B. Hence, the impulse response remains unaffected by initial discontinuities.
5.11 Fundamental Limitation of the Laplace Transformed Models

The resolution of inconsistency inherent in the Laplace domain dynamics is discussed in detail in Chapter 6. The two initializations A and B happen to be mutually consistent for some linear cases. However, this is not true of the linear systems, in general; especially, it is not true for the impulse responses of the non-trivial chemical engineering systems involving phase changes, mixing with reaction, and interacting capacities of material, thermal, and mechanical engineering capacities mentioned in introduction (see the next section on linearized systems).

Hence, for such systems the Laplace transform approach that uses pre-initial values of dependent variable (0^- values), would be less accurate as it would yield post-initial values (0^+ values) that are inconsistent with physical principles (Chapter 6).

5.12 Fundamental and Practical Limitations of the Linearized Models

Effect of the transformation of the models through linearization (using Taylor’s series expansion, with the system assumed in the vicinity of the initial state), on the evaluation of initial discontinuities through alternative approaches, is now discussed. The condenser Example 2 exhibited identical initial discontinuities via approaches A & B for impulse in \( F \) (Eq. (5.34.e)). However, if the model is linearized (Section 3.4.3), the initial discontinuity in \( T \), calculated via initialization A, would be:

\[
T(0^+) - T(0^-) = \frac{M \{ T^0 - T(0^-) \} }{N(0^-)}
\]  \( (5.48) \)

which is not equal to the one estimated from initialization B (Eq. (5.34.e)). Hence, the system that is unaffected by initial discontinuities originally, would be affected by it upon linearization. However, for impulse in \( L \), approach A exhibits the same initial discontinuities upon linearization as that calculated from the maiden nonlinear model (Eq. 5.36):

\[
T(0^+) - T(0^-) = \frac{M \Delta H / C_p}{N(0^-)}
\]  \( (5.36) \)
This was not equal to the one estimated from initialization B (Eq. (5.38)). Hence, this system that is affected by discontinuities originally would remain affected by it upon linearization. The same is true for the gravity-flow tank and isothermal CSTR systems.

However, if the closed loop stirred tank heater of Example 3 is linearized, the initial discontinuity, via initialization A, would turn out to be the same as that calculated from initialization B (Eq. (5.41)). Hence, this system that is affected by discontinuities originally, interestingly, would be unaffected by it upon linearization. Exactly the same happens for the constant holdup CSTR.

The variable-volume non-isothermal CSTR of Example 1 perturbed by impulse in the exit flow rate remains unaffected by discontinuities before and after linearization (Eq. (5.20)). Many systems were analyzed, i.e., gas phase pressurized CSTR, semi batch reactor, bimolecular reaction CSTR, two phase CSTR, flash distillation, interacting and coupled systems, etc. It was found that many systems are affected by the discontinuities. And, only a very few of them, get rid of this effect upon linearization. However, many other systems remained unaffected in their maiden nonlinear form. And, among them, some cases showed the effect of discontinuities upon linearization. Single component condenser and variable-volume CSTR for feed rate change presented here, are such examples. Thus, all the above four possibilities of appearance/disappearance of the effect, exist for the chemical engineering systems. Various linearized models are presented in Chapter 3.

So, if a system is affected/unaffected by an initial discontinuity in the linearized form, in general, nothing can be said about the effect/non effect of the discontinuity on the corresponding nonlinear system. This is an important result, because linearized systems generally behave in the same manner as the maiden nonlinear systems for near normal operations, and the practical linear control systems are designed on this basis of the operations in the neighborhood of the normal operation. However, as shown above, in particular, the initial discontinuous response of a linearized model can be significantly different from the initial response of the actual system and can deviate significantly from the normal operation. These facts elicit the limitations of using the linearized transformed models instead of the native models for initialization A for singular inputs.
Furthermore, the Laplace transformation approach that uses pre-initial values would be less accurate in treating those linearized cases, which were affected by the discontinuities under the impulse inputs. These limitations of the Laplace transformation were stated at the end of the preceding sub-section and would be discussed in detail in Chapter 6. Limitations of the models transformed through symbolic differentiations and manipulations are discussed in Section 5.13.

5.12.1 Special cases

Some systems also undergo order reduction and reduction to standard systems (i.e., not containing derivative of input) upon linearization. These are discussed here.

Consider the non-isothermal CSTR of Section 3.1 and assume constant holdup volume. Through the above analysis, it is seen that the temperature response of this system is affected by discontinuities for an impulse perturbation in the feed stream concentration $C_{Ao}$. Upon linearization, the temperature response of this system reduces to a standard second-order system for feed concentration perturbation. However, it remains affected by initial discontinuities.

The concentration response of the same system (Section 3.1.1) is found to be affected by discontinuities for impulse perturbation in the jacket temperature $T_j$. Upon linearization, this system too, reduces to a standard second-order one (Eq. 3.5) and remains affected by discontinuities.

Consider the linear isothermal constant holdup CSTR under feed concentration perturbation of Section 3.2. This model was a standard second-order system (i.e., not containing the derivative of input) and was not affected by initial discontinuities for step perturbation. However, for the impulse perturbation in Section 4.2.4, it is found to behave as a second-order system with numerator-dynamics and is affected by the discontinuities (as given by Eq. (4.13)).

A few systems also undergo simultaneous order-reduction upon linearization due to pole-zero cancellation (Ahuja, 2010; 2011). These are: temperature response of a constant volume non-isothermal CSTR for zero reaction enthalpy under jacket temperature perturbation (as shown through Eq. 3.77), the same system under feed flow rate perturbation, and the variable volume stirred tank heater under feed rate perturbation.
(as shown in Section 3.7.1 through Eq. 3.40), which reduced to standard first-order systems. The first one is affected by initial discontinuities in its maiden nonlinear form but is unaffected by them upon linearization. The remaining two are not affected by initial discontinuities in nonlinear, as well as, linearized adaptations.

5.13 Limitations of the Symbolically Transformed Models

In this section, several models obtained from mathematical transformations of the condenser model are considered, and upon inconsistent initialization, their numerical results are plotted simultaneously with the results of the original mathematically non-transformed explicit ODE model Eqs. (5.29') through (5.33) used above in Example 2 (non-transformed model). The transformed models considered are: (a) model of symbolic differentiations and manipulations of Eqs. (5.29) through (5.32) for index reduction (transformed model I) (Vieira and Biscaia Jr, 2001); (b) Explicit ODE model consisting of Eqs. (3.15), (3.16), (3.17), (3.22), and (3.23) (transformed model II, of Section 3.4.2), obtained through symbolic differentiations and manipulations of the condenser model; and (c) Explicit ODE model consisting of Eqs. (5.29) through (5.33) (transformed model III), which uses mathematically transformed Eq. (5.29) instead of Eq. (5.29') of the non-transformed model. Narrowing down of the working ranges of inconsistent initial conditions for these transformed models is also discussed. The inconsistent initialization problems for the step and the impulse perturbations arising from the mathematical transformations are thoroughly explained next.

5.13.1 Inconsistency in the symbolically transformed models

This inconsistency was discussed at length in the literature review Section 2.3.1. To illustrate the inconsistency arising out of symbolic manipulations and differentiations, consider a perturbation in the molar feed rate $F$ introduced into the single component condenser model of Section 3.4.2 (transformed model II). In the two alternative explicit models of Section 3.4.2, $L$ was calculated from the equation derived after symbolic manipulations, i.e., Eq. (3.23) (at constant volume). The discontinuities analysis exposing their inconsistency is presented below, and the numerical results are discussed subsequently.
**Step perturbation in F**

Inconsistency, during numerical solutions, is anticipated due to the following two reasons:

- The numerical integration of the set of Eqs. (3.15), (3.16), (3.17), (3.22), and (3.23) require initializations of $N$ and $T$. However, if these values are either chosen quite different from their initial steady state values, or any combination of the values of $N$ and $T$ is chosen arbitrarily; those values of $N$ and $T$ would be mutually inconsistent. This would happen because they don’t satisfy the algebraic Eqs. (3.17) and (3.18). Hence, Eq. (3.23), derived from them, would yield a wrong value of $L$, initially and afterwards. This will lead to gross errors and wrong or no convergence at all.

- It is clear that if one starts with mutually consistent or initial steady state conditions (as explained above) for all the other variables except $F$ ($F$ suffers a discontinuous step input from $t \to 0^-$ to $t \to 0^+$), the value of $L$ at $t \to 0^+$ should remain at its original value at $t \to 0^-$ (from a physical observation, the dynamic lag in the condenser would prevent a discontinuity in $L$). However, the new initial value of $F$, i.e., $F(0^+)$ is substituted in Eq. (3.23) during the numerical integration, which gives a wrong initial value of $L(0^+)$. Thus, this wrong value would be used for $L$ at $t \to 0^+$ and, hence, subsequently. The original value $L(0^-)$ would have been obtained only if the initial value $F(0^-)$ was substituted into Eq. (3.23). This would lead to a completely wrong initialization of $L$. This initial discontinuity in $L$ would cause a discrepancy in the system, even if, one starts with the consistent or initial steady state conditions for all the other variables except $F$. The problems will be compounded during numerical integration, in case, one starts with inconsistent initialization pointed above (results for such a case are discussed in Section 5.13.2 below).

**Impulse perturbation in F**

Nevertheless, for impulse input, the second problem does not come in, since the input variable $F$ doesn’t change in a stepwise manner. If, in the symbolically manipulated explicit model of Section 3.4.2, one starts with a mutually consistent set of initial conditions, the results would converge to the consistent values. However, the impulse input will cause initial jump discontinuities in the dependent variables whose magnitude
will depend upon the magnitude of the input. So, these variables jump to mutually inconsistent post-initial conditions, even if they started with consistent pre-initial or steady state values (consistent by default). This leads to the first problem mentioned above. The same is true for other DAE approaches that use symbolic manipulations for index reduction.

5.13.2 Numerical Results

Step perturbation in $F$ with singular initial conditions

In the models transformed through symbolic differentiations and manipulations, the presence of initial discontinuities involves singular initial conditions even for step inputs, and, thus, they have inconsistent initial conditions. To illustrate the resultant effects and limitations of the mathematical transformation of models, the numerical results of the non-transformed model of condenser, are plotted together with those of mathematically transformed model I. A numerical integration must converge to the consistent final steady state values, irrespective of whether the integration is started with a consistent or an inconsistent set of values. The computations are done, keeping this objective in mind, to get a plausible solution set. However, it is seen below that the transformed models don’t converge to the consistent steady state values.

The literature study for the step perturbation to the index-2 model of single component condenser (Eqs. (5.29) through (5.32)) assumed constant volume, and applied symbolic manipulation and differentiation of these equations to convert the model to index-1 DAE model (transformed model I) in order to employ the integration code DASSL. Since the results were not converging with the discontinuous step function, consistent initialization was achieved based on the fact that initial steady state can be used as a consistent set of initial conditions. Hence, the system was assumed to be at the initial steady state at $0^-$ time, then, at $0^+$ time, the system was rapidly initialized to the actual $0^+$ state of Table 5.4 and the discontinuous step perturbation was approximated by a smoothed function; smoothing was based on the response to a step perturbation into the first tank of the $n$ tanks-in-series model of total time constant $\tau$ (Vieira and Biscaia Jr, 2001). To draw a clear conclusion, the parameter values, magnitude of the input and the
Table 5.4  Parameters for the Condenser Example

For Section 5.13

\[ \Delta H = 4.5 \times 10^3 \text{ J/mol} \]
\[ F(0^-) = 50 \text{ mol/s} \]
\[ L(0^-) = 50 \text{ mol/s} \]
\[ A = 1.2 \times 10^{10} \text{ Pa} \]
\[ UA_h = 1.0 \text{ W/K} \]
\[ F(0^+) = 30 \text{ mol/s} \]
\[ T(0^+) = 488.63 \text{ K} \]
\[ B = 3816 \text{ K} \]
\[ C_p = 3.35 \times 10^4 \text{ J/mol-K} \]
\[ T_f = 283 \text{ K} \]
\[ N(0^-) = 532.43 \text{ mol} \]
\[ C = -46 \text{ K} \]
\[ R = 8.314 \text{ J/mol-K} \]
\[ T_v = 373 \text{ K} \]
\[ k = 6.89 \times 10^{-2} \text{ (mol/s)/mol} \]
\[ n = 1 \]
\[ \tau = 10^{-6} \]

initial conditions were kept the same as in the reference study as given in Table 5.4. A case of a step perturbation in \( F \) from 50 mol/s to 30 mol/s was considered. The consistent initial steady state values were calculated in the present study corresponding to the constant parameters given in Table 5.4 by zeroing the derivatives in Eqs. (5.29) and (5.30) and, using (5.31), and (5.32). These are: \( L(0^-) = 50 \text{ mol/s}, N(0^-) = 725.725 \text{ mol}, T(0^-) = 507.195 \text{ K} \). Similarly, the final steady state values assuming constant volume are calculated: \( L(\infty) = 30 \text{ mol/s}, N(\infty) = 725.039 \text{ mol}, T(\infty) = 507.135 \text{ K} \). If the volume is allowed to vary, the initial steady state set remains the same, and the final steady values can still be calculated by including Eq. (5.33) for the non-transformed model. The final steady state values of \( L(\infty) \) and \( T(\infty) \) remain the same as that for the constant volume case, but \( N(\infty) = 435.414 \text{ mol} \).

The results of the non-transformed and transformed model I are plotted together in Figs. 5.16, 5.17, and 5.18. However, as seen from these figures, the reference study profiles converge to neither of the two sets of the final steady state values; this is due to the fact that mathematically transformed models were used in this study. According to the initial conditions in Table 5.4, \( N \) and \( T \) were initialized at values that were inconsistent with their initial steady state values (singular initial conditions due to initial discontinuities). Thus, there must be initial discontinuities in \( L \) and \( P \) as seen physically.

This initial discontinuity for \( L \) is seen in Fig. 5.16 for the non-transformed model curve. However, the reference study curve only exhibits a discontinuity of 5%, and its behavior is sharper. In Fig. 5.17, \( N \) shows a monotonic decrease for the non-transformed
Figs. 5.16 and 5.17 Numerical solutions of non-transformed and transformed models—Step response respectively of liquid exit flow rate ($L$), and moles ($N$) of vapor in condenser to perturbation in molar feed rate ($F$). 2. Vieira & Biscaia Jr, 2001
model before converging to the consistent value of 435.414 mol. The reference study curve also exhibits a monotonic decrease in \( N \) but converges to an inconsistent value of 100.930 mol, thus exhibiting erroneous solution profile. Also, \( T \) in Fig. 5.18 for the reference study decreases and converges to a value of 413.663 K instead of 507.105 K, whereas the non-transformed model curve rises and converges correctly to 507.105 K.

**Impulse perturbation in \( F \)**

Result of non-transformed model for the condenser (that uses Eq. (5.29) for energy balance) is plotted along with the result of transformed model III (that uses Eq. (5.29) instead). The rest of Eqs. (5.30) through (5.33) were kept common in both these cases. The transformed model III would exhibit wrong numerical integrations because Eq. (5.29') was obtained from the differentiation and manipulation of the original equations. These two single component condenser models, were solved for impulse perturbation in \( F \). Initial conditions \( T(0^+) \) and \( N(0^+) \) were obtained by including impulse in the cause and
carrying out the integration at initial time (initialization A). Since, the energy balances in the two cases were different, different initial conditions were obtained in the two cases presented. The initial discontinuity for perturbation in \( F \) to the non-transformed model was given by Eq. (5.34). This initial discontinuity happened to be the same from the initialization procedures A and B of the framework. The value of initial discontinuity using the transformed model III is calculated through initialization A as:

\[
T(0^+) - T(0^-) = \frac{M \left( T_0 - T(0^+) \right)}{N(0^+)}
\]  

(5.49)

A magnitude of the impulse perturbation of \(-100\) mol (13\% of initial steady-state \( N \)) was considered. The results converge to the initial steady-state values. The same parameter values of Table 5.4 as in the above case of step perturbation (except \( T(0^+) \) and \( N(0^+) \)) were applied. The results are presented in Fig. 5.19 for \( T \).

**Fig. 5.19** Numerical solutions of non-transformed and transformed models—Impulse response of temperature of vapor in condenser to a perturbation in feed molar flow rate of magnitude of \(-100\) mol
The curve for the transformed model III exhibits a significant error of 10%. So, the first principles model Eq. (5.29'), rather than Eq. (5.29), obtained after differentiation and manipulations should be used for the condenser system. Transformed model II converged to 731.562 mol against the correct value of 725.039 mol (not shown in Figs.).

However, the non-transformed model curves in Figs. 5.16-5.19 are converging to the consistent final steady state values for all the variables $T$, $P$, $L$ and $N$ (not shown on the Figs. for some). Hence, this model provides accurate solutions, that converge to the right values even for a wide range of inconsistent initial conditions, in addition to being simple (no symbolic manipulations needed), direct, and computationally efficient.

The results of this section clearly signify that the results of the transformed models I and II are inaccurate, and the errors increase at inconsistent initializations. These errors are attributed to the symbolic manipulations and differentiations as elicited in Section 5.13.1; with initial discontinuities, the differentiations of the original equations cause singularity and the resultant singular and inconsistent initial conditions in the output. This fact is also appropriate for the case of impulse inputs that put the systems far off from their consistent initial steady state.

**Working range of inconsistent initial conditions**

Since impulse inputs put the system decently far from the consistent initial steady state, the range of the applicability of the solvers needs to be specified, especially, if the system is relatively stiff. The working range of initial discontinuities was tested by increasing/decreasing a variable from its consistent initial value (keeping others fixed) until the solvers gave an error message. The computations were performed on a PC with Intel Core 2 CPU, 1.66 GHz and 0.5 GB of RAM. The numerical integrations were carried out using the ODE solvers, RKF45, BS, STIFF, etc. from Polymath. The range (of positive values) are expressed as percentage of the consistent value (of Tables 5.1 and 5.2), and the CPU times correspond to the extreme value of this range.

The constant holdup CSTR of Section 5.4 was a stiff system of slow and fast dynamics combined, as $T$ changed very slowly compared to $C_A$. STIFFBS, generally meant for the stiff systems, was very slow outside the range of $T(0^+)$ of 133%, and took 30.09 s of CPU time. The BS solver that works for the non-stiff problems, worked in the
range of 251%, took around 10.35 s; RKF45 (took 4.63 s) and RKF56 (took 5.79 s) worked faster in the range of 333% and 384%, respectively. However, STIFF was the best with a tremendous working range of (0 K – 2.0 \times 10^7 K), i.e., 60,060%, taking only 3.47 s.

The non-transformed condenser model was immediately solved with all the solvers in the range of 717% except STIFFBS, which worked in the range of 60% and took 45 s. All the above results converged to the consistent steady state values.

For the condenser transformed model II, the working ranges of all the solvers was similar and was only of (50 K – 400 K), i.e., 72%. All the solvers solved immediately except STIFFBS, which took 31.25 s at 50 K. So, the working range of this transformed model is very narrow as compared to the above non-transformed models.

The error messages flashed by the solvers were: (a) BS: Internal Error Trapped ODEINT_BS: Too many steps in routine odeint; (b) STIFF & STIFFBS: Internal Error Trapped ODEINT_ST & ODEINT_BSST: Too many steps in routine odeint; (b) STIFFBS: Internal Error Trapped: Step size underflow; (c) STIFF: Division by zero; and, (d) Overflow error in all the solvers.

The working deviations of various for transformed battery model simulations are cited (Wu and White, 2001) for comparison: for positive values, these are, 0% (MAPLE®), 14.2% (DASSL), 544% (DAEIS); and, reported as 871% (Soares and Secchi, 2005), and 5,053% (with JACOBIAN®) (Methekar et al., 2011). Thus, they depend very strongly on the solver used, whereas, the solvers for non-transformed ODE models worked over wider inconsistencies.

It is emphasized that the working of the proposed methodology is, in no way, limited to the establishment of an initial steady state, \( a \ text{priori} \), at \( t \rightarrow 0^- \). The steady states are included here, only to check the convergence and the plausibility of our results.

5.14 Outcomes Revisit

To wind up the discussion, it is concluded that the two ways of initializations (A and B), in general, are mutually inconsistent. However, initialization A accurately models the singularity and the initially discontinuous systems for operations not too far away from the normal operating conditions.
Step responses of the original, un-manipulated models, however, are not affected by initial discontinuities, even though they can exhibit initial discontinuities and singularity due to the derivatives of inputs.

The numerical solutions, obtained using the symbolically transformed models I, II, and III, including that based on the smoothening of the inputs, exhibited incorrect values. Nevertheless, non-transformed explicit ODE model of single-component condenser exhibits (formulated in Section 3.4.1) consistent convergence and accounts for changes in volume. Furthermore, the solutions for the non-transformed models for all the systems presented in Chapter 3 can be obtained quite efficiently using an ODE solver that works over a wide range of the mutually inconsistent initial values of the output variables.

The post-initial conditions, calculated via the inclusion of impulse in the cause (initialization A), satisfactorily predict the system behavior within an error of the order of 10% for small magnitude of the inputs. Initialization C is, however, inadequate. These effects are illustrated by computer simulation of the nonlinear models of single-component condenser, non-isothermal CSTR and closed-loop stirred tank heater systems, in this chapter. The closeness of initialization A to initialization B is quantified in these examples. The superiority of initialization B was discussed in the last chapter, and was substantiated there through computer simulations of the nonlinear models of gravity-flow tank and interacting two-tank systems and the calculations of time-to-empty these flow-level tanks.

First, the post-initial conditions are obtained from the direct methods A and B proposed; these are used subsequently for the numerical solutions using an ODE solver through the framework proposed (Fig. 5.1). However, for the numerical solutions of the impulse responses, the values of the impulse input terms in the equations must be substituted equal to zero, since the magnitude of these terms have already been included in the model while calculating the initial conditions. Thus, for the impulse response, this framework corresponds to route (b) of the preliminary analysis presented in Fig. 4.1, and followed in Sections 4.2 through 4.8 of the last chapter; wherein, all the initial conditions of output variables are used at \( t \to 0^+ \) with the input variable equated to zero, i.e., the initial discontinuities are accounted for in the initial conditions of the output variables.