7 Conclusions and Recommendations

7.1 Conclusions

A methodological framework for the analysis of initial discontinuities and the estimation of the initial conditions for the lumped-parameter chemical engineering systems for the singular inputs is proposed. The following conclusions can be drawn from this study:

• Lumped-parameter chemical engineering systems contain derivative of the input terms in their models when solved for one of the output variables, and, thus, exhibit numerator dynamics behavior upon linearization. These physical systems and their models present themselves with initial discontinuities for the singular inputs. Their range of assorted solution profiles and the corresponding characteristic conditions are obtained for negative real part poles and represented concisely on the real axis. These exhibit different behavior than the standard systems; the profiles exhibiting maximum/minimum are also important from design perspective.

• The inclusions of singularity via the cause (initialization A) and the effects (initialization B) give the same solutions for many systems, but mutually inconsistent solutions for many others as their models are affected by singularity. Initial conditions via initialization A are obtained by the integration of the models between $0^-$ and $0^+$ times, prior to carrying out the analytical or numerical solution. These initial conditions satisfactorily predict the system behavior within an error of the order of 10% vis-à-vis initialization B for operations not very far away from the 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. The applicability of initialization A procedure was suggested by its conformity to the definitely known cases, and to the Laplace transform treatment for linear systems.

• The solutions obtained by including singularity in the effects and the applications of physical balances (initialization B) have been found to be more accurate and conform to the physical facts than the ones calculated solely from a theoretical perspective (initialization A). This effect is substantiated by carrying out numerical experiments.
and comparing the results with the experimental results of flow-level tanks. Further
evidence to this effect is provided by carrying out the analysis of the calculations of
time required for emptying the flow-level tanks.

- The approach of using a continuous function for an impulse can’t reveal the true
asymptotic behavior as it can’t catch up with the correct initial conditions. The
symbolically transformed models and the linearized models, also, can’t predict the
correct initial conditions, and, thus, lead to erroneous solution profiles and
inconsistent convergence. In general, the non-transformed models work for
operations over a wider range of the mutually inconsistent initial values of the output
variables, as compared to the symbolically transformed models.

- For linear systems, it is revealed that the post-initial conditions obtained through
initialization A and \( \mathcal{L} \) approach are invariably the same. The \( \mathcal{L} \), approach that uses
the post-initial conditions obtained through physical balances on the effects is more
exact and resolves several inconsistencies vis-à-vis the \( \mathcal{L} \) approach, especially for
complex chemical engineering cases under an impulse.

### 7.2 Recommendations for future work

- The present models can be extended further to deal with the problem of
discontinuity/inconsistency in initial/boundary condition specifications in
distributed-parameter systems, for example how to handle the situation when
Dirichlet’s boundary conditions are used and there is a discrepancy between the
initial condition inside the domain and the value at the boundary.

- Future work can explore direct methods for other complex models and see how the
computational effort scales with the model complexity and the way the algorithms
are implemented, for example it would be challenging to treat discontinuity in
fractional order ODE/PDE models, Volterra-Laguerre models, empirical models, etc.
**Notations**

- **$A$**: Antoine’s constant [Pa]; Cross-sectional area of the U-tube manometer column [m$^2$]
- **$A_h$**: Surface area for heat transfer [m$^2$]
- **$A_T, A_P$**: Cross-section area of tank and pipe in gravity-flow tank, respectively [m$^2$]
- **$A_1, A_2$**: Cross-section area of the first and the second tank of the interacting liquid-level tanks, respectively [m$^2$]
- **$B$**: Antoine’s constant [K]
- **$b$**: Damping coefficient in suspension system [N·m/(N·s)]
- **$C$**: Antoine’s constant [K]
- **$C_p$**: Specific heat [J/(mol·K)]
- **$C_{A_0}, C_A, C_R$**: Concentration of $A$ in feed, $A$ in tank and $R$ in tank, resp. for a CSTR [mol/m$^3$]
- **$D_p$**: Diameter of the pipe in gravity-flow tank [m]
- **$E$**: Reaction activation energy [J/mol]
- **$f$**: Fanning friction factor [-]
- **$F$**: Molar feed rate to a condenser [mol/s]
- **$g$**: Acceleration due to gravity [m/s$^2$]
- **$h$**: Level of liquid in gravity-flow tank [m]
- **$h_1, h_2, H_1, H_2$**: Level in first and second tanks in interacting tanks and corresponding deviation variables, respectively [m]
- **$h, H$**: Level of liquid in gravity-flow tank and the corresponding deviation variable, respectively [m]
- **$\Delta H$**: Heat of condensation of vapor in condenser [J/mol]
- **$\Delta H_R$**: Reaction enthalpy at the reaction temperature [J/mol]
$k, k_o$  Constant of proportionality for condenser $[\text{mol/s mol}]$; First-order rate constant of reaction $A \rightarrow B$ and the same at a very high temperature, respectively $[\text{1/s}]$

$k_s$  Spring constant of suspension system $[\text{N/m}]$

$K, K'$  Steady-state gains of the transfer functions

$L$  Condenser liquid exit molar flow rate $[\text{mol/s}]$; Length of pipe in gravity-flow tank [m]; Total length of the U-tube manometer column [m]

$\mathcal{L}$  Laplace operator

$M$  Magnitude of impulse (general)

$M_A, M_R, M_I$  Molecular weights of $A, R$ and inert in a CSTR

$m$  Mass of the car body [kg]; Mass of the U-tube manometer liquid column [kg]

$N$  Moles of vapor in condenser [mol]

$P^*$  Vapor pressure [Pa]

$\Delta P$  Pressure difference applied to the U-tube manometer column [Pa]

$Q$  Heat transfer rate [W]

$q, Q$  Inflow rate to gravity-flow tank (or first tank of interacting system) and corresponding deviation variable $[\text{m^3/s}]$

$q_{21}, q_2, Q_{21}, Q_2$  Inflow and outflow of the second tank of interacting tank system and corresponding deviations, respectively $[\text{m^3/s}]$

$R$  Universal gas constant $[\text{J/mol-K}]$

$s$  Laplace parameter

$t$  Time [s]

$T, T_o, T_J$  Temperatures in the tank, in feed, and in jacket, respectively [K]

$u, U$  Velocity of U-tube manometer liquid column, and its deviation from the pre-initial state $[\text{m/s}]$

$u_p, U_p$  Velocity in the pipe of gravity-flow tank and corresponding deviation variable, respectively $[\text{m/s}]$
**$U_h$** Overall heat transfer coefficient $\left[ \frac{W}{m^2 \cdot K} \right]$

**$u(t)$** Unit step input (general)

**$v_{in}, v_{out}$** Inlet and outlet volumetric flow rate through a tank $\left[ \frac{m^3}{s} \right]$

**$V$** Volume of vapor in condenser, fluid in CSTR & stirred-tank-heater $[m^3]$

**$x$** Displacement of the wheel in car wheel suspension example $[m]$

**$y$** Displacement of the car body in car wheel suspension example $[m]$

**$z$** $(n^2 + m^2 + nm) / (n + m)$, a characteristic parameter for a numerator-dynamics system, where $n$ & $m$ are system constants

**Greek letters**

- **$\rho$** Density $\left[ \frac{kg}{m^3} \right]$
- **$\mu$** Viscosity $[Pa \cdot s]$
- **$\tau_d$** Dead time in stirred tank heater $[s]$
- **$\delta(t)$** Unit impulse function (Dirac function)
- **$\tau_1, \tau_2$** Time constants for the first tank and the second tank of the two interacting tanks system $[s]$
- **$\zeta$** Damping coefficient

**Subscripts and superscripts**

- **$imp$** Impulse
- **$i$** Inflection
- **$max$** Maximum
- **$min$** Minimum
- **$s$** Initial steady states
- **$st$** Step
- **$-$** Over-bar, deviation from initial steady state
- **$'$** First differential
- **$''$** Second differential
- **$n$** $n^{th}$ differential
- **$-n$** $n^{th}$ integral
### Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CSTR</td>
<td>Continuous flow stirred tank reactor</td>
</tr>
<tr>
<td>DAE</td>
<td>Differential and algebraic equations</td>
</tr>
<tr>
<td>DDE</td>
<td>Delay differential equation</td>
</tr>
<tr>
<td>FOPDT</td>
<td>First order plus dead time</td>
</tr>
<tr>
<td>NRMSD</td>
<td>Normalized root mean square deviation</td>
</tr>
<tr>
<td>ODE</td>
<td>Ordinary differential equation</td>
</tr>
<tr>
<td>PID</td>
<td>Proportional integral derivative control</td>
</tr>
<tr>
<td>RMSD</td>
<td>Root mean square deviation</td>
</tr>
</tbody>
</table>