# Numerical Solution of Dynamic Flash Equations

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# Erklärung

Hiermit erkläre ich, dass ich die vorliegende Arbeit selbstständig und eigenhändig sowie onhe unerlaubte fremde Hilfe und ausschließlich unter Verwendung der aufgeführten Quellen und Hilfsmittel angefertigt habe.

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Berlin, den 27.07.2015

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**Abstract**

This thesis concerns simulation and control of two-phase flash separators, which are important and ubiquitous components of many industrial processes. The topic will be motivated, and two dynamic models that are proposed in literature will be presented: a full model and one based on simplifying physical assumptions. In general, the system is described by a hybrid physical/empirical system of differential-algebraic equations (DAEs) with a high degree of nonlinearity. It is claimed in the literature that the simplified model has an increased d-index.

Relevant literature pertaining to the solvability of such systems in a behaviour setting using the concept of the strangeness index, as well as suitable numerical methods, is reviewed.

This framework is then used to explore the two models and the impact of the dependencies of the empirical terms on the structure of the DAEs, resulting in deriving explicit conditions for both systems to be index 1. In particular, the index of the simplified system depends on the choice of control and state variables, and which variables are used for feedback. The claims made in the literature can be clearly understood from the behaviour setting - taking a different choice of control variable, or a carefully constructed feedback matrix, leads to an index 1 formulation.

A suitable test case is presented based on a simple alkane-hydrocarbon flash, using appropriate (if simple) closure models and physical data from a steady-state analysis in the literature. The test case is implemented in Matlab® with the systems constructed to be index 1.

Finally, some numerical results for the test problem are presented and analysed, with both systems and solvers compared. It is apparent that second system is a good input-output model for the full system under these conditions, although it does not provide enough information to determine the phase distribution of the contents of the flash drum.

# Zusammenfassung in deutscher Sprache

## Simulation von dynamischen Flash-Verdampfern

In dieser Arbeit wird die Simulation und Kontrolle von Zwei-Phasen-Flash-Separatoren, die ein wichtiger Bestandteile vieler industrieller Prozesse sind, betrachtet. Zwei-Phasen-Flash Separatoren können mittels hybrider Modellierung von physikalischen und empirischen Beobachtungen durch ein System von stark nichtlinearen differential-algebraischen Gleichungen (DAEs) beschrieben werden. Die Modelle basieren auf physikalischen Erhaltungssätzen sowie systemspezifischen Funktionen, die das Verhalten im Phasen-Gleichgewicht annähern. Es werden zwei in der Literatur vorgeschlagene dynamische Modelle vorgestellt. Das erste Modell ist ein vollständiges Modell der Flash-Dynamik und das zweite Modell ist eine auf physikalischen Annahmen basierende Vereinfachung. In der Literatur wird behauptet, dass das DAE-System des vereinfachten Modells einen höheren Index aufweist als beim vollständigen Modell.

Zunächst wird in der Arbeit ein Überblick der Literatur in Bezug auf die Klassifizierung des Index von Deskriptor-Systemen mittels des Behavior-Ansatzes gegeben. Dabei wird das Strangeness-Index-Konzept zugrunde gelegt. Neben der theoretischen Betrachtung werden auch numerische Methoden vorgestellt.

Die Lösbarkeit der beiden Modelle wird in Bezug auf die Auswirkungen der empirischen Terme auf die Struktur des DAE-Systems untersucht. Explizite Bedingungen für die empirischen Funktionen werden hergeleitet, die garantieren, dass beide Systeme Differentations-Index 1 haben. Der Index des vereinfachten Systems hängt dabei von der Wahl der Regelungs- und Zustandsvariablen ab. Die in der Literatur getroffenen Behauptungen können durch den Behavior-Ansatz verifiziert werden. Durch eine andere Wahl der Regelungsvariablen oder eine sorgfältig gewählte Feedback-Regelung kann jedoch eine Index-1-Formulierung garantiert werden.

Als Testproblem wird eine einfache Kohlenwasserstofftrennung mit geeignetem empirischen Modell und physikalischen Daten von einer Analyse des stationären Zustandes betrachtet. Das Testproblem wird als Index-1-Formulierung in Matlab® implementiert.

Abschließend werden einige numerische Ergebnisse für das Testproblem vorgestellt und analysiert. Das volle und vereinfachte System werden mit verschiedenen Lösern verglichen. Es ist ersichtlich, dass das vereinfachte System das Eingangs-Ausgangs-Verhalten des Gesamtsystems unter diesen Bedingungen gut darstellt, obwohl nicht genug Informationen vorliegen um die Phasenverteilung im Flash-Verdampfer zu bestimmen.

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# Contents

# 1 Introduction: Dynamic Flash Equations

A "flash drum" is an industrial separation unit that is used to disengage liquid and vapour phases from a mixed stream. The flash vessel is essentially a large enclosed tank, which may be vertical or horizontal, where sufficient space is allowed for vapour-liquid disengagement. In a typical flash vessel, as depicted in Figure 1 below, a multiphase feed $F(t)$ with composition $w(t)$ is cooled (or heated) to a controlled temperature $T_c$, and then fed into the vessel. This temperature must be selected to induce a phase separation at the pressure (P) in the vessel. Liquid is drawn off from the bottom of the vessel as $L(t)$ with composition $x(t)$ and vapour is drawn from the top as $V(t)$ with composition $y(t)$. During operation, the flash vessel maintains (time-varying) hold-up or inventory of both liquid and vapour phases, $M_l$ and $M_v$ respectively. In general, the operating temperature of the flash vessel is not equal to the control temperature due to the energetic requirements of the flash process. The heating element acts on the system only through a delay that is inversely proportional to the feed velocity (the time taken to reach the tank), but this delay is usually neglected in simulation.

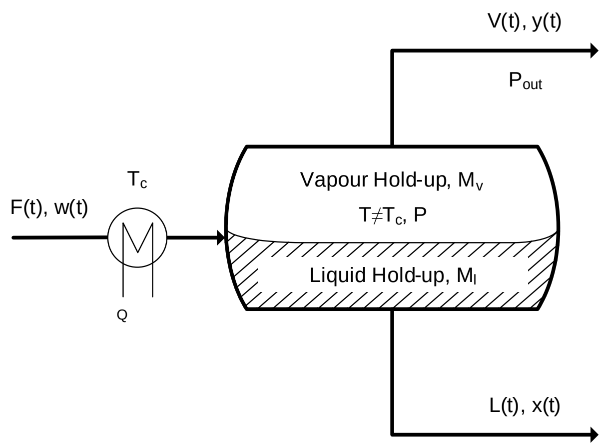


Figure 1: Schematic depiction of adiabatic flash vessel

Flashing is ubiquitous in many chemical processes, for example, Benzene-Toluene-Xylene pre-separation [1, 18], petrochemical applications, waste water processing [8], and desalination [27].

Separation is typically the most expensive part of industrial processing and hence a great deal of effort is expended to optimize separation processes [22]. In order to optimise and control the behaviour of a flash vessel, a good understanding of the dynamic behaviour of the system is required. Detailed dynamic models of flash drums are explored in [11, 12, 17, 27]. Simulation of flash vessel dynamics is also an important step in the simulation of distillation columns, which can be viewed as a linked network of flash vessels - typically each stage or tray of a distillation column is treated as its own equilibrium flash stage [21, 22].

Simulation work on flash drums does not generally consider a discrete, fine grained spatial variation and is instead based on simulating the mass and energy inventories of the vessel. This is done due to the serious uncertainties that persist in the of simulation multiphase, multicomponent flows, and the long history of validated empirical thermodynamic models that are available [22].

This work considers the solution of isothermal flash problems, which are the simplest class of flash problems. The system simulated here is assumed to operate at a given, possibly time-varying operational temperature. This simplifies the resulting system by removing the energy balance [22], as schematically represented by Figure 2 below. Now, the heating element is assumed to instantly change the vessel temperature instead of the feed temperature.

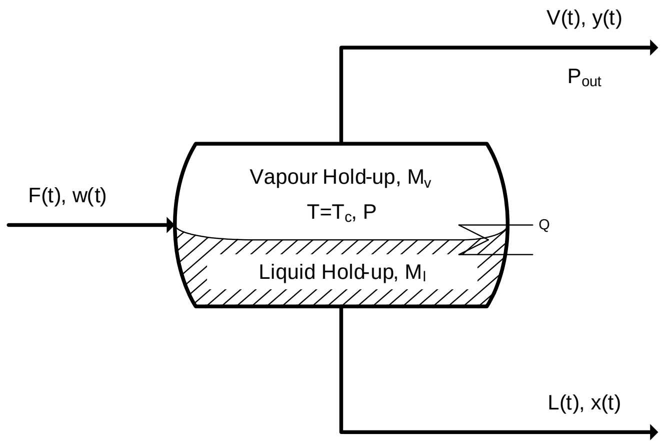


Figure 2: Schematic depiction of isothermal flash vessel

Additionally, this work considers equilibrium based methods, which are simpler to handle compared to rigorously derived rate-based methods such as the MERSHQ equations in [22], which are typically used for highly accurate steady-state simulation. This simplification amounts to assuming that the flash vessel operates in thermodynamic equilibrium, but equilibrium theoretically requires infinite residence time. Rate-based models estimate this deviation; for example, the software package ChemSep ® [14] makes use of rate-based methods to solve steady-state flash vessel problems. A more detailed survey of the underlying thermodynamic processes is given in [4].

The flash vessel models that are considered here are presented in [5]. They are derived from a mass balance on the vessel, along with the equilibrium assumptions which are presented in more detail in Section 5.1. The two systems are presented as systems of nonlinear differential-algebraic equations (DAEs).

## 1.1 Full Dynamic Flash

The first system presented in [5] attempts to describe the control of an isothermal flash drum in full detail. Let the feed enter at a rate $F(t)$ with $N_c$ components, and let the molar fraction of each component $i$ be denoted as $w_i$. The vapour phase is enriched with the volatile components of the feed and the liquid phase is enriched with the heavier components. This is represented by the following differential equation for each species, $i$:

$$\frac{dM_i}{dt} = F(t)w_i(t) - L(t)x_i(t) - V(t)y_i(t) \quad i = 1, 2..N_c$$

These are supplemented by the following constraints:

$$\begin{aligned}
M(t) &= \sum_{i=1}^{N_c} M_i(t) \\
M(t) &= M_l + M_v \\
M_i &= M_l x_i(t) + M_v y_i(t) \quad i = 1, 2..N_c \\
y_i &= K_i(T, P)x_i(t) \quad i = 1, 2..N_c \\
C_T &= \frac{M_v}{\rho_v(T, P, y)} + \frac{M_l}{\rho_l(T, P, x)} \\
L &= \psi^L(P, M) \\
V &= \psi^V(P - P_{out}) \\
0 &= \sum_{i=1}^{N_c} (y_i - x_i) = \sum_{i=1}^{N_c} (K_i(T, P) - 1)\, x_i
\end{aligned}$$

Here, $M_l$ and $M_v$ are the molar hold-ups (inventories) of the liquid and vapour phases respectively, and $x_i$ and $y_i$ are the molar fractions of component $i$ in these phases. $L$ and $V$ are the exiting flow rates of the different phases. $P$ is the pressure, $T$ is the temperature, $C_T$ is the tank volume, $\rho$ indicates molar density and $P_{out}$ is the outlet pressure. The function $\psi_V$ relates to the valve equation and $\psi_L$ relates to the hydrodynamics of the tank.

The advantage of this formulation is that it is possible to account for the impact of the species densities on the equilibrium dynamics and the tank hydrodynamic properties. This model is reported to have differentiation index 1 [5] (as defined in Section 2.1), but it is reported to be highly stiff, as the pressure changes much faster than the composition. There are $N_c$ nonlinear differential equations and $2N_c + 6$ algebraic equations. As it is intended for temperature to be a control, this formulation is undetermined by a single component, having a state space dimension of $3N_c + 7$.

## 1.2 Simplified Dynamic Flash

In [5], it is suggested that the full flash problem given previously can be simplified by assuming $M_v(t) \approx 0$, as this tends to be two to three orders of magnitude less than $M_l$. The resulting system is as follows:

$$\begin{aligned}
\frac{dM}{dt} &= F(t) - L(t) - V(t) \\
\frac{dx_i}{dt} &= \frac{1}{M(t)} \left[ F(t) \left( w_i(t) - x_i(t) \right) - V(t) \left( y_i(t) - x_i(t) \right) \right] \quad i = 1, 2..N_c
\end{aligned}$$

This system is supplemented by the following constraints:

$$\begin{aligned}
y_i &= K_i(T, P) x_i(t) \quad i = 1, 2..N_c \\
L &= \psi^L(P, M) \\
0 &= \sum_{i=1}^{N_c} (y_i - x_i) = \sum_{i=1}^{N_c} \left( K_i(T, P) - 1 \right) x_i
\end{aligned}$$

This system contains $N_c + 1$ differential equations and $2N_c + 2$ algebraic equations. Here, the system is underdetermined by degree $2$, meaning that the control (nominally $T$) and an additional variable need to be fixed. It is suggested that the pressure be explicitly specified in order to give a solvable system. This can be justified by the potential loss of accuracy in the prediction of pressure due to neglecting the presence of vapour hold-up.

This simplification is done to reduce the stiffness of the problem given above, and intends to provide a good approximation to the full system behaviour without carrying the extra equations in terms of the phase densities. This can also be advantageous as these are not always known with confidence. This DAE is reported to have differentiation index 2 [5]. This suggests that, although the model describes simplified physical behaviour, the mathematical model appears to exhibit more complicated solution behaviour.

## 1.3 Scope of This Work

These two systems are high-level "physical" models, and describe direct consequences of physical and thermodynamic laws (such as the conservation of mass, or the Gibbs' phase rule). As is typical in engineering, these models rely on (mostly) empirical closure models to describe the in-depth behaviour of the real system. For example, in the above models, $K_i(T, P, x, y)$ refers to an empirical law describing the vapour-liquid equilibrium behaviour for species $i$ as, potentially, a function of the temperature, pressure and composition of all species present. Which model is appropriate to use depends hugely on the species present and the process conditions, and there are a large range of highly complex, nonlinear models in common use [21].

DAEs do not in general share the nice solvability properties of ordinary differential equations (ODEs) [15]. Not every system of DAEs is solvable, and even if the system is solvable, the index (roughly a measure of the difficulty of solving the system, see Section 2.1) of the system depends on the partial derivatives of the system, i.e. the way in which the constraints and the differential equations interact. Since the choice of closure models affects the coupling of the differential and algebraic variables, it is worth considering what impact the choice of closure models has on the structure (and solvability) of the problem.
A behaviour form approach is used to investigate the systems in the sense of the strangeness index presented in [15]. In fact, in Sections 3.2 and 4.2, explicit conditions on the choice of closure models required for the problems to have index $1$ are derived.

In this work, these two sets of systems are compared, and the reason behind the reported curious difference in index between the systems is investigated. Conditions for the second system to be index $1$ are derived and explored in Section 4.2.

This is followed by establishing a test case system for simulation, which concerns a simple multicomponent hydrocarbon flash drum based on the example in [22]. The relevant equations are developed and a method for finding consistent initial conditions based on a steady-state solution algorithm is presented and applied.

Finally, the systems are implemented for various test conditions using two solvers, one implicit Runge-Kutta type and one backwards difference routine. The results are compared between the solvers, test cases and systems of equations in Matlab®.

# 2 Literature Review

In this section, a survey of some necessary background literature is presented. In the first half, a theoretical framework for the analysis of the solution behaviour of nonlinear DAE control problems is presented. In particular, the concept of the strangeness index is introduced and formalised. Methods for determining the index, both in the general case and specialized for the semi-implicit nature of the systems above, are presented. A method to construct strangeness-free/index 1 problems (in terms of Hypothesis 1) is presented.

The second part of this review focuses on a selection of numerical methods suitable for solving low-index DAEs. Together, these sections give a complete theoretical approach to the solution of an arbitrary nonlinear DAE by conversion to a lower index problem.

## 2.1 Analysis of Nonlinear DAEs

Here, the approach to analyse general nonlinear DAEs is reviewed, based on the framework given in [15]. A fundamental tool for classification of DAEs is that of the index, which is used to understand the behaviour of the system. In the broadest sense, the index is a measure of the difficulty of solving the problem by describing the "distance" from the problem to a well-behaved problem with the same solution set. Higher index systems must generally be converted into lower index systems before they can be solved. A generic DAE, without control, takes the form:

$$F\left(t, x, \dot{x}\right) = 0 \tag{2.1}$$

In this form, $x \in \mathbb{D}_x \subseteq \mathbb{R}^n$ and $\dot{x} \in \mathbb{D}_{\dot{x}} \subseteq \mathbb{R}^n$ take values in their respective admissible sets. Consider square, real-valued problems such that $F : (\mathbb{I} \times \mathbb{D}_x \times \mathbb{D}_{\dot{x}}) \mapsto \mathbb{R}^n$. It is assumed that the system in (2.1) is solvable, i.e. these sets are non-empty. It can occur that there are multiple solutions [6], but it is assumed that this is handled by suitable restriction on $\mathbb{D}_x$ such that the problem is uniquely solvable on $\mathbb{I}$. There are two index concepts referenced here (although others exist). The first is the differentiation index [5], which, roughly speaking, determines how far the system is from a purely differential system. More precisely, the differentiation index is the number of times the equations (2.1) must be derived with respect to time until the system can be formulated as a regular implicit ODE problem (for possibly extended $x := \left[x^T \ \dot{x}^T ...\right]^T$):

$$G\left(t, x, \dot{x}\right) = 0$$

This method is advantageous in that the solution of such problems is well characterised. Clearly, an ODE system has differentiation index $0$. However, this work considers non-square DAE control systems with $n$-dimensional state space $x$, and $m$-dimensional control $u$, of the form:

$$F\left(t, x, \dot{x}, u\right) = 0 \tag{2.2}$$

Again, the state and state-derivatives $x \in \mathbb{D}_x \subseteq \mathbb{R}^n$ and $\dot{x} \in \mathbb{D}_{\dot{x}} \subseteq \mathbb{R}^n$ take values in some admissible sets $\mathbb{D}_x$ and $\mathbb{D}_{\dot{x}}$ respectively, and the control takes admissible values $u \in U_{ad} \subseteq \mathbb{R}^m$. Only real-valued problems are considered, such that $F : (\mathbb{I} \times \mathbb{D}_x \times \mathbb{D}_{\dot{x}} \times U_{ad}) \mapsto \mathbb{R}^l$.

Any output equations are neglected as they are assumed to be uniquely solvable, and further, the flash problems considered in this work have $y(t,x,u) = x$ (or some subset thereof).

The only way to apply the the differentiation index to (2.2) is to fix a consistent and sufficiently smooth control $u$, and require that the resulting system is square (i.e. of dimension $n$). Instead, the approach presented here uses the strangeness index in a behaviour setting to determine solution behaviour.

The strangeness index is roughly a measure of how far the system is from a decoupled system of differential and algebraic equations. This approach accounts for the well-behavedness of purely algebraic variables [15]. By contrast, the d-index of a purely algebraic equation is higher than that of an ODE. The intention is to convert the problem into a set of decoupled differential and algebraic variables. The advantages of this method include the treatment of non-square systems and the fact that it does not involve state transformations. This last point is important in the behaviour setting as it allows the variables to maintain their original, physical interpretation. Hence, variables can be interpreted as states or controls in the natural physical setting.

The definition of the strangeness index is given for general DAEs and so the first step must be conversion into a behaviour form [19]:

$$z = \begin{bmatrix} x \\ u \end{bmatrix}$$

Effectively, the control variables are treated as state variables and hence the problem (2.2) is rewritten as $F(t,z,\dot{z}) = 0$. Here, we will consider $u \in \mathbb{R}^m$, and hence the dimension of $z$ is $n+m$. The nonlinear derivative array for this system is formed as follows:

$$\mathcal{F}_k\left(t,z,\dot{z},\ldots,z^{(k+1)}\right) := \begin{bmatrix} F(t,z,\dot{z}) \\ \frac{d}{dt}F(t,z,\dot{z}) \\ \vdots \\ \frac{d^k}{dt^k}F(t,z,\dot{z}) \end{bmatrix} \tag{2.3}$$

The strangeness-index is defined in terms of the following hypothesis (Hypothesis 4.30 in [15]):

**Hypothesis 1.**
*Consider a system of the form $F(t,z,\dot{z}) = 0$. Then there exist constant integers $\mu$, $a$, $d$, $v$ and $r$ such that the following conditions hold. Let $\mathbb{L}_\mu$, defined as follows:*

$$\mathbb{L}_\mu = \left\{ z_\mu \in \mathbb{I} \times \mathbb{R}^{n+m} \times \ldots \times \mathbb{R}^{n+m} \middle| \mathcal{F}_\mu(z_\mu) = 0 \right\}$$

*be non-empty, and for $z^0_\mu = \left(t, z_0, \dot{z}_0, \ldots, z_0^{(\mu+1)}\right) \in \mathbb{L}_\mu$, there is neighbourhood in which:*

1. *$\mathbb{L}_\mu \subseteq \mathbb{R}^{(\mu+2)(m+n)+1}$ forms a manifold of dimension $(\mu+2)(m+n)+1-r$*
2. *rank $\left(\mathcal{F}_{\mu,\left[z,\dot{z},\ldots,z^{(\mu+1)}\right]}\right) = r$ on $\mathbb{L}_\mu$*
3. *corank $\left(\mathcal{F}_{\mu,\left[z,\dot{z},\ldots,z^{(\mu+1)}\right]}\right)$ − corank $\left(\mathcal{F}_{\mu-1,\left[z,\dot{z},\ldots,z^{(\mu+1)}\right]}\right) = v$ on $\mathbb{L}_\mu$, where by definition corank $\left(\mathcal{F}_{0,\left[z,\dot{z},\ldots,z^{(\mu+1)}\right]}\right) = 0$*
4. *rank $\left(\mathcal{F}_{\mu,\left[\dot{z},\ldots,z^{(\mu+1)}\right]}\right) = r - a$ on $\mathbb{L}_\mu$ and there exist smooth, full rank, matrix valued functions $Z_2$ of size $(\mu+1)\,l \times a$ and $T_2$ of size $(m+n)\times(m+n-a)$ such that, on $\mathbb{L}_\mu$, the following hold:*

i $Z_2^T \mathcal{F}_{\mu,\left[\dot{z},\ldots,z^{(\mu+1)}\right]} = 0$
ii rank $\left(Z_2^T \mathcal{F}_{\mu,z}\right) = a$
iii $Z_2^T \mathcal{F}_{\mu,z} T_2 = 0$

5. *Let $d = l - a - v$. Then, on $\mathbb{L}_\mu$, rank $(F_{,\dot{z}} T_2) = d$ and there exists a smooth, full rank, matrix valued function $Z_1$ s.t. $Z_1^T F_{,\dot{z}} T_2$ has full rank*

**Remark 2.1.**

1. *If $F$ is sufficiently smooth and satisfies the hypothesis with $\mu$, $a$, $d$, $v$, $r$ then, locally, solutions to the following reduced system coincide with the original system:*

$$Z_1^T F(t, z, \dot{z}) := \hat{F}_1(t, z, \dot{z}) = 0 \qquad (d)$$
$$Z_2^T \mathcal{F}_\mu(t, z, \mathcal{H}(\overline{\omega}_0)) := \hat{F}_2(t, z) = 0 \qquad (a)$$

   *The existence of such functions is guaranteed using the implicit function theorem , see Theorem 4.13 in [15]. Here, $Z_2$ removes the components of $\mathcal{F}_\mu$ that are associated with the derived variables $\dot{z}, \ldots, z^{(\mu+1)}$ and extracts the algebraic system. Analogously, $Z_1$ extracts the differential parts of $F$.*
   *It is also possible to have a set of redundant equations in addition to the above ($\hat{F}_3 = 0$), which can be discarded. This is particularly relevant in the case of automatic model generation, where redundant constraints may form part of the original system.*
2. *The reduced system, defined above, is strangeness-free, but can still have undetermined coefficients, i.e. it is possible to have $m + n \geq a + d$.*
3. *$\omega_0$ are the free variables in the system (manifold parameters), evaluated at the linearisation point.*

**Theorem 2.1.** *Necessary condition for regularity of a control problem*
*If $F$ is sufficiently smooth and satisfies Hypothesis 1 with constant $\mu$, $a$, $d$, $v$, $r$, with $v = 0$ and $n = a + d$, and additionally*

$$\text{rank} \begin{bmatrix} \hat{F}_{1,\dot{x}} \\ \hat{F}_{2,x} \end{bmatrix} = a + d$$

*then the control problem is regular and strangeness free - which implies the problem is uniquely solvable fixing any consistent $u$, i.e. as a free system, and of d-index at most $1$.*

*Proof.*
Firstly, observe that it is sufficient to consider the reduced system locally ($\hat{F}_1, \hat{F}_2$). The proof is given in [15], and follows as the reduced order model is strangeness free so all hypothesis conditions must hold. □

**Theorem 2.2.** *Existence of a regular closed-loop system under feedback control*
*If the Hypothesis above is satisfied with constant $\mu$, $a$, $d$, $v$, $r$, and $n = a + d$, then the closed-loop problem is regular and strangeness free, with a linear state feedback controller given by:*

$$u(t) = Kx(t) + w(t)$$

*In particular, there exists a $K$ such that*

$$\text{rank} \begin{bmatrix} \hat{F}_{1,\dot{x}} \\ \hat{F}_{2,x} + \hat{F}_{2,u} K \end{bmatrix}$$

*is non-singular. The function $w(t)$ can be used to satisfy initial condition requirements on $u$.*

*Proof.*
The form follows directly from the previous theorem with $u(t) = Kx(t) + w(t)$. The existence of the matrix $K$ follows from Corollary 3.81 in [15]. $\square$

Additionally, the problems considered in this work are quasi-linear and semi-implicit [26], in that they admit the following structure (in behaviour form as before):

$$\begin{aligned} E_1(t,z)\,\dot{z}(t) &= f(t,z) \\ 0 &= h(t,z) \end{aligned} \tag{2.4}$$

For problems in the above (2.4) form, the following simpler alternative test for strangeness-free problems exists, taken from [26]:

**Theorem 2.3.** *Strangeness-free semi-implicit DAEs*
*Let $E_1(t,z) \in \mathbb{R}^{d\times m+n}$ and $h(t,z) \in \mathbb{R}^{a\times m+n}$ define a semi-implicit quasi-linear DAE as in Equation 2.4 above. Further, let the following conditions hold:*

1. *rank $(E_1) = d$ is constant for all $(t,z) = (t,x,u) \in (\mathbb{I}\times\mathbb{D}_x\times U_{ad})$*
2. *rank $(h_z) = a$ is constant for all $(t,z) = (t,x,u) \in (\mathbb{I}\times\mathbb{D}_x\times U_{ad})$, where $h_z$ is the partial derivative of $h$ with respect to the extended state variable $z$.*
3. *rank $\begin{bmatrix} E_1 \\ h_z \end{bmatrix} = d + a$ is constant (and full) for all $(t,z) = (t,x,u) \in (\mathbb{I}\times\mathbb{D}_x\times U_{ad})$*

*then, the system given by equation 2.4 is strangeness free, i.e. it satisfies Hypothesis 1 with $s = 0$ and hence has d-index at most $1$.*

*Proof.*
It will be shown, based on [26], that if a solvable DAE in the form of (2.4) fulfils the rank conditions, it will automatically satisfy Hypothesis 1 with $\mu = s = 0$.
Firstly, consider the form of the DAE, with arguments omitted:

$$0 = F = \begin{bmatrix} E_1\dot{z} - f \\ -h \end{bmatrix}$$

For this system, it is clear that:

$$\text{rank}\left(\mathcal{F}_{0,z,\dot{z}}\right) = \text{rank}\begin{bmatrix} \frac{\partial}{\partial z}\left(E_1\dot{z} - f\right) & E_1 \\ -h_z & 0 \end{bmatrix} = a + d$$

Therefore, the second hypothesis condition holds. The third condition holds by definition for $\mu = 0$. The fourth condition holds with:

$$Z_2 = \begin{bmatrix} 0 \\ \tilde{Z}_2 \end{bmatrix}$$

such that rank $\left(Z_2^T\mathcal{F}_{0,z}\right) = $ rank $\left(\tilde{Z}_2^T h_z\right) = a$, and $T_2$ satisfies the conditions with range $(T_2) = \ker(h_z)$. The third assumption gives that $F_zT_2$ will have rank $d$. $\square$

**Remark 2.2.**

1. *This formulation provides a faster and more convenient method to verify that the given problems are (or are not) strangeness-free.*
2. *The above holds equally for semi-explicit DAEs, with $E = \begin{bmatrix} I & 0 \end{bmatrix}$ and suitable splitting of $z$.*

## 2.2 Numerical Solution of Nonlinear DAEs

The numerical treatment of general DAEs in the form of (2.2) is based on well-studied methods for ODEs [15]. However, difficulties arise from problems with non-zero strangeness, including that the discretization may not have a unique solution even if the DAE does. Therefore, it may be useful or even necessary to conduct index-reduction prior to solving the equation [15], and this has been implemented automatically in some solvers such as SOLVEDAES/GENDA [16].

In the preceding section, a method for converting a general nonlinear DAE into an equivalent strangeness-free formulation is presented. In this section, numerical methods for the solution of the resulting strangeness-free formulation will be briefly discussed. Since the problems considered later will be semi-explicit, the discussion will be limited to these problems for simplicity, although the methods are not limited to these problems. Consider a DAE in the following form:

$$\begin{aligned} \dot{x} &= F_1\left(t, x, y\right) \\ 0 &= F_2\left(t, x, y\right) \end{aligned} \tag{2.5}$$

This form follows from (2.4) above, with $E = \begin{bmatrix} I & 0 \end{bmatrix}$ partitioned such that $x$ represents the state variables whose derivatives explicitly occur, while $y$ includes the remaining states (and the control in behaviour form by assumption).

It is also worth noting that finding consistent initial conditions, including suitable values for the derivatives, is required for the numerical solution of a DAE [24]. Finding such initial conditions can be achieved by a nonlinear equation solver, typically Newton's method, and this is automatically implemented in many available DAE codes, for example DASSL [6], SOLVEDAES/GENDA [16] and the Matlab® routines for DAEs [24]. However, finding suitable starting conditions can still pose difficulties, particularly for higher index problems [24]. In this work, initial conditions are found using the theory for steady-state flash problems, see Section 5.5, and so this is not considered further in this section.

For simplicity, this discussion will consider mostly constant stepsizes. This facilitates ease of notation, and many of the presented results with regard to order of accuracy are derived in terms of constant stepsizes only. However, varying (and intelligent) stepsize selection is highly important for the practical implementation of modern codes, which attempt to balance local contributions to the error in terms of the desired tolerance. Since local discretization errors can be related to the local gradient, solvers can take larger steps away from rapidly changing solutions without loss of accuracy. These approaches can be used for fully explicit d-index $1$ DAEs without modification, but can cause problems in higher-index systems [15].

### 2.2.1 Single Step Methods

The first family of methods considered here are the single-step Runge-Kutta methods. This discussion is based heavily on the review by Hairer and Wanner [13]. These can be understood be considering a generic ODE:

$$\dot{x} = f\left(t, x\right), \quad x\left(0\right) = x_0 \tag{2.6}$$

Assume that there exists a time discretization such that the time interval $[0, T]$ is divided into $t_i$, with $t_0 = 0$, and for simplicity assume a constant stepsize $h$ such that $t_{i+1} = t_i + h$. Let

$x_n \approx x(t_n)$ be the approximate solution at timestep $n$. For this system, a general Runge-Kutta method is given in terms of internal steps $X_i$, and for a method with $s$ steps the update scheme is as follows:

$$
\begin{aligned}
k_i &= f(t_n + c_i h, X_i) = \dot{X}_i \quad i = 1, 2..., s \\
X_i &= x_n + h \sum_{j=1}^{s} a_{i,j} k_j \quad i = 1, 2..., s \\
x_{n+1} &= x_n + h \sum_{i=1}^{s} b_i k_i
\end{aligned}
$$

Clearly, the method is defined fully by the vectors, $b$ and $c$, and the matrix $A$ with elements $a_{i,j}$. Different methods can be represented in Butcher-Tableau form as follows:

$$
\begin{array}{c|c}
c & A \\
\hline
 & b^T
\end{array}
$$

The presence of terms $a_{i,j}$ with $j \geq i$ distinguish implicit methods, i.e. those that require the solution of (possibly nonlinear) equations at every timestep. For example, the simplest implicit method is the Implicit Euler method, given by:

$$
\begin{array}{c|c}
1 & 1 \\
\hline
 & 1
\end{array}
$$

which gives rise to:

$$x_{n+1} = x_n + hf(t_n + h, x_n + k_1) = x_n + hf(t_{n+1}, x_{n+1})$$

A method is called stiffly accurate [13] if $b_i = a_{s,i}$ for all $i$, and this means that method maintains its order of accuracy even when solving stiff problems.

In order to extend the methods to the DAE case via a direct method, consider a perturbation of the semi-explicit DAE in (2.5):

$$
\begin{aligned}
\dot{x} &= F_1(t, x, y) \\
\varepsilon \dot{y} &= F_2(t, x, y)
\end{aligned}
$$

Applying the numerical method to this problem gives:

$$
\begin{aligned}
k_i &= F_1(t_n + c_i h, X_i, Y_i) = \dot{X}_i \quad i = 1, 2..., s \\
l_i &= F_2(t_n + c_i h, X_i, Y_i) = \varepsilon \dot{Y}_i \quad i = 1, 2..., s \\
X_i &= x_n + h \sum_{j=1}^{s} a_{i,j} k_j \quad i = 1, 2..., s \\
Y_i &= y_n + h \sum_{j=1}^{s} a_{i,j} l_j \quad i = 1, 2..., s \\
x_{n+1} &= x_n + h \sum_{i=1}^{s} b_i k_i \\
y_{n+1} &= y_n + h \sum_{i=1}^{s} b_i l_i
\end{aligned}
$$

Taking the limit as $\varepsilon \to 0$, the method for a semi-explicit DAE follows:

$$\begin{aligned} k_i &= F_1\left(t_n + c_i h, X_i, Y_i\right) \quad i = 1, 2..., s \\ 0 &= F_2\left(t_n + c_i h, X_i, Y_i\right) \quad i = 1, 2..., s \\ X_i &= x_n + h\sum_{j=1}^{s} a_{i,j} k_j \quad i = 1, 2..., s \\ x_{n+1} &= x_n + h\sum_{i=1}^{s} b_i k_i \end{aligned}$$

Theorem 5.16 from [15] gives that this systems inherits the order of accuracy from the ODE case, for a stiffly accurate Runge-Kutta method with invertible matrix $A$ .

Of interest are a subset of implicit Runge-Kutta methods called collocation methods, which can be understood in terms of the following general idea. First, a set of collocation nodes are selected in the area of interest, and then a finite space of candidate solutions is chosen; typically a number polynomials of a given order. The coefficients of the polynomials are then determined in order to satisfy the ODE/DAE at the collocation nodes [13], as well as to chain continuously with the other polynomials. The simplest collocation method is the trapezoidal rule, which can be viewed as solution by piecewise parabolas that satisfy the ODE/DAE at the node the points, and is given by the following tableau:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \tag{2.7}$$

An important consideration in the use of collocation methods is the choice of collocation points, which are chosen according to different integral quadrature rules. A popular family of methods for DAEs are the implicit methods based on Radau quadrature known as Radau IIA methods. The first such methods were proposed by Butcher in [7], but proved to have poor damping and stability properties [13]. The so-called Radau IIA methods were extended by Ehle [9] to have improved stability properties. The methods possess an order of accuracy of $2s-1$ for ODEs, where $s$ is the number of stages. The methods of $3^{rd}$ and $5^{th}$ order are as follows [13]:

$$\begin{array}{c|cc} \frac{1}{3} & \frac{5}{12} & -\frac{1}{12} \\ 1 & \frac{3}{4} & \frac{1}{4} \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array} \qquad \begin{array}{c|ccc} \frac{4-\sqrt{6}}{10} & \frac{88-7\sqrt{6}}{360} & \frac{269-169\sqrt{9}}{1800} & \frac{-2+3\sqrt{6}}{225} \\ \frac{4+\sqrt{6}}{10} & \frac{269+169\sqrt{9}}{1800} & \frac{88+7\sqrt{6}}{360} & \frac{-2-3\sqrt{6}}{225} \\ 1 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \\ \hline & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \end{array}$$

It is shown in [15] that these Radau IIA methods retain their order of accuracy when applied to strangeness free DAEs (under the assumption of constant stepsize).

Radau quadrature is not the only possibility. The trapezoidal rule ((2.7) above) belongs to a class of collocation methods based on Lobatto quadrature [12]. These methods have the following structure (in terms of the Butcher Tableau):

$$a_{1,j} = 0 \qquad a_{s,j} = b_j$$

The methods of $4^{th}$ and $6^{th}$ order are as follows [13]:

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{5}{24} & \frac{1}{3} & \frac{-1}{24} \\ 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array} \qquad \begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2}-\frac{\sqrt{5}}{10} & \frac{11-\sqrt{5}}{120} & \frac{25-\sqrt{5}}{120} & \frac{25-13\sqrt{5}}{120} & \frac{-1+\sqrt{5}}{120} \\ \frac{1}{2}+\frac{\sqrt{5}}{10} & \frac{11-sqrt5}{120} & \frac{25+13\sqrt{5}}{120} & \frac{25+\sqrt{5}}{120} & \frac{-1-\sqrt{5}}{120} \\ 1 & \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12} \\ \hline 1 & \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12} \end{array}$$

These methods are stiffly accurate and have ODE accuracy order $2s-2$ for a method with $s$ stages [12]. Note however, that the first stage is "free" as $X_1 = x_n$, so they should be compared in terms of computational work to other methods of $s-1$ stages. These methods have worse analytical stability properties compared to Radau IIA methods, and hence can have tight stepsize restrictions. However, these are mitigated in practice by use of adaptive stepsizes, where small steps are taken near rapid changes to ensure accuracy and then the stepsize is relaxed away from fast transience. In testing on numerous examples, [12] showed that adaptive Lobatto methods have similar performance to existing Radau-type and BDF codes for singularly perturbed ODEs. However, [2] has reported on serious difficulties arising in solving particular stiff DAEs, even of d-index $1$, using symmetric (Lobatto) methods. This is reportedly due to undamped error terms arising for certain pathological cases. It is unclear if this effect is likely to be encountered in practice.

### 2.2.2 Linear Multi-step Methods

Another approach applied to the solution of DAEs is to use multistep methods, which estimate the value of the discrete solution at timestep $n$ in terms of the values at multiple, normally preceding, timesteps (as opposed to only at $t_{n-1}$, as in the single step methods above). Typically a linear combination of the previous states is used, which for an ODE as per (2.6) can be expressed as:

$$\sum_{i=0}^{k} \alpha_{k-i} x_{n-i} = h \sum_{i=0}^{k} \beta_{k-i} f\left(t_{n-i}, x_{n-i}\right)$$

In order for the method to give an expression for $x_n$ and consist of $k$ steps, it is required that $\alpha_k \neq 0$ and ${\alpha_0}^2 + {\beta_0}^2 \neq 0$ [15]. An intuitive way to select these coefficients is to replace the differential term with the analytic derivative of the polynomial interpolating the solution points $x_{n-k}$ to $x_n$ [6]. This then gives an implicit nonlinear equation to solve for $x_n$ at each step. These methods are called backwards difference formulae (BDF) methods and are often considered the most successful method for solving low index DAEs [6]. They are implemented in many codes such as DASSL [6], SOLVEDAES/GENDA (optional) [15] and implemented in Matlab® as an option for *ode15s* [23]. These methods all have $\beta_k = 1$ and $\beta_i = 0\ \forall i \neq k$, posses an order of accuracy of $k$ in the ODE case, and have declining stability properties with increasing order [6].

BDF methods are stable up to order $k < 7$ [6], and the set of coefficients $\alpha_{k-i}$ are given as follows [15]:

| | $i=0$ | $i=1$ | $i=2$ | $i=3$ | $i=4$ | $i=5$ | $i=6$ |
|---|---|---|---|---|---|---|---|
| $k=1$ | $1$ | $-1$ | | | | | |
| $k=2$ | $\frac{3}{2}$ | $-2$ | $\frac{1}{2}$ | | | | |
| $k=3$ | $\frac{11}{6}$ | $-3$ | $\frac{3}{2}$ | $-\frac{1}{3}$ | | | |
| $k=4$ | $\frac{25}{12}$ | $-4$ | $3$ | $-\frac{4}{3}$ | $\frac{1}{4}$ | | |
| $k=5$ | $\frac{137}{60}$ | $-5$ | $5$ | $-\frac{10}{3}$ | $\frac{5}{4}$ | $-\frac{1}{5}$ | |
| $k=6$ | $\frac{147}{6}$ | $-6$ | $\frac{15}{2}$ | $-\frac{20}{3}$ | $\frac{15}{4}$ | $-\frac{6}{5}$ | $\frac{1}{6}$ |

The extension of such methods directly to explicit DAEs as in the from of (2.5) above follows in the same was as indicated for Runge-Kutta methods. Starting with a system of ODEs:

$$\begin{aligned} \dot{x} &= F_1\left(t, x, y\right) \\ \varepsilon\dot{y} &= F_2\left(t, x, y\right) \end{aligned}$$

Applying a BDF method to this system gives:

$$\begin{aligned} \sum_{i=0}^{k} \alpha_{k-i} x_{n-i} &= hF_1\left(t_n, x_n, y_n\right) \\ \varepsilon \sum_{i=0}^{k} \alpha_{k-i} y_{n-i} &= hF_2\left(t_n, x_n, y_n\right) \end{aligned}$$

Then, applying the limit $\varepsilon \to 0$ gives the direct application of the BDF method to an explicit DAE:

$$\begin{aligned} \sum_{i=0}^{k} \alpha_{k-i} x_{n-i} &= hF_1\left(t_n, x_n, y_n\right) \\ 0 &= F_2\left(t_n, x_n, y_n\right) \end{aligned}$$

Since such a method requires knowledge of $k-1$ preceding timesteps, at the beginning of the integration, the method must determine the initial few values using a different routine, for example implicit Euler. Therefore, despite the higher accuracy of the BDF method chosen, this can have serious consequences if the stepsize for this initial method is incorrectly specified, particularly for index $3$ or higher problems - as illustrated in examples in [6].

As before, theoretical results exist giving the applicability of these methods to strangeness-free DAEs, in particular Theorem $5.27$ in [15] gives that the BDF methods listed above maintain their order of accuracy when applied to strangeness free, regular DAEs as long as all of the required initial steps $(x_0, ... x_{n-1})$ are consistent.

# 3 System 1 Analysis

This section considers System 1, as given in Section 1.1 above, using the analytical tools presented in Section 2.1. First, the problem is posed as a system of DAEs in the behaviour setting. Then, the strangeness index of the system is determined in terms of requirements on the external empirical functions $K_i$, $\psi$ and $\rho$. Finally, consideration is given to the regularity of the resulting free and closed-loop systems.

## 3.1 Posing System 1 as a DAE in Behaviour Form

For System 1, let the variables be coded as $z_i$, with the index as follows:

Table 1: Variable assignment in behaviour form for System 1

| Index | Original Variable | Comments |
|---|---|---|
| $1, 2..N_c$ | $M_i$ | Molar hold-up of species $i$ |
| $N_c+1, N_c+2 ...2N_c$ | $x_i$ | Liquid fraction of species $i$ |
| $2N_c+1, 2N_c+2 ...3N_c$ | $y_i$ | Vapour fraction of species $i$ |
| $3N_c+1, 3N_c+2$ | $M_l$, $M_v$ | Phase molar hold-ups |
| $3N_c+3$ | $M$ | Total mass |
| $3N_c+4, 3N_c+5$ | $L(t)$, $V(t)$ | Phase outflows |
| $3N_c+6, 3N_c+7$ | $T$, $P$ | Temperature and pressure |

The inhomogeneities, which are considered to be specified externally, will be denoted as $\phi_i$ for $i = 1, 2...N_c + 2$, with the following indices:

Table 2: Inhomogeneity assignment in behaviour form for System 1

| Index | Original Variable | Comments |
|---|---|---|
| $1, 2..N_c$ | $F(t)w_i(t)$ | Inflow of species $i$ |
| $N_c+1$ | $C_T$ | Tank volume |
| $N_c+2$ | $P_{out}$ | Outlet pressure |

This enables System 1 to be written in behaviour form:

$$0 = \frac{dz_i}{dt} - \phi_i + z_{(3N_c+4)}z_{(N_c+i)} + z_{(3N_c+5)}z_{(2N_c+i)} \quad i = 1, 2..N_c \tag{3.1}$$

$$0 = z_i - z_{(3N_c+1)}z_{(N_c+i)} - z_{(3N_c+2)}z_{(2N_c+i)} \quad i = 1, 2..N_c \tag{3.2}$$

$$0 = z_{(2N_c+i)} - K_i\left(z_{(3N_c+6)}, z_{(3N_c+7)}\right) z_{(Nc+i)} \quad i = 1, 2..N_c \tag{3.3}$$

$$0 = z_{(3N_c+3)} - \sum_{i=1}^{N_c} z_i \tag{3.4}$$

$$0 = z_{(3N_c+3)} - z_{(3N_c+1)} - z_{(3N_c+2)} \tag{3.5}$$

$$
\begin{aligned}
0 =& \phi_{(Nc+1)} - z_{(3N_c+2)} \left(\rho_v \left(z_{(3N_c+6)}, z_{(3N_c+7)}, z_{(2Nc+1)}, z_{(2Nc+2)} \dots z_{(3N_c)}\right)\right)^{-1} && (3.6)\\
& - z_{(3N_c+1)} \left(\rho_l \left(z_{(3N_c+6)}, z_{(3N_c+7)}, z_{(Nc+1)}, z_{(Nc+2)} \dots z_{(2N_c)}\right)\right)^{-1} && (3.7)\\
0 =& z_{(3N_c+4)} - \psi_L \left(z_{(3N_c+7)}, z_{(3N_c+3)}\right) && (3.8)\\
0 =& z_{(3N_c+5)} - \psi_V \left(z_{(3N_c+7)} - \phi_{(N_c+2)}\right) && (3.9)\\
0 =& \sum_{i=1}^{N_c} \left(K_i \left(z_{(3N_c+6)}, z_{(3N_c+7)}\right) - 1\right) z_{(Nc+i)} && (3.10)
\end{aligned}
$$

Let the above equations define a nonlinear descriptor system with $F(t, z, \dot{z}) = 0$, where $\dot{z}$ represents the time derivative of the state variable $z$. $F$ is a system consisting of $3N_c + 6$ equations.

Formally, $F : \mathbb{I} \times \mathbb{D}_z \times \mathbb{D}_{\dot{z}} \mapsto \mathbb{R}^{3N_c+6}$, with $\mathbb{D}_z \subset \mathbb{R}^{3N_c+7}$, $\mathbb{D}_{\dot{z}} \subset \mathbb{R}^{3N_c+7}$ and $\mathbb{I} = [0, T]$.

In order to assess the strangeness index of the problem, the derivative array must be formed. Hence, the ordinary time derivative of the equations in (3.1-3.10) is given in Appendix A.1 as Equations (A.1-A.9). This system is referred to as $\dot{F}(t, z, \dot{z})$ for ease of notation, and defines an operator $\dot{F} : \mathbb{I} \times \mathbb{D}_z \times \mathbb{D}_{\dot{z}} \mapsto \mathbb{R}^{3N_c+6}$. Together, these equations define a derivative array as per Hypothesis 1.

At this point, it is requited to introduce some assumptions about the admissible states $\mathbb{D}_z$ and $\mathbb{D}_{\dot{z}}$, the external functions, and the inhomogeneities $\phi_i$.

**Assumption 3.1.** *System 1 assumptions*

1. *The allowed states $\mathbb{D}_z \subset \mathbb{R}^{3N_c+7}$ are such that:*

$$
\begin{aligned}
&z_i \in \mathbb{R}^+ && \forall i \in \{1, 2 \dots, N_c\} \cup \{3N_c + 1, 3N_c + 2 \dots, 3N_c + 7\}\\
&z_i \in \mathbb{R}^+ \cup \{0\} && \forall i \in \{N_c + 1, N_c + 2 \dots, 3N_c\}
\end{aligned}
$$

   *where $\mathbb{R}^+$ is the positive real axis.*
2. *The phase densities $\rho$, the equilibrium coefficients $K_i$ and the outflows $\psi$ satisfy:*

$$
\begin{aligned}
&\rho_v : \left(\mathbb{D}_{\{z_{2N_c+1}, \dots, z_{3N_c}\} \cup \{z_{3N_c+6}, z_{3N_c+7}\}} \subset \mathbb{D}_z\right) \mapsto \mathbb{R}^+\\
&\rho_l : \left(\mathbb{D}_{\{z_{N_c+1}, \dots, z_{2N_c}\} \cup \{z_{3N_c+6}, z_{3N_c+7}\}} \subset \mathbb{D}_z\right) \mapsto \mathbb{R}^+\\
&K_i : \left(\mathbb{D}_{\{z_{3N_c+6}, z_{3N_c+7}\}} \subset \mathbb{D}_z\right) \mapsto \mathbb{R}^+ && \forall i \in \{1, 2 \dots, N_c\}\\
&\psi_v : \left(\mathbb{D}_{z_{3N_c+7}} \subset \mathbb{D}_z\right) \mapsto \mathbb{R}^+\\
&\psi_l : \left(\mathbb{D}_{\{z_{3N_c+3}\} \cup \{z_{3N_c+7}\}} \subset \mathbb{D}_z\right) \mapsto \mathbb{R}^+
\end{aligned}
$$

3. *Further, all required partial derivatives of $\rho_l, \rho_v$ and $K_i$ are assumed to exist, which requires regularity of the equilibrium and phase equations.*

**Remark 3.1.** *Physical implications of Assumptions 3.1*

1. *Assumptions 1 and 2 require the existence of two phases, i.e. the system does not allow for the degenerate case where the conditions are out of the two-phase regime, and one of the phase hold-ups is zero. This case is trivially solved by setting the single phase outflow and composition equal to the input. Difficulties arise when the mass hold-ups* $z_{3N_c+1}$ *and* $z_{3N_c+2}$ *are different orders of magnitude [5]. Unfortunately, due to lower density of the gas phase in general, this is a common occurrence and motivates the assumptions that lead to System 2. This difficulty is readily apparent from the Jacobian analysis in Appendix A.3, where a small value of* $M_v = z_{3N_c+1}$ *directly implies ill-conditioned blocks* $J_{2,2}$ *and* $J_{6,6}$.
2. *Assumption 2 requires that all of the components have non-zero equilibrium coefficients, which is true from a physical perspective. However, equilibrium coefficients of "heavy" non-distributing components can be many orders of magnitude lower than other components in the system. This leads to extremely ill-conditioned blocks in the Jacobian system, such as block* $J_{32}$*, and can make the resulting problem stiff [5].*

## 3.2 Solvability

In the course of the investigation of the solvability of System 1, a set of additional criteria were determined, which dictate the index behaviour of the system. In the interest of brevity, an additional assumption is defined here, and the following work will characterise the behaviour of the system if the following holds:

**Assumption 3.2.** *System 1 extended assumptions*
*In addition to Assumptions 3.1, assume that the following terms are not simultaneously zero, i.e. given*

$$
\begin{aligned}
\alpha_1 &:= z_{(3N_c+2)}\rho_v^{-2}(\cdot)\frac{\partial\rho_v(\cdot)}{\partial z_{(3N_c+6)}} + z_{(3N_c+1)}\rho_l^{-2}(\cdot)\frac{\partial\rho_l(\cdot)}{\partial z_{3N_c+6}} \\
\alpha_2 &:= z_{(3N_c+2)}\rho_v^{-2}(\cdot)\frac{\partial\rho_l(\cdot)}{\partial z_{(3N_c+7)}} + z_{(3N_c+1)}\rho_l^{-2}(\cdot)\frac{\partial\rho_l(\cdot)}{\partial z_{(3N_c+7)}} \\
\alpha_3 &:= \sum_{i=1}^{N_c}\left(\frac{\partial K_i\left(\cdot\right)}{\partial z_{(3N_{c+6})}} z_{(Nc+i)}\right) \\
\alpha_4 &:= \sum_{i=1}^{N_c}\left(\frac{\partial K_i\left(\cdot\right)}{\partial z_{(3N_{c+7})}} z_{(Nc+i)}\right) \\
\xi_{7,i} &:= K_i - 1, \quad i = 1, 2 \ldots N_c
\end{aligned}
$$

*it holds that the row vector:*

$$
\begin{bmatrix} \xi_{7,1} & \xi_{7,2} & \cdots & \xi_{7,N_c} & \alpha_3 & \alpha_4 \end{bmatrix}
$$

*is non-zero* $\forall t, z \in \mathbb{I} \times \mathbb{D}_z$*, and further, if anywhere the above holds with* $\alpha_3 = \alpha_4 = 0$*, then additionally it is required that:*

$$
|\alpha_1| + |\alpha_2| > 0,\ \forall (t, z) \in \{(t, z) \in (\mathbb{I} \times \mathbb{D}_z)\,;\, \alpha_3\left(t, z\right) = \alpha_4\left(t, z\right) = 0\}
$$

**Remark 3.2.** *On the extended assumptions for System 1*

1. *Note that Assumption 3.2 is stronger than the physical assumptions given in Assumption 3.1.*
2. *The physical interpretation of* $\alpha_3, \alpha_4 \neq 0$ *is that the vapour-liquid equilibrium coefficient* $K_i$ *has a non-zero dependence on either temperature or pressure. Note that under the physical assumptions (3.1), the molar liquid fractions* $z_{N_c+i}$ *are non-negative, and under natural physical assumptions it should hold that* $\frac{\partial K_i}{\partial T} > 0$*, while* $\frac{\partial K_i}{\partial P} < 0$*, so there is no possibility of cancellation. From a modelling perspective, the equilibiurm is strongly a function of both temperature and pressure [21], and hence these are not restrictive assumptions at all.*
3. *If both* $\alpha_3$ *and* $\alpha_4$ *are zero, the conditions of Assumption 3.2 can still hold, as long as* $K_i \neq 1\, \forall i$ *and* $\alpha_1, \alpha_2$ *are not both zero. The case where* $K_i = 1$ *is of some physical interest, as it corresponds to an azeotrope [21, 22], a case where the equilibrium functions combine in a particularly pathological fashion, and the liquid and vapour products contain equal fractions of the species in question. In this case, no useful separation occurs, and hence care must be taken when operating separators near azeotropic conditions. It is perhaps appropriate that structural issues in the mathematical analysis occur under the same conditions.*

4. *The condition on $\alpha_1$, $\alpha_2$ follows if the phase densities $\rho_v$ and $\rho$ depend on at least one of $T$ or $P$. These conditions make intuitive sense in the context of the model. If temperature and pressure are able to influence the system via the equilibrium coefficient $K_i$, then the assumption holds with $\alpha_3$, $\alpha_4 \neq 0$. If this does not hold, the effect of $T$ and $P$ must still be felt in the phase densities.*

Here, the solvability concepts presented above are applied to System 1. In order to test Hypothesis 1, the following lemmas about the structure of the Jacobian of the derivative array are required:

**Lemma 3.1.** *Structure of the Jacobian of the derivative array*
*The matrix $\mathcal{F}_{1|[z,\dot{z},\ddot{z}]} \in \mathbb{R}^{(6N_c+12)\times(6N_c+14)}$ for the system defined by (3.1-3.10) is given as follows:*

$$\mathcal{F}_1|_{z,\dot{z},\ddot{z}} = \begin{array}{c} \begin{bmatrix} 0 & J_{1,2} & J_{1,3} & J_{1,4} & I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ I_{N_C} & J_{2,2} & J_{2,3} & J_{2,4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & J_{5,2} & J_{5,3} & J_{5,4} & 0 & J_{5,6} & J_{5,7} & J_{5,8} & I_{N_c} & 0 & 0 & 0 \\ 0 & J_{6,2} & J_{6,3} & J_{6,4} & I_{N_c} & J_{6,6} & J_{6,7} & J_{6,8} & 0 & 0 & 0 & 0 \\ 0 & J_{7,2} & 0 & J_{7,4} & 0 & J_{7,6} & I_{N_C} & J_{7,8} & 0 & 0 & 0 & 0 \\ J_{8,1} & J_{8,2} & J_{8,3} & J_{8,4} & J_{8,5} & J_{8,6} & J_{8,7} & J_{8,8} & 0 & 0 & 0 & 0 \end{bmatrix} \end{array} \begin{array}{c} (N_c) \\ (N_c) \\ (N_c) \\ (6) \\ (N_c) \\ (N_c) \\ (N_c) \\ (6) \end{array} \tag{3.11}$$

*Closed expressions for each block of this matrix are provided in Appendix A.3.*

*Proof.*
The result follows from direct computation, and is given in full in Appendix A.3. □

**Lemma 3.2.** *Ranks of Jacobians*
*Under Assumption 3.1, along the additional Assumption 3.2, the following matrix ranks are constant:*

1. *rank* $(\mathcal{F}_0|_{z,\dot{z}}) = 3N_c + 6$
2. *rank* $(\mathcal{F}_0|_{\dot{z}}) = \mathcal{M}_0 = N_c$
3. *rank* $(\mathcal{F}_1|_{z,\dot{z},\ddot{z}}) = 6N_c + 12$
4. *rank* $(\mathcal{F}_1|_{\dot{z},\ddot{z}}) = \mathcal{M}_1 = 4N_c + 6$

*Proof.*
The result follows from a series of elementary row operations, and is given in full in Appendix A.4. □

**Theorem 3.1.** *System 1 strangeness index*
*Under Assumption 3.1, the DAE system defined by (3.1-3.10) has a well-defined strangeness index $s = 0$, with $v = 0$, $d = N_c$ and $a = 2N_c + 6$ as per Hypothesis 1 if, and only if, Assumption 3.2 is also satisfied.*

*Proof.*

1. The manifold
$$\mathbb{L}_0 = \{z \in \mathbb{I} \times \mathbb{D}_z \times \mathbb{D}_{\dot{z}} | F_0(z) = 0\}$$
is embedded in $\mathbb{R}^{2(3N_c+7)+1}$ with $r = (3N_c + 6)$ equations specified, which gives a manifold dimension $3N_c + 10$.
2. The rank condition rank $(\mathcal{F}_1|_{z,\dot{z},\ddot{z}}) = r = (3N_c + 6)$ follows from Lemma 3.2.
3. The third condition is satisfied with $\nu = 0$ as $F_{|z,\dot{z}}$ has full row rank.

4. rank $\left(F_{[\dot{z}]}\right) = N_c = r - a \implies a = 2N_c + 6$, by Lemma 3.2. It follows $Z_2$ should have dimension $(3N_c + 6) \times (2N_c + 6)$ and $T_2$ should have dimension $(3N_c + 7) \times (N_c + 1)$. Suitable matrices $Z_2$ and $T_2$ are given as follows:

$$Z_2 = \begin{array}{cc} \begin{bmatrix} 0 & 0 & 0 \\ I_{N_c} & 0 & 0 \\ 0 & I_{N_c} & 0 \\ 0 & 0 & I_6 \end{bmatrix} & \begin{array}{c} (N_c) \\ (N_c) \\ (N_c) \\ (6) \end{array} \end{array} \in \mathbb{R}^{3N_c+6\times 2Nc+6} \tag{3.12}$$

$$T_2 = \begin{array}{cc} \begin{bmatrix} X_1 & v_1 \\ X & 0 \\ X_2 & v_2 \\ Y & v \end{bmatrix} & \begin{array}{c} (N_c) \\ (N_c) \\ (N_c) \\ (7) \end{array} \end{array} \in \mathbb{R}^{3N_c+7\times N_c+1} \tag{3.13}$$

The determination of these matrix elements and verification that they satisfy the requirements given in Hypothesis 1 is non-trivial and is presented in detail in Appendix A.5. The expressions are derived for the case where $\alpha_3,\ \alpha_4 \neq 0$. However, a similar form is apparent if Assumption 3.2 holds with $\alpha_1,\ \alpha_2 \neq 0$ and $K_i \neq 1$.

5. According to the Hypothesis, $d = l - a - v = 3Nc + 6 - 2N_c + 6 = N_c$, and this should match the rank of $F_{\dot{z}} T_2$. This condition is satisfied for the $T_2$ given in (3.13), and this is verified in Appendix A.5. A suitable matrix $Z_1$ is given as:

$$Z_1 = \begin{bmatrix} I_{N_c} \\ 0 \\ 0 \end{bmatrix} \in \mathbb{R}^{3N_c+6\times N_c} \tag{3.14}$$

$\square$

Also note that System 1, as defined by Equations (3.1-3.10), can be written explicitly in terms of the derivatives in the form of (2.4), that is:

$$\begin{aligned} E_1 \dot{z} &= f_1(t, z) \\ 0 &= h(t, z) \end{aligned}$$

Where:

$$E_1 = \begin{bmatrix} -I_{N_c} & 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{N_c \times 3N_c+7} \tag{3.15}$$

$$f_1(t, z) = \begin{bmatrix} -\phi_1(t) + z_{(3N_c+4)} z_{(N_c+1)} + z_{(3N_c+5)} z_{(2N_c+1)} \\ -\phi_2(t) + z_{(3N_c+4)} z_{(N_c+2)} + z_{(3N_c+5)} z_{(2N_c+2)} \\ \vdots \\ -\phi_{N_c}(t) + z_{(3N_c+4)} z_{(N_c+N_c)} + z_{(3N_c+5)} z_{(2N_c+N_c)} \end{bmatrix} \tag{3.16}$$

$$
h(t,z) = \begin{bmatrix} z_1 - z_{(3N_c+1)}z_{(N_c+1)} - z_{(3N_c+2)}z_{(2N_c+1)} \\ \vdots \\ z_{N_c} - z_{(3N_c+1)}z_{(2N_c)} - z_{(3N_c+2)}z_{(3N_c)} \\ z_{(2N_c+1)} - K_1(\cdot)\, z_{(Nc+1)} \\ \vdots \\ z_{(3N_c)} - K_{N_c}(\cdot)\, z_{(2Nc)} \\ z_{(3N_c+3)} - \sum_{i=1}^{N_c} z_i \\ z_{(3N_c+3)} - z_{(3N_c+1)} - z_{(3N_c+2)} \\ \phi_{(Nc+1)}(t) - z_{(3N_c+2)}\left(\rho_v(\cdot)\right)^{-1} - z_{(3N_c+1)}\left(\rho_l(\cdot)\right)^{-1} \\ z_{(3N_c+4)} - \psi_L(\cdot) \\ z_{(3N_c+5)} - \psi_V(\cdot) \\ \sum_{i=1}^{N_c}\left(K_i(\cdot) - 1\right) z_{(Nc+i)} \end{bmatrix} \tag{3.17}
$$

This is in fact a semi-explicit formulation of the DAE. As shown in Appendix A.6, the DAE system comprising of (3.15-3.17) only has an s-index of $0$ if the following block is non-singular (see Equation A.16 and the derivation thereof):

$$
\begin{bmatrix} (\alpha_{23} - \alpha_{22}) & \alpha_{24} & \alpha_{25} \\ (\alpha_{27} - \alpha_{26}) & \alpha_{28} & \alpha_{29} \end{bmatrix} \tag{3.18}
$$

Clearly, under Assumption 3.1 and the additional conditions in Assumption 3.2, the system is known to be strangeness index $0$. Therefore, it must hold that this block has full rank. However, it is of interest to explore the possibility of this block being poorly scaled - i.e. numerically close to a rank deficient matrix.

**Corollary 3.1.** *Semi-explicit representation of strangeness index for System 1*
*If the block matrix given in (3.18) above (and as (A.16) in Appendix A.6) , with terms defined in Appendix A.2, is non-singular, then the DAE system given in (3.1-3.10) corresponding to (3.15-3.17), satisfies the conditions of Theorem 2.3, and hence is strangeness free and of d-index at most* $1$.

*Proof.*
The proof is given in Appendix A.6. □

If these expressions are formed explicitly:

$$
\alpha_{23} - \alpha_{22} = \left( \sum_{i=1}^{N_c} \frac{\left(\xi_{1,i} + K_i(\cdot)\,\xi_{2,i}\right)\left(z_{(N_c+i)} - z_{(2N_c+i)}\right)}{-\left(z_{(3N_c+1)} + K_i(\cdot)\, z_{(3N_c+2)}\right)} \right) - \left(\rho_v^{-1}(\cdot) - \rho_l^{-1}(\cdot)\right)
$$

$$
\alpha_{27} - \alpha_{26} = \left( \sum_{i=1}^{N_c} \frac{\left(K_i(\cdot) - 1\right)\left(z_{(N_c+i)} - z_{(2N_c+i)}\right)}{-\left(z_{(3N_c+1)} + K_i(\cdot)\, z_{(3N_c+2)}\right)} \right)
$$

As defined in Appendix A.2, $\xi_{1,i}$ depends on $\frac{\partial \rho_l(\cdot)}{\partial z_{(N_c+i)}}$ and $\xi_{2,i}$ depends on $\frac{\partial \rho_v(\cdot)}{\partial z_{(2N_c+i)}}$. In both cases, so long as there is a mixing rule in place, i.e. a dependence of the mixture molar density on composition in either phase, these terms will not be zero. Additionally, the inverse densities (i.e., molar volumes) are not physically likely to be near equal unless the operation is near the supercritical region. Therefore, there is no physically relevant case with two distinct phases where the first element is likely to be near zero. The denominator is non-zero by Assumption 3.1. The remaining elements in the first row are:

$$\alpha_{24} = -z_{(3N_c+2)} \sum_{i=1}^{N_c} \frac{\xi_{10,i}\theta_{i,1}}{\xi_{13,i}} + \alpha_1$$

$$\alpha_{25} = -z_{(3N_c+2)} \sum_{i=1}^{N_c} \frac{\xi_{10,i}\theta_{i,2}}{\xi_{13,i}} + \alpha_2$$

The remaining terms on the final row are as follows:

$$\alpha_{28} = \textstyle\sum_{i=1}^{N_c} \left[1 + \frac{(K_i(\cdot)-1)z_{(3N_c+2)}}{\left(z_{(3N_c+1)}+K_i(\cdot)z_{(3N_c+2)}\right)}\right] \left(\frac{\partial K_i(\cdot)}{\partial z_{(3N_c+6)}} z_{(N_c+i)}\right)$$
$$\alpha_{29} = \textstyle\sum_{i=1}^{N_c} \left[1 + \frac{(K_i(\cdot)-1)z_{(3N_c+2)}}{\left(z_{(3N_c+1)}+K_i(\cdot)z_{(3N_c+2)}\right)}\right] \left(\frac{\partial K_i(\cdot)}{\partial z_{(3N_c+7)}} z_{(N_c+i)}\right)$$

It is observed that $\alpha_{28}$ and $\alpha_{29}$ are dependent on partial derivatives of the vapour equilibrium function $K_i$. This is an equivalent condition to $\alpha_4$ and $\alpha_3$ not both being zero, which is easily apparent from Appendix A.2. In particular, if $K_i = 1$ , then $\alpha_{28} \rightarrow \alpha_3$ and $\alpha_{29} \rightarrow \alpha_4$. Conversely, if $\alpha_3 = \alpha_4 = 0$, it follows that $\theta_{i,1} = \theta_{i,2} = 0$ and then, $\alpha_{24} \rightarrow \alpha_1$ and $\alpha_{25} \rightarrow \alpha_2$. This shows how this condition is equivalent to Assumption 3.2 for the system to be strangeness-free.

From a physical standpoint, $K_i$ is a strong function of both temperature and pressure. Therefore, it is unlikely that these partial derivatives will be small enough to pose numerical difficulties in determining rank. Firstly, any physical system should respect $\frac{\partial K_i(\cdot)}{\partial z_{(3N_c+6)}} > 0$ as vapour pressure increases with temperature. Since most vapour-liquid equilibrium models are essentially based on modifications to Raoult's Law [21] (as given in Equation (5.3) in Section 5.1), which is exponential with respect to temperature, the sum of partial derivatives is not near zero unless all of the equilibrium constants are near zero, which suggests that the fundamental assumption of operation in a two-phase region is violated. Therefore, it does not appear likely that the system will exhibit behaviour near a system of higher strangeness index under any realisable conditions if the equilibrium function $K_i$ depends on temperature and/or pressure (as per Assumption 3.2).

Given the higher index of the related problem reported in literature [5], it is of interest to consider the system as being of index one higher, i.e. with $s = 1$. It is desired to test if, by assuming that Assumption 3.2 does not hold (at least numerically), the system would satisfy the hypothesis for $\mu = 1$. This leads to the following theorem:

**Theorem 3.2.** *System 1 with higher strangeness index*
*Under Assumption 3.1, the DAE system defined by (3.1-3.10) satisfies Hypothesis 1 with $\mu = 1$, with $v = 0$, $d = N_c$ and $a = 2N_c + 6$ if, and only if, the additional Assumption 3.2, also holds.*

*Proof.*

1. The manifold
$$\mathbb{L}_1 = \{z_1 \in \mathbb{I} \times \mathbb{D}_z \times \mathbb{D}_{\dot{z}} | \mathcal{F}_1(z_1) = 0\}$$
is embedded in $\mathbb{R}^{3(3N_c+7)+1}$ with $r = 2(3N_c+6)$ equations specified, which gives a manifold dimension $3N_c + 10$.
2. The rank condition $\operatorname{rank}(\mathcal{F}_1|_{z,\dot{z},\ddot{z}}) = r = 2(3N_c+6)$ follows from Lemma 3.2.

3. The third condition is satisfied with $\nu = 0$ as $\mathcal{F}_1|_{z,\dot{z},\ddot{z}}$ has full row rank.
4. rank $\left(\mathcal{F}_{1,[\dot{z},\ddot{z}]}\right) = 4N_c + 6 = r - a \implies a = 2N_c + 6$, by Lemma 3.2. It follows that $Z_2$ should have dimension $(6N_c + 12) \times (2N_c + 6)$ and $T_2$ should have dimension $(3N_c + 7) \times (N_c + 1)$. Suitable matrices are given below, and are motivated in Appendix A.5:

$$Z_2 = \begin{array}{c} \left[\begin{array}{ccc} 0 & 0 & 0 \\ I_{N_c} & 0 & 0 \\ 0 & I_{N_c} & 0 \\ 0 & 0 & I_6 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{array}\right] \end{array} \begin{array}{c} (N_c) \\ (N_c) \\ (N_c) \\ (6) \\ (N_c) \\ (N_c) \\ (N_c) \\ (6) \end{array} \in \mathbb{R}^{6N_c+12\times 2Nc+6}$$

$$T_2 = \left[\begin{array}{cc} X_1 & v_1 \\ X & 0 \\ X_2 & v_2 \\ Y & v \end{array}\right] \begin{array}{c} (N_c) \\ (N_c) \\ (N_c) \\ (7) \end{array} \in \mathbb{R}^{3N_c+7\times N_c+1}$$

   This is the same $T_2$ as found previously, as the matrix $\dot{F}_{\dot{z},\ddot{z}}$ has an empty left nullspace. Again, the matrix $T_2$ is given for the case where $\alpha_3,\ \alpha_4 \neq 0$, but a similar form can be derived if Assumption 3.2 holds with $\alpha_3,\ \alpha_4 = 0$ and $\alpha_1,\ \alpha_2 \neq 0$.
5. As before, the Hypothesis requires $d = l - a - v = 3Nc + 6 - 2N_c + 6 = N_c$, which is fulfilled and the same $Z_1$ defined above is suitable here as well.

□

**Remark 3.3.** *Necessary assumptions for system with $\mu = 1$*

1. *The necessity of Assumption 3.2 follows from the manipulations in Appendix A.4 and in particular the discussion around Equation (A.13). If Assumption 3.2 does not hold, the matrices in question cannot have sufficient rank to satisfy the conditions in Hypothesis 1. This is clear from the discussion around Equation (A.14).*
2. *This implies that, in the unlikely event that Assumption 3.2 does not hold, the DAE system is not strangeness 1. It may potentially have higher strangeness or not possess a well-defined index.*

**Corollary 3.2.** *Regularity of System 1 control problem*
*Viewing $z_{3N_c+6}$ (temperature) as the control, and under Assumption 3.1, System 1 in the form of (2.4) as described by (3.15-3.17), satisfies the regularity conditions in Theorem 2.1 and hence is regular as a free system if, and only if, at least one of the following hold for all $(t,z) \in (\mathbb{I} \times \mathbb{D}_z)$:*
1. $\alpha_4 \neq 0$
2. $K_i \neq 1\ i = 1,2,..N_c$ *and* $\alpha_2 \neq 0$

*Proof.*
A condition for regularity is as follows, from Theorem 2.1:

$$\text{rank}\left[\begin{array}{c} \hat{F}_{1,\dot{x}} \\ \hat{F}_{2,x} \end{array}\right] = a + d$$

Note that, per Theorem 3.1, under Assumption 3.2 , $a + d = 3N_c + 6$. For the strangeness 0 formulation, it holds that, using the form of (2.4):

$$\hat{F}_1 = F_1 = -E_1\dot{z} + f_1\left(t, z\right)$$
$$\hat{F}_2 = F_2 = h\left(t, z\right)$$

As this system is in behaviour form, with $z = \left[\begin{array}{cc} x & u \end{array}\right]$ and $E_{1,\dot{z}} = \left[\begin{array}{cc} E_{1,\dot{x}} & 0 \end{array}\right]$, it holds that:

$$-E_{1,\dot{x}} = \left[\begin{array}{cccc} I_{N_c} & 0 & 0 & 0 \end{array}\right] \in \mathbb{R}^{N_c \times 3N_c+6}$$

where the last block is shortened by one row as the control is removed. For $h_x$:

$$h_x = \left[\begin{array}{cccc} I_{N_C} & J_{2,2} & J_{2,3} & \tilde{J}_{2,4} \\ 0 & J_{3,2} & I_{N_c} & \tilde{J}_{3,4} \\ J_{4,1} & J_{4,2} & J_{4,3} & \tilde{J}_{4,4} \end{array}\right] \in \mathbb{R}^{2N_c+6 \times 3N_c+7}$$

where the tildes represent the matrix blocks after deletion of the control column. This is essentially a repeat of the analysis conducted for the semi-implicit case with a column deletion, which leads to the following conclusion if the column corresponding to the control is removed $\left(z_{(3Nc+6)}\right)$:

$$\text{rank}\left[\begin{array}{c} \hat{F}_{1,\dot{x}} \\ \hat{F}_{2,x} \end{array}\right] = a + d \iff \text{rank}\left[\begin{array}{cc} (\alpha_{23} - \alpha_{22}) & \alpha_{25} \\ (\alpha_{27} - \alpha_{26}) & \alpha_{29} \end{array}\right] = 2$$

The result then follows from the discussion and proof of Corollary 3.1 above, in particular the working in Appendix A.6. □

Clearly, the assumption on the problem being regular as free system is stricter than that of the system with the control, which can be seen because the requirement in Corollary 3.2 above implies Assumption 3.2, but not vice-versa. Additionally, it is apparent that the system can be made regular by feedback (actually any) control so long as Assumption 3.2 still applies.

# 4 System 2 Analysis

This section considers System 2, as given in Section 1.2 above, using the analytical tools presented in Section 2.1. As before, the problem is first posed as a system of DAEs in the behaviour setting. Then, the strangeness index of the system is determined in terms of requirements on the external empirical functions $K_i$ and $\psi$. Particular attention is paid to the claims of higher index behaviour reported in the literature. Finally, consideration is again given to the regularity of the resulting free and closed-loop systems.

## 4.1 Posing System 2 as a DAE in Behaviour Form

For System 2, let the variables be coded as $z_i$, with the index as follows:

Table 3: Variable assignment in behaviour form for System 2

| Index | Original Variable | Comments |
|---|---|---|
| $1, 2..N_c$ | $x_i$ | Liquid fraction of each species $i$ |
| $N_c + 1, N_c + 2 \ldots 2N_c$ | $y_i$ | Vapour fraction of each species $i$ |
| $2N_c + 1$ | $M$ | Total molar hold-up |
| $2N_c + 2, 2N_c + 3$ | $L(t),\ V(t)$ | Phase outflows |
| $2N_c + 4, 2N_c + 5$ | $T, P$ | Temperature and pressure |

The inhomogeneities, which are considered to be specified externally, will be denoted as $\phi_i$ for $i = 1, 2 \ldots N_c + 1$, with the following indices:

Table 4: Inhomogeneity assignment in behaviour form for System 2

| Index | Original Variable | Comments |
|---|---|---|
| $1, 2..N_c$ | $w_i(t)$ | Inflow fraction of each species $i$ |
| $N_c + 1$ | $F(t)$ | Total inflow |

It is important to note that the phase densities are no longer required, since the hold-up in the vessel is assumed to be only liquid. Therefore, the pressure (or some other variable) can be explicitly specified. This will be handled in a natural way using the behaviour approach by treating it as another variable in an underdetermined system.

This enables System 2 to be written in behaviour form:

$$0 = z_{(2N_c+1)}\frac{dz_i}{dt} - \phi_{(N_c+1)}\left(\phi_i - z_i\right) + z_{(2N_c+3)}\left(z_{(N_c+i)} - z_i\right) \quad i = 1, 2..N_c \tag{4.1}$$

$$0 = z_{(N_c+i)} - K_i\left(z_{(2N_c+4)}, z_{(2N_c+5)}\right) z_i \quad i = 1, 2..N_c \tag{4.2}$$

$$0 = \frac{dz_{(2N_c+1)}}{dt} - \phi_{(N_c+1)} + z_{(2N_c+2)} + z_{(2N_c+3)} \tag{4.3}$$

$$0 = z_{(2N_c+2)} - \psi_L\left(z_{(2N_c+1)}, z_{(2N_c+5)}\right) \tag{4.4}$$

$$0 = \sum_{i=1}^{N_c}\left(K_i\left(z_{(2N_c+4)}, z_{(2N_c+5)}\right) - 1\right) z_{(i)} \tag{4.5}$$

Let the above equations define a nonlinear descriptor system with $F(t, z, \dot{z}) = 0$, where $\dot{z}$ represents the time derivative of the state variable $z$. $F$ is a system consisting of $2N_c + 3$ equations.

Formally, $F : \mathbb{I} \times \mathbb{D}_z \times \mathbb{D}_{\dot{z}} \mapsto \mathbb{R}^{2N_c+3}$, with $\mathbb{D}_z \subset \mathbb{R}^{2N_c+5}$, $\mathbb{D}_{\dot{z}} \subset \mathbb{R}^{2N_c+5}$ and $\mathbb{I} = [0, T]$.

Just as before, it is required to introduce some assumptions about the allowed state spaces $\mathbb{D}_z$ and $\mathbb{D}_{\dot{z}}$, as well as the external functions, $K_i$ and $\psi$, and the inhomogeneities $\phi_i$.

**Assumption 4.1.** *System 2 assumptions*

1. *The allowed states $\mathbb{D}_z \subset \mathbb{R}^{2N_c+5}$ are such that:*

$$\begin{aligned} &z_i \in \mathbb{R}^+ && \forall i \in \{2N_c+1, 2N_c+2..., 2N_c+5\} \\ &z_i \in \mathbb{R}^+ \cup \{0\} && \forall i \in \{1, 2..., 2N_c\} \end{aligned}$$

   *where $\mathbb{R}^+$ is the positive real axis.*
2. *The outflow $\psi_L$ and the VLE coefficients $K_i$ satisfy:*

$$\begin{aligned} &\psi_L : \left(\mathbb{D}_{\{z_{2N_c+1}\}\cup\{z_{2N_c+5}\}} \subset \mathbb{D}_z\right) \mapsto \mathbb{R}^+ \\ &K_i : \left(\mathbb{D}_{\{z_{2N_c+4}, z_{2N_c+5}\}} \subset \mathbb{D}_z\right) \mapsto \mathbb{R}^+ \qquad \forall i \in \{1, 2..., N_c\} \end{aligned}$$

3. *Further, all required partial derivatives of $\psi^L$ and $K_i$ are assumed to exist, which requires regularity of the equilibrium and phase outflow functions.*

**Remark 4.1.** *Physical implications of Assumption 4.1*

1. *As in the assumptions made for System 1, Assumptions 1 and 2 require the existence of two phases and do not allow for a single phase system. Since the vapour hold-up is set to zero, it is claimed [5] that the difficulties that arise in System 1 could be prevented. Unfortunately, this is a highly non-physical assumption.*
2. *Again the second assumption only holds if all of the components have non-zero equilibrium coefficients. This is true from the physical perspective but may cause problems numerically as the equilibrium coefficients of non-distributing components can be many orders of magnitude lower than those of the light components.*

## 4.2 Solvability

This section will begin by defining the additional assumptions that will be shown to be sufficient to give index $1$ solution behaviour.

**Assumption 4.2.** *System 2 extended assumptions*
*In addition to Assumption 4.1, assume that the following terms are not simultaneously zero, i.e. given*

$$\alpha_2 := \sum_{i=1}^{N_c} \left( \frac{\partial K_i(\cdot)}{\partial z_{(3N_{c+4})}} z_i \right)$$
$$\alpha_3 := \sum_{i=1}^{N_c} \left( \frac{\partial K_i(\cdot)}{\partial z_{(3N_{c+5})}} z_i \right)$$

*it holds that the row vector:*

$$\begin{bmatrix} \alpha_3 & \alpha_4 \end{bmatrix}$$

*is non-zero $\forall t, z \in \mathbb{I} \times \mathbb{D}_z$.*

**Remark 4.2.** *On the extended assumptions for System 2*
*This condition is similar to, but more strict than, Assumption 3.2 for System 1, and all of the commentary in Remark 3.2 applies here as well. Since the phase densities do not enter in the system, there is no way for the temperature and pressure to play a role if the partial derivatives of $K_i$ with respect to these terms are zero. This is in contrast to the System 1 case, see Assumption 3.2, where the phase densities provide additional terms can prevent rank deficiency in the Jacobians.*

The solvability concepts presented in Section 2.1 are applied to System 2. In order to test Hypothesis 1, the following lemmas about the structure of the Jacobian of the derivative array are required:

**Lemma 4.1.** *Structure of the Jacobian of the derivative array*
*The matrix $\mathcal{F}_{1,[z,\dot{z},\ddot{z}]} \in \mathbb{R}^{(4N_c+6)\times(6N_c+15)}$ for the system defined by (4.1-4.5) is given as follows:*

$$\mathcal{F}_1|_{z,\dot{z},\ddot{z}} = \begin{array}{c} \begin{bmatrix} J_{1,1} & J_{1,2} & J_{1,3} & J_{1,4} & 0 & 0 & 0 & 0 & 0 \\ J_{2,1} & I_{N_c} & J_{2,3} & 0 & 0 & 0 & 0 & 0 & 0 \\ J_{3,1} & 0 & J_{3,3} & 0 & 0 & J_{3,6} & 0 & 0 & 0 \\ J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4} & J_{4,5} & J_{4,6} & J_{4,7} & 0 & 0 \\ J_{5,1} & 0 & J_{5,3} & J_{5,4} & I_{N_c} & J_{5,6} & 0 & 0 & 0 \\ J_{6,1} & J_{6,2} & J_{6,3} & J_{6,4} & 0 & J_{6,6} & 0 & 0 & J_{6,9} \end{bmatrix} \end{array} \begin{array}{c} (N_c) \\ (N_c) \\ (3) \\ (N_c) \\ (N_c) \\ (3) \end{array} \in \mathbb{R}^{4N_c+6\times 6N_c+15} \tag{4.6}$$

*Closed expressions for each block of this matrix are provided in Appendix B.3.*

*Proof.*
The result follows from direct computation, and is given in full in Appendix B.3. □

**Lemma 4.2.** *Ranks of Jacobians*
*For the system defined by (4.1-4.5) under Assumptions 4.1 and 4.2, the following matrix ranks are constant:*

1. *rank* $(\mathcal{F}_0|_{z,\dot{z}}) =$ *rank* $(F|_{z,\dot{z}}) = 2N_c + 3$
2. *rank* $(\mathcal{F}_0|_{\dot{z}}) = \mathcal{M}_0 = N_c + 1$

*Proof.*
The result follows from a series of elementary row operations and is given in full in Appendix B.4. □

**Theorem 4.1.** *System 2 strangeness index*
*Under Assumption 4.1, the DAE system defined by (4.1-4.5) has a well-defined strangeness index $s = 0$, with $v = 0$, $d = N_c + 1$ and $a = N_c + 2$ as per Hypothesis 1 if, and only if, Assumption 4.2 is also fulfilled.*

*Proof.*
In order to verify that the Hypothesis holds for $\mu = 0$, note that:

1. The manifold
$$\mathbb{L}_0 = \{z \in \mathbb{I} \times \mathbb{D}_z \times \mathbb{D}_{\dot{z}} | F_0(z) = 0\}$$
is embedded in $\mathbb{R}^{2(2N_c+5)+1}$ with $r = (2N_c + 3)$ equations specified, which gives a manifold dimension $3N_c + 8$.
2. The rank condition rank $(\mathcal{F}_0|_{z,\dot{z}}) = r = (2N_c + 3)$ follows from Lemma 4.2.
3. The third condition is satisfied with $\nu = 0$ as $F_{|z,\dot{z}}$ has full row rank.
4. rank $(F_{\dot{z}}) = N_c + 1 = r - a \implies a = N_c + 3$, by Lemma 3.2. It follows that $Z_2$ has dimension $(2N_c + 3) \times (N_c + 2)$ and $T_2$ has dimension $(2N_c + 5) \times (N_c + 4)$. Suitable matricies are derived in Appendix B.5 and found to be:
$$Z_2 = \begin{bmatrix} 0 & 0 \\ I_{N_c} & 0 \\ 0 & 0 \\ 0 & I_2 \end{bmatrix} \begin{matrix} (N_c) \\ (N_c) \\ (1) \\ (2) \end{matrix} \in \mathbb{R}^{2N_c+3 \times Nc+2}$$
$$T_2 = \begin{bmatrix} I_{N_c} & 0 \\ \tilde{Y}_1 & \tilde{Y}_2 \\ Y_1 & Y_2 \end{bmatrix} \begin{matrix} (N_c) \\ (N_c) \\ (5) \end{matrix} \in \mathbb{R}^{2N_c+5 \times Nc+3}$$
5. From Hypothesis 1, $d = l - a - v = 2Nc + 3 - N_c - 2 = N_c + 1$. It is required that rank $(F|_{\dot{z}} T_2) = d$, which is verified in Appendix B.5. A suitable matrix $Z_1$ is given as:
$$Z_1 = \begin{bmatrix} I_{Nc} & 0 \\ 0 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{matrix} (N_c) \\ (N_c) \\ (1) \\ (1) \\ (1) \end{matrix} \in \mathbb{R}^{2N_c+3 \times N_c+1}$$

□

Therefore, despite the claim that System 2 is d-index 2 in [5], this work concludes that the system defined by (4.1-4.5) is in fact strangeness-free, and hence possesses d-index at most $1$, once a suitable choice of state and control variables is made.

An equivalent check to those above is to test the conditions given in Theorem 2.3. First, note that the system defined by Equations (4.1-4.5) can be written in a semi-implicit form as follows:
$$E_1 \dot{z} = f_1(t, z)$$
$$0 = h(t, z)$$

Where:

$$E_1 = \begin{bmatrix} -z_{(2N_c+1)} I_{N_c} & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & & \cdots & 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$
$$= \begin{bmatrix} \tilde{E}_1 & 0 & \hat{E}_1 \end{bmatrix} \in \mathbb{R}^{N_c+1 \times 2N_c+5} \tag{4.7}$$

$$f_1(t,z) = \begin{bmatrix} -\phi_{(N_c+1)}(\phi_1 - z_1) + z_{(2N_c+3)}\left(z_{(N_c+1)} - z_1\right) \\ \vdots \\ -\phi_{(N_c+1)}(\phi_{N_c} - z_{N_c}) + z_{(2N_c+3)}\left(z_{(2N_c)} - z_{N_c}\right) \\ -\phi_{(N_c+1)} + z_{(2N_c+2)} + z_{(2N_c+3)} \end{bmatrix} \tag{4.8}$$

$$h(t,z) = \begin{bmatrix} z_{(N_c+1)} - K_1(\cdot) z_1 \\ \vdots \\ z_{(2N_c)} - K_{N_c}(\cdot) z_{N_c} \\ z_{(2N_c+2)} - \psi_L(\cdot) \\ \sum_{i=1}^{N_c} (K_i(\cdot) - 1) z_i \end{bmatrix} \tag{4.9}$$

As shown in Appendix B.6, the DAE system resulting from (4.7-4.9) only has an s-index of $0$ if the following vector is non-singular (not the zero vector):

$$\begin{bmatrix} \alpha_2 & \alpha_3 \end{bmatrix} \tag{4.10}$$

**Corollary 4.1.** *Semi-implicit representation of strangeness index for System 2*
*Under the assumptions that the vector given in (4.10) above is non-zero, with terms defined in Appendix B.2, then the DAE system given in (4.1-4.5) corresponding to (4.7-4.9), satisfies the conditions of Theorem 2.3, and hence is strangeness free and d-index at most $1$ once suitable controls are applied.*

*Proof.*
The proof is given in Appendix B.6. □

As before, the expressions in this block are equivalent the conditions established in Assumption 4.2, which further confirms that system can have d-index 1, in apparent contradiction with [5]. As before, this is not a strict requirement for a physical system as the equilibrium coefficient is known to be a strong function of temperature [21], and neglecting this dependence is a large simplification.

This analysis in the behaviour setting indicates that it is possible to obtain a strangeness-free system, for some choice of input (control) and state variables. In order to determine which, consider the matrix $\begin{bmatrix} E \\ h_z \end{bmatrix}$, as derived in Appendix B.6, with the columns labelled back in the physical variables:

$$\begin{array}{c} \\ (N_c) \\ (N_c) \\ (1) \\ (1) \\ (1) \end{array} \begin{array}{c} \begin{array}{ccccccc} x_1,\ldots x_{N_c} & y_1,\ldots y_{N_c} & M & L & V & T & P \end{array} \\ \begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & I_{N_c} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\partial \psi_L}{\partial M} & 1 & 0 & 0 & \frac{\partial \psi_L}{\partial P} \\ 0 & 0 & 0 & 0 & 0 & \alpha_2 & \alpha_3 \end{bmatrix} \end{array} \tag{4.11}$$

Clearly, this matrix is full rank under the conditions of Corollary 4.1 above, and hence strangeness-free as an under-determined behaviour system. However, it is apparent from the structure of (4.11) that the choice of control and state variables is limited by the column of zeros (corresponding to variable $V$). Unlike System 1, this problem has two undetermined variables, which can be interpreted either as two controls or a control and a fixed parameter.

First, consider the choice of inputs and state variables as proposed in the original source [5]. Here, temperature is viewed as the control and the pressure is fixed. If these "controls" are viewed as general inputs, the matrix (4.11) will be rank deficient once the corresponding columns are excluded. This leads to the following result:

**Corollary 4.2.** *Regularity of System 2 control problem with $u = [T, P]$*
*Viewing $[z_{2N_c+4}, z_{2N_c+5}]$ (temperature and pressure) as the controls, and under Assumptions 4.1 and 4.2, System 2 in the form of (2.4) as described by (4.7-4.9), does not satisfy the regularity conditions in Theorem 2.1, and hence is not regular as a free system or with arbitrarily chosen controls.*

*Proof.*
As before, this result follows directly from the conditions in Theorem 2.1, with the necessary condition obtained by deleting the columns corresponding to the control in the semi-implicit representation, see Appendix B.6 and (4.11) above. Here, the column of zeros leads directly to rank deficiency. □

This means that, for the choice of state and control variables in the literature, the problem is not strangeness-free. This has implications for the numerical solution of the problem, and may lead to requirements on the differentiability of the inputs. However, the behaviour analysis indicates that it is possible to arrive at a strangeness-free formulation (possibly for different choices of input).

There are two possible ways to proceed. Firstly, one may consider whether it is possible to correct this rank deficiency, and hence produce a strangeness-free system, by placing restrictions on the input functions. It turns out that it is possible to regularize this system via feedback control on the condition that the feedback depends on $V$, as this is needed to "correct" the rank deficiency in (4.11).

**Corollary 4.3.** *Regularization of System 2 DAE under feedback control with $u = [T, P]$*
*Viewing $[z_{2N_c+4}, z_{2N_c+5}]$ (temperature and pressure) as the controls, and under Assumption 4.1, System 2 in the form of (2.4) as described by (4.7-4.9), satisfies the conditions in Theorem 2.2 and hence is regular as a closed-loop system under proportional state feedback control, if and only if the elements in the feedback matrix $K$ corresponding to state variable $z_{2N_c+3}$ (vapour outflow, $V$) are non-zero.*

*Proof.*
This follows from the structure of (4.11). Under suitable feedback, defined in Corollary 4.3, $\frac{\partial T}{\partial V} \neq 0$ and hence full rank is obtained in (4.11). □

Another way to view this issue is to conclude that the component $V$ is effectively undetermined. The behaviour approach suggests that this variable should be set as an input, and therefore, for the rest of this work, the vapour rate, $V$, will be treated as a control variable and set by feedback with respect to $P$. The same physical relationship used in System 1 is applied here (i.e. $V(t) = \psi_V(P, P_{out})$, with $P_{out}$ taken as constant).

In effect, this is adding the same outlet vapour relation (Equation (3.9)) from System 1 to System 2 in place of one of the controls. The temperature will be used for control and the pressure will be treated as a state variable.

This will be done for three reasons. Firstly, this gives a d-index 1 DAE as per the following corollaries. This also presents the closest possible structural analogue to System 1, which facilitates easy comparison between the systems. Lastly, this makes sense from a physical standpoint as the vapour outlet rate should depend on the pressure differential across the valve. This discussion motivates the following corollaries:

**Corollary 4.4.** *Regularity of System 2 control problem with* $u = [V, T]$
*Viewing* $[z_{2N_c+3}, z_{2N_c+4}]$ *(vapour outflow and temperature) as the controls, and under Assumption 4.1 and additionally requiring* $\alpha_3 \neq 0$*, System 2 in the form of (2.4) as described by (4.7-4.9),satisfies the regularity conditions in Theorem 2.1, and hence is regular as a free system.*

**Corollary 4.5.** *Regularization of System 2 DAE under feedback control with* $u = [V, T]$
*Again viewing* $[z_{2N_c+3}, z_{2N_c+4}]$ *(vapour outflow and temperature) as the controls, and under Assumption 4.1 and additionally requiring* $\alpha_3 \neq 0$*, System 2 in the form of (2.4) as described by (4.7-4.9), satisfies the conditions in Theorem 2.2 for any* $K$ *and hence is regular as a closed-loop system under proportional state feedback control*

*Proof.*
This follows from the preceding discussion and the form of (4.11). The additional requirement of $\alpha_3 \neq 0$ is analogous to Assumption 4.2 above, when the temperature control is ignored (i.e. in order to maintain full row rank of (4.11) when the temperature column is excluded). □

Of course, the choice of input variable in the simulation has no bearing on the physical, real-world system. It is not guaranteed that $V$ is available as a control, or that it can be measured with sufficient accuracy to be used for feedback control (or that it can be measured at all). As this work does not concern a specific physical vessel, it is impossible to conclude whether such instrumentation is available. However, in general, controlling vapour outflow rate can be achieved relatively easily by a control valve. In fact, this is a standard, practical method for regulating pressure inside process units [25], so this does not seem like a physically unrealistic expectation.

# 5 Sample Problem: Hydrocarbon Flash

The analysis given previously is now applied to create a d-index 1 model of the isothermal flash separation of mixed alkanes. In order to describe a physically relevant case, suitable closure models are required. As this work is focussed more on the structural aspects of the underlying DAE systems, an effort is made to restrict these closures to the simplest examples of their type, although in principle much more complicated models could be used.

## 5.1 Vapour-liquid Equilibrium

The fundamental tool for describing the interphase thermodynamic equilibrium between liquid and vapour mixtures is the equilibrium condition [21]:

$$\bar{f}_i^L\left(T,P,x_1,x_2...,x_{N_c}\right)=\bar{f}_i^V\left(T,P,y_1,y_2...,y_{N_c}\right) \tag{5.1}$$

This states that the fugacity of the species $i$ in the mixture is equal in both phases. The fugacity can be understood as the relative equilibrium contribution of each phase. For the vapour phase, the fugacity is defined relative to the partial pressure of the pure component ($y_iP$), and the fugacity coefficient $\bar{\phi}_i^V$:

$$\bar{f}_i^V\left(T,P,y_1,y_2...,y_{N_c}\right)=\bar{\phi}_i^V\left(T,P,y_1,y_2...,y_{N_c}\right)y_iP$$

For the liquid phase, if an equation of state (EOS) is available, the same formulation applies. However, in the absence of a reliable liquid phase equation of state, a common approach [21] is to define a activity coefficient $\gamma_i$ and use the fugacity of the liquid species at its saturation conditions:

$$\bar{f}_i^L\left(T,P,x_1,x_2...,x_{N_c}\right)=\gamma_i\left(T,P,x_1,x_2...,x_{N_c}\right)x_iP_i^{sat}\left(T\right)\phi_i^{L,sat}\left(T,P\right)$$

In terms of flash calculations, a useful concept derived from the above is the species equilibrium coefficient, $K_i$. From the fundamental relation 5.1, it follows that [22]:

$$\bar{\phi}_i^V\left(T,P,y_1,y_2...,y_{N_c}\right)y_iP=\gamma_i\left(T,P,x_1,x_2...,x_{N_c}\right)x_iP_i^{sat}\left(T\right)\phi_i^{L,sat}\left(T,P\right)$$

For illustrative purposes here, low pressure ideal solution behaviour will be assumed, which is essentially that the fugacity and activity coefficients are unity [21]. In general, these would be supplied by equation of state models such as the Peng-Robinson EOS and activity coefficient models respectively [21]. Combining this with the Lewis-Randall rule (which says that the species fugacity is proportional to the mole fraction and pure species fugacity) [21], gives the following expression for the relative volatility of species $i$:

$$K_i\left(T,P\right)=\frac{y_i}{x_i}=\frac{P_i^{vap}\left(T\right)}{P}$$

For the vapour pressure, the simplest description is given by the Antoine equation [20]:

$$P_i^{vap}\left(T\right)=10^{\left(A_i-\frac{B_i}{T+C_i-273.15}\right)} \tag{5.2}$$

where the parameters $A,B,C$ are determined experimentally. Taking these equations together gives a simple model of the equilibrium:

$$K_i\left(T,P\right)=\frac{10^{\left(A_i-\frac{B_i}{T+C_i-273.15}\right)}}{P} \tag{5.3}$$

## 5.2 Mixture Molar Densities

It is required to provide closure relations for the various densities in System 1. For simplicity, ideal solution behaviour is assumed and hence the volumetric effects of mixing are neglected. For the liquid phase, this gives the density as follows:

$$\rho_l \left(T, P, x_1, x_2..., x_{N_c}\right) = \frac{1}{\sum_{i=1}^{N_c} \left(\frac{x_i}{\rho_i^{Ref}}\right)} \tag{5.4}$$

Here, $\rho_i^{Ref}$ is the reference liquid molar density, which is given at a reference temperature. The effect of temperature on the species liquid molar density is neglected as it is a weaker function of temperature than the vapour density. A reference pure component liquid molar volume can be determined at an arbitrary temperature from the critical properties of the fluid using the Rackett equation [20], where $T_R$ is the desired reference temperature:

$$V_R = V_c Z_c^{\left(1-\frac{T_R}{T_c}\right)^{\frac{2}{7}}} \tag{5.5}$$

The vapour density is given by an equation of state. For illustrative purposes, the ideal gas law will serve equally well in this context [21]:

$$\rho_v \left(T, P, y_1, y_2..., y_{N_c}\right) = \frac{n}{V} = \frac{RT}{P} \tag{5.6}$$

Here, $R$ is the universal gas constant in appropriate units.

## 5.3 Tank Hydrodynamics

Part of the data required for the models is a method of choosing how the phase outflows respect the hydrodynamic constraints of the vessel itself. These constraints are described by functions $\psi_l$ and $\psi_v$. These functions could depend on vessel geometry, valve characteristics and other complications. In order to avoid such complexity, it is assumed that the vessel cross-sectional area is constant, and that the liquid density is consistent enough to eliminate composition dependence from the hydrostatic head. Then, Torricelli's principle [22] implies that the flow should be proportional to the square of the liquid hold-up, which suggests the following model:

$$\psi_l = C_l \sqrt{M} \tag{5.7}$$

The constant, $C_l$, will be determined based on the reference steady-state solution. For the vapour phase exit rate, the pressure differential establishes a similar driving force via a proportional valve equation, where the square terms better account for compressible flow:

$$\psi_v = C_v \sqrt{P^2 - P_{out}^2} \tag{5.8}$$

## 5.4 Physical Properties

The following thermo-physical properties are found in [20], and are provided by the Thermodynamics Research Center (TRC) data bank, College Station, Texas, USA.

Table 5: Critical properties for isothermal flash species from [20]

| Species | $mw_i$ $[g\ mol^{-1}]$ | $T_c$ $[K]$ | $P_c$ $[bar]$ | $V_c$ $[cm^3 mol^{-1}]$ | $Z_c$ $[\,]$ |
|---|---|---|---|---|---|
| Propane | 44.10 | 369.80 | 42.48 | 200.00 | 0.276 |
| Butane | 58.12 | 425.12 | 37.96 | 255.00 | 0.274 |
| Pentane | 72.15 | 469.80 | 33.70 | 311.00 | 0.268 |
| Hexane | 86.20 | 507.60 | 30.25 | 368.00 | 0.264 |

Coefficients for the Antoine Equation (5.2), returning pressure in bars with input temperature in kelvins, are provided in the same source:

Table 6: Antoine coefficients for isothermal flash species from [20]

| Species | $A_i$ | $B_i$ | $C_i$ |
|---|---|---|---|
| Propane | 3.928 | 803.99 | 247.04 |
| Butane | 3.932 | 935.77 | 238.80 |
| Pentane | 3.978 | 1064.84 | 232.00 |
| Hexane | 4.00 | 1170.88 | 224.32 |

## 5.5 Hydrocarbon Flash - Base Case

A base-case, steady-state example is selected here, based on that given in [22]. The example is a time invariant simple isothermal flash of a mixed hydrocarbon feed, with composition as supplied below:

Table 7: Base case feed data for isothermal flash

| Component | Flow Rate $kmol/h$ | Fraction $[\,]$ | Type |
|---|---|---|---|
| propane | 10 | 0.1 | Light |
| n-butane | 20 | 0.2 | Distributing |
| n-pentane | 30 | 0.3 | Distributing |
| n-hexane | 40 | 0.4 | Heavy |
| Total | 100 | | |

The isothermal flash conditions are a temperature of $T^{Ref} = 366.5K$, and an absolute pressure of $P^{Ref} = 6.89$ bar. Although the example includes exiting compositions as well, since the equilibrium constants given in [22] do not align exactly with those resulting from the data in [20], it is required to re-calculate the exiting flows and compositions in order to achieve mass balance. Additionally, the source does not provide hydrodynamic information for $\psi_l$ and $\psi_v$, or information about the tank volume $C_T$. Therefore, the well known Rachford-Rice

Iteration [21, 22] is used to determine $L, V, x_i$ and $y_i$ for this system at steady-state. Once this is complete, the remaining data $C_T, M, \psi_l$ and $\psi_v$ can be specified in a consistent manner.

The Rachford-Rice Iteration for composition-independent equilibrium coefficients [22] is as follows:

1. Set $\Psi := \frac{V}{F}$, then solve the following function for zero (using Newton's Method or equivalent):
$$f(\Psi) = \sum_{i=1}^{N_c} \frac{w_i (1 - K_i)}{1 + \Psi (K_i - 1)}$$
2. It then follows that
$$x_i = \frac{w_i}{1 + \Psi (K_i - 1)}$$
$$y_i = \frac{K_i w_i}{1 + \Psi (K_i - 1)}$$
$$L = F - V$$

Applying this procedure to the given problem using an initial guess $\Psi = 0.129$ from [22] gives a solution for the data in Table 6 at $\Psi = 0.1689$. For these conditions, the exiting compositions are given below:

Table 8: Base case steady-state outflow data

| Component | Liquid Rate $L$ $\left[kmol\, h^{-1}\right]$ | Fraction $x_i$ $[\,]$ | Vapour Rate $V$ $\left[kmol\, h^{-1}\right]$ | Fraction $y_i$ $[\,]$ |
|---|---|---|---|---|
| propane | 4.7947 | 0.0577 | 5.2053 | 0.3082 |
| n-butane | 14.5133 | 0.1746 | 5.4867 | 0.3249 |
| n-pentane | 26.0974 | 0.3140 | 3.9026 | 0.2311 |
| n-hexane | 37.7078 | 0.4537 | 2.2922 | 0.1357 |
| Total | 83.1132 | 1 | 16.8868 | 1 |

Of course, this steady-state solution does not uniquely specify the vessel dynamics - there is not enough information to specify the tank size based on this alone. Therefore, an assumption must be made about the size of the tank. Using the molar volumes as determined using Equation (5.5) and data in Table 5, the volumetric liquid discharge at steady-state is found to be $\sim 11.4m^3h^{-1}$.

Optimal sizing of flash vessels is a large and well surveyed subject [10, 22], and should be based on ensuring sufficiently low liquid velocity for phase disengagement (see Souders-Brown equation [10]). Such concerns are outside the scope of this example and hence a very crude approximation is to be made. Based on classical flash drum sizing heuristics [10], the drum should have a half-full draining time of approximately $4$ minutes. This gives a drum volume of $\sim 1.5m^3$, and assuming even volumetric phase split, the molar liquid hold-up can be determined from the molar density based on Equation (5.5) and the data in Table 5. The vapour density at this condition is given by Equation (5.6) and this allows the vapour hold-up and a total reference hold-up to be estimated. Together, this allows consistent specification of the constants from Section 5.3. The base case steady-state solution parameters are summarized in Table 9. It can be easily verified that these parameters solve Systems 1 and 2 when at steady-state (i.e. all derivatives are zero), combined with the state equation information in Table 8.

Table 9: Base case system dynamic parameters

| Parameter | Symbol | Reference Value | Unit |
|---|---|---|---|
| Tank Volume | $C_T$ | 1.500 | $m^3$ |
| Liquid Hold-up | $M_l$ | 5.4563 | $kmol$ |
| Vapour Hold-up | $M_v$ | 0.1696 | $kmol$ |
| Total Hold-up | $M^{Ref}$ | 5.6259 | $kmol$ |
| Liquid Discharge Constant | $C_l$ | 35.041 | $kmol^{1/2}h^{-1}$ |
| Vapour Discharge Constant | $C_v$ | 2.4771 | $kmol\, h^{-1}\, Bar^{-1}$ |

## 5.6 Test Cases

Now that the problem is fully defined, it remains to select some test cases to allow comparison of the two systems considered in this work. Note that, following on from the discussion in Section 4.2, System 2 is implemented with the vapour outflow rate $V$ as a control using the same valve equation used in System 1 for comparison. The temperature is controlled in both systems in the same way.

In the first test, a time varying temperature profile is established such that the temperature-response curve of the systems can be compared. The temperature is set to ramp-up, hold, ramp-down and hold with time, such that the temperature obeys the following equation on $t \in [0, 48]$:

$$T\left(t\right) = \begin{cases} T^{Ref} + \frac{T^{Max} - T^{Ref}}{12} & 0 \leq t \leq 12 \\ T^{Max} & 12 < t \leq 18 \\ T^{Max} - \frac{T^{Max} - T^{Min}}{24} & 18 < t \leq 42 \\ T^{Min} & 42 < t \leq 48 \end{cases}$$

For illustration set $T^{Min} = T^{Ref} - 50$ and $T^{Max} = T^{Ref} + 50$, which gives the response of the system at a large range of operating temperatures. This profile is shown in Figure 3.

It is noted that this control output is smooth, although not differentiable at the switch points. This should not pose any difficulty, as the systems have been formulated to be strangeness-free problems. This implies that there is no requirement on the differentiability of the input functions, and it should be possible to use the systems as is for switch simulation as well.

The second test involves varying the feed conditions at constant temperature (i.e. the free system with the reference temperature maintained). These are typical disturbances in operational units and hence comparing these dynamics in the different models is of interest.

For the varying feed, observe that the base case conditions contain a large portion of heavy components ($70\%$ n-pentane and n-butane). As a somewhat extreme example, the response to a linear ramp to a light-dominated feed is simulated. Additionally, the feed rate ($F$) is increased by $50\%$ over the same period. The composition of the feed species transitions linearly between the following states:

Table 10: Test Case 2 feed data for isothermal flash

| | $t = 0$ | $t = 48h$ |
|---|---|---|
| Component | Initial Fraction $w_i$ | Final Fraction $w_i$ |
| propane | 0.1 | 0.4 |
| n-butane | 0.2 | 0.3 |
| n-pentane | 0.3 | 0.2 |
| n-hexane | 0.4 | 0.1 |
| | Initial Flow Rate $kmol\,h^{-1}$ | Final Flow Rate $kmol\,h^{-1}$ |
| $F$ | 100 | 150 |

This is illustrated in Figure 4.

In the final test, a simple proportional-only control is implemented as a demonstration. The same time-varying input functions in Test Case 2 are used, but this time the temperature profile is selected by proportional feedback. Based on the results of Test Case 2, the liquid outflow rate was selected as the control target and the objective is assumed to be mitigating the effect of the varying input conditions, i.e. to keep the liquid outflow as close as possible to the initial state given in Table 8.
The control input now has the following structure:

$$T(t, L) = T^{Ref} + k(L - L_0) \tag{5.9}$$

Here, $L_0 = 83.11\ kmol\,h^{-1}$ from Table 8, and the gain is set as $k = 3$ based on manual tuning. The gain was noted to have a strong effect on the simulation time by increasing the stiffness of the problem and driving the number of timesteps taken by the solver up.

The liquid outflow is a reasonable choice of feedback control variable as it is likely to be possible to measure this quantity online, instead of requiring measurement of compositions or distributions inside the vessel. Additionally, the liquid outflow rate is an important physical parameter from the point of view of downstream conditions, and control of this parameter may be industrially relevant. Disruptions in flash vessel output can cause control problems for downstream distillation columns, for example see [25].

The inputs used in Test Case 1 and Test Cases 2 and 3 are illustrated below:

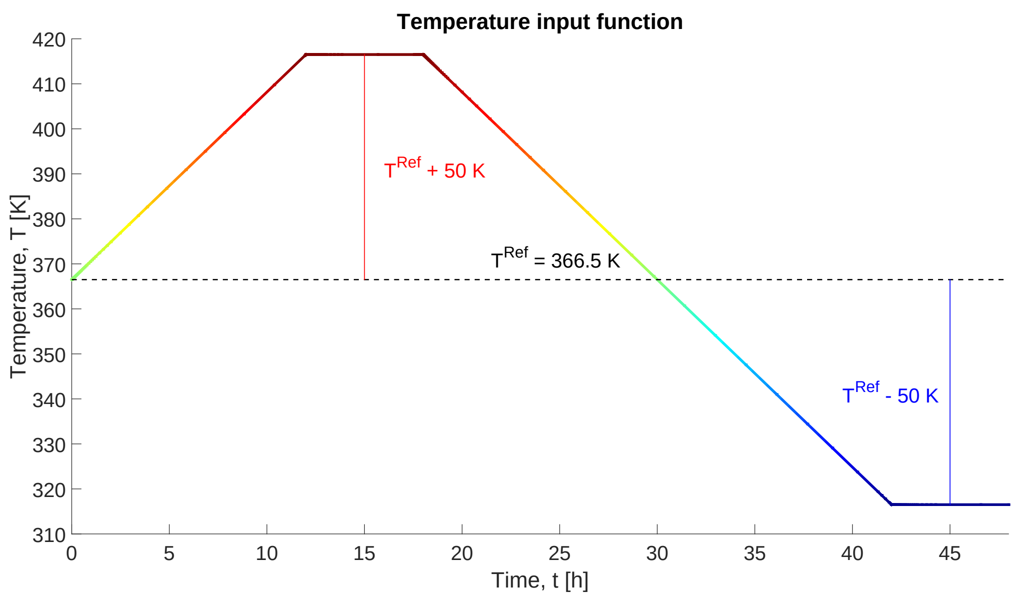


Figure 3: Temperature input function for Test Case 1

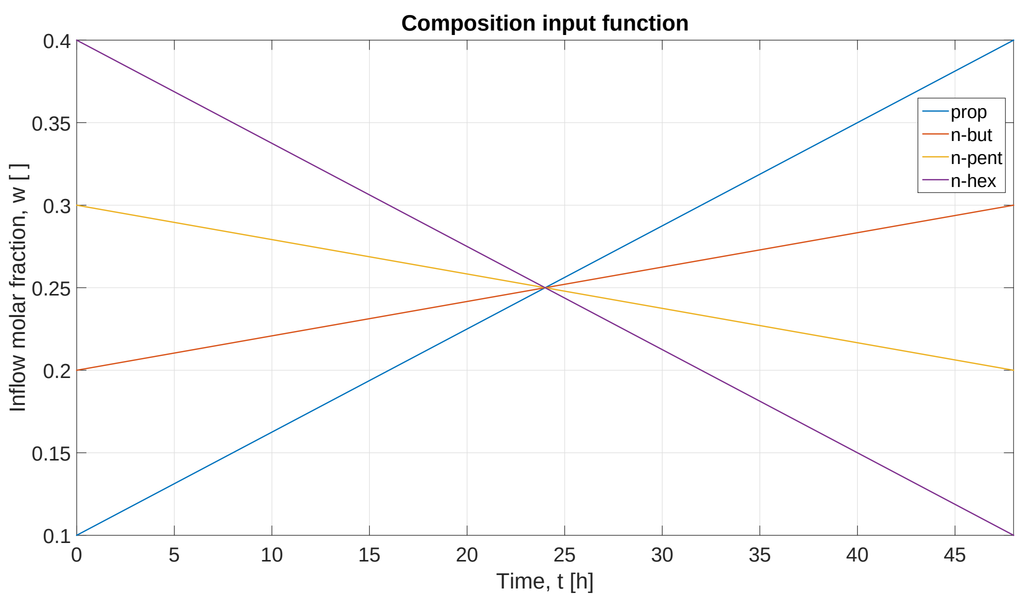


Figure 4: Feed composition input function for Test Cases 2 and 3

## 5.7 Output Metrics

In order to interpret and compare the multivariate state space solutions of the two systems, some outputs will be defined. It is also intended to use the types of outputs that are, in principal, of interest in the context of the problem. The first is the flash ratio:

$$\Psi\left(t\right) = \frac{V\left(t\right)}{F\left(t\right)}$$

This is a measure of the (molar) extent of vaporisation in the separator. Another important performance indicator for a flash vessel is the composition difference between the exiting phases. This can be quantified by the split or separation ratio [22] for each species $i$:

$$SR_i\left(t\right) = \frac{y_i\left(t\right)V\left(t\right)}{x_i\left(t\right)L\left(t\right)}$$

Finally, the relative separation power for any two species $i$ and $j$ is defined as:

$$SP_{i,j}\left(t\right) = \frac{SR_i\left(t\right)}{SR_j\left(t\right)}$$

In general, it is desired to operate such that the separation ratios are all far from unity and the separation power between key components is as high as possible. Which components are considered "key" is dependent on the operating requirements, but here the focus will be on the separation of distributing components, namely n-butane to n-pentane.

It is not necessarily apparent that these metrics can be measured accurately and easily in the real world. Some of these metrics depend on composition, which is difficult to determine online, and hence these will not be used for feedback purposes. However, they are still useful in characterising the theoretical performance of the separator.

Other feasible physical measurements would include internal pressure, which is almost always monitored in elevated-pressure vessels [25].

# 6 Numerical Results

In order to solve the problems set up in the previous section, two commercially available solvers implemented in Matlab® were used. Matlab® is used as an environment due to the small size of the problem and the convenience of the syntax. As will be demonstrated here, Matlab® possesses suitable inbuilt methods to solve stiff d-index 1 DAEs. This section begins by describing the two codes used to solve the sample problem developed in the previous section. The underlying numerical details and applicability of these methods is handled in the section on numerical methods (Section 2.2). The discussion here is limited to implementation information for the different solvers, for example the stepsize control used and other specific details. More details about the structure of the code written for this project and a link to the source can be found in Appendix C. A copy of the code is provided along with this document.

Next, the performance of the solvers over the test cases and systems studied here is presented and analysed. Once the controls have been fixed as per the set up in Sections 3.2 and 4.2, Systems 1 and 2 are both d-index $1$, square and of state dimension $3N_c + 6 = 18$ and $2N_c + 3 = 11$ respectively.

Finally, this section contains some results and technical interpretation of the resulting solutions for the various cases, and compares the outputs of the two systems under the various conditions tested.

## 6.1 About the Solvers

The first solver used is the *ode15s* routine, which is able to handle d-index 1 semi-implicit DAEs. This disucssion is based on the original implementation notes in [23] and [24]. The underlying numerical method is based on a so-called numerical differentiation routine [23], where the order of the method is selected dynamically between second and fifth order.

This can be understood as an extension of the BDF methods discussed in Section 2.2. For simplicity, in the ODE case, the BDF methods are given by:

$$\sum_{i=0}^{k} \alpha_{k-i} x_{n-i} = hF_1\left(t_n, x_n\right)$$

Now, the method used by *ode15s* is given by [24]:

$$\sum_{i=0}^{k} \alpha_{k-i} x_{n-i} + \kappa\gamma_l\left(y_n - y_n^0\right) = hF_1\left(t_n, x_n\right)$$

Here, $\kappa$ is an empirically tuned parameter, $\gamma_j$ is is the $j^{th}$ harmonic number $\left(\gamma_j = \sum_{k=0}^{j} \frac{1}{j}\right)$ and $y_n^0$ is an estimate, given by, for the $k^{th}$ order NDF:

$$y_n^0 = \sum_{m=0}^{k} \nabla^m y_{n-1}$$

The expression $\nabla^m y_{n-1}$ is the $m^{th}$ order numerical backwards difference formula, given by [23]:

$$\nabla^m y_n = \sum_{i=0}^{m} \binom{m}{i} (-1)^i y_{n-i}$$

This term is based on the leading error term of the BDF method. Including this term reduces the stability of the method but increases accuracy; it is reported [23] that the method here achieves the same accuracy as the corresponding BDF method with $\sim 26\%$ larger average stepsize. The additional term is not used in the fifth order method as the penalty to the stability region is judged to be too severe.

The solver uses a simplified Newton iteration to solve the resulting nonlinear system, using an approximation to the Jacobian. The initial stepsize is estimated based on the initial Jacobian, and convergence of the solver is monitored online. The approximation of the Jacobain is retained between iterations and is only updated (either by call to a user supplied function or numerically estimated) if the stepsize or order of the method changes, or if the solver estimates more than four iterations are required for convergence. If the solver expects more than four iterations are required, it will first refresh the Jacobian, and should that fail, the stepsize is reduced [23].

The second method is the *ode23t* routine, which is based on the single-step Trapezoidal rule with a 'free' interpolant. This method is formally of order $2$, so is not expected to be competitive with *ode15s* at high tolerances [23], but because of the low overhead, it is possible for *ode23t* to outperform the multistep solver at crude tolerances. As a Lobatto method (formally anyway), the discussion in Section 2.2 applies, especially that the method provides low numerical damping [23] but may possibly have additional stability issues when applied to DAEs [3].

While the literature is not explicitly clear in the case *ode23t* [23, 24], it is assumed that the stepsize and Jacobian methods are similar to those used in the other *ode23* solvers and the above methods given for *ode15s*.

## 6.2 Solver Comparison

The performance of the solvers at various specified absolute (element-wise) error tolerances is given in Figures 5 and 6 below. The simulations were repeated 100 times each, and the times indicated are the arithmetic mean of the run times, excluding the time required to find consistent initial conditions. Initial conditions were handled separately, but in the same manner for both systems as per Section 5.5 above. The time for finding initial conditions was $\mathcal{O}\left(10^{-3}\right)\ s$.

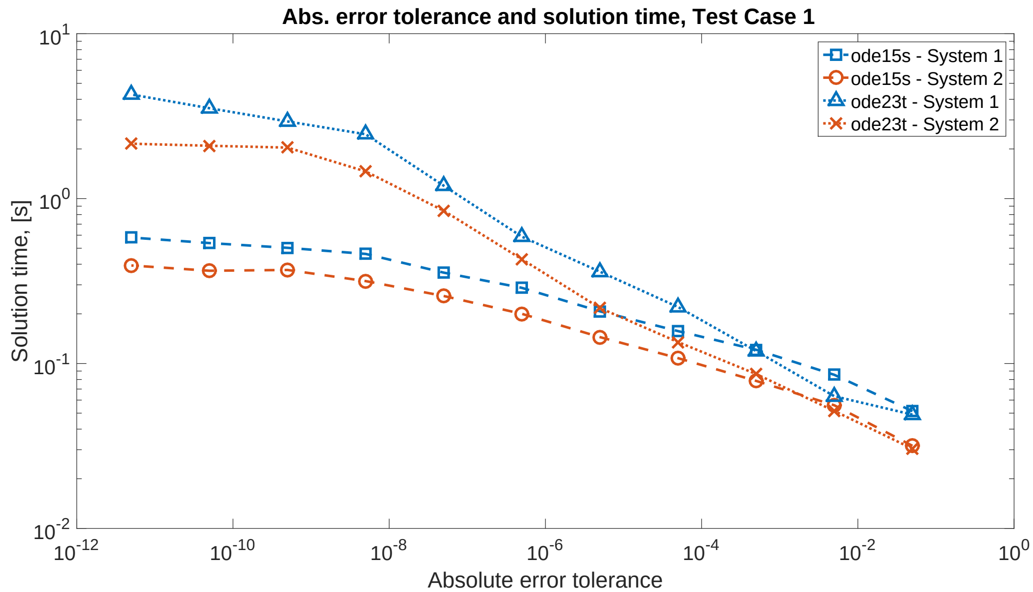


Figure 5: Solution time - absoulte error tolerance plot for ode15s and ode23t, Test Case 1, average of 100 repeats.

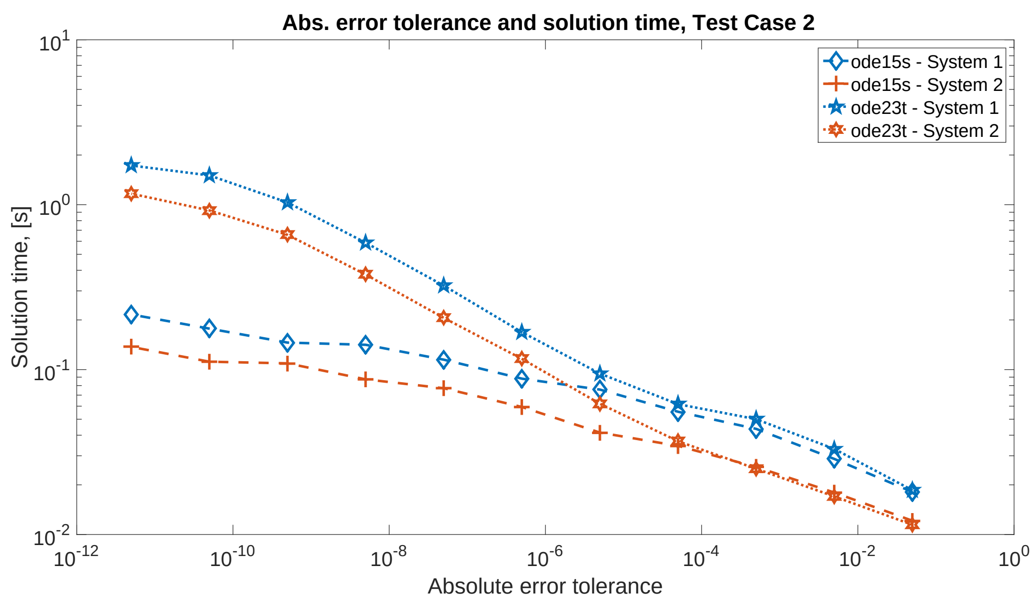


Figure 6: Solution time - absolute error tolerance plot for ode15s and ode23t, Test Case 2, average of 100 repeats.

It is readily apparent that, for Test Cases 1 and 2 at low tolerances, the different solvers are nearly equivalent. As the tolerance is made more stringent, the numerical difference routine, *ode15s*, exhibits superior scaling. In both cases, the larger and more complex System 1 takes more time.

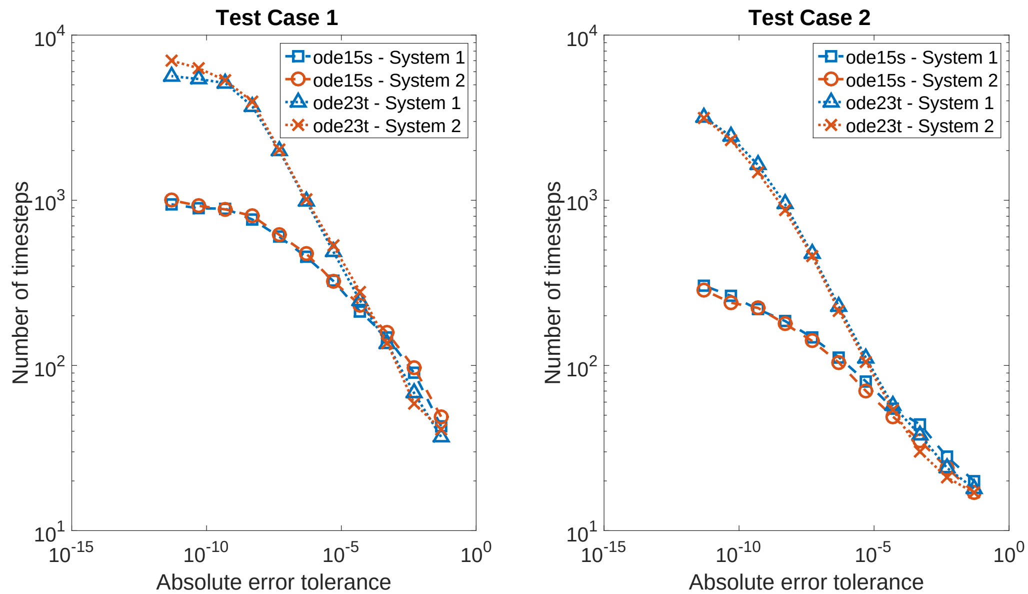


Figure 7: Number of timesteps - absolute error tolerance plot for ode15s and ode23t, Test Cases 1 and 2 compared , average of 100 repeats.

A similar trend is observed from the number of timesteps needed at each level of accuracy, plotted in Figure 7. Here, it is apparent that at low tolerances, the numerical difference method requires more steps but still solves more quickly. For tighter tolerances, *ode23t* requires tens times as many steps. This is likely due to the lower order of accuracy of the trapezoidal rule and the stability issues characteristic of Lobatto methods applied to DAEs as discussed in Section 2.2. Both systems require a similar number of steps to solve, which implies the extra time needed for System 1 is only a product of the system being larger.

Considering Test Case 3, the first observation is the addition of the control term drastically increases the computational load, as evidenced by Table 11 below.

Table 11: Comparison of the solution time and number of timesteps for Test Cases 2 and 3, both systems of equations and two tolerances.

| | Abs. Tolerance | Test case | System 1 | | System 2 | |
|---|---|---|---|---|---|---|
| | | | ode15s | ode23t | ode15s | ode23t |
| Solution time, 100 repeats, $[s]$ | $5 \times 10^{-5}$ | 3 | 7.630 | 4.455 | 2.856 | 0.468 |
| | | 2 | 0.055 | 0.062 | 0.034 | 0.036 |
| | $5 \times 10^{-7}$ | 3 | 13.050 | 59.499 | 3.813 | 9.566 |
| | | 2 | 0.086 | 0.164 | 0.058 | 0.113 |
| Timesteps, 100 repeats, $[\,]$ | $5 \times 10^{-5}$ | 3 | 5716 | 1306 | 2887 | 354 |
| | | 2 | 55 | 57 | 49 | 54 |
| | $5 \times 10^{-7}$ | 3 | 8741 | 14867 | 4013 | 3389 |
| | | 2 | 112 | 227 | 104 | 214 |

Enabling the control increases the solution time by a factor of $\mathcal{O}\left(10^2\right)$ at an absolute error tolerance of $5 \times 10^{-5}$, for both solvers and systems. This is most likely due to the changing Jacobian which causes the solver to take smaller steps and re-estimate the Jacobian more frequently. As can be seen in Appendix A.3, the Jacobian has a large dependence on the equilibrium coefficients, $K_i$, which are exponential in temperature. It is also observed that the computational savings from using System 2 are far greater under these conditions. This is possibly attributable to the lack of coupling of temperature into the balance equations in System 2 (as the densities do not appear), which means the impact of changing temperature on the Jacobian is not as high as is the case in System 1.

It is interesting to observe that the multistep solver, *ode15s*, is slower than the explicit solver under these conditions, and by a substantial margin. This is the opposite of the trend observed in the uncontrolled simulation (Test Case 2). For the second system of equations, *ode23t* is over five times faster than *ode15s*. This is due to the higher number of steps required by *ode15s* under these conditions, although it is not immediately apparent why the stepsize routine enforces so many timesteps.

Looking at the case where the tolerance is tightened to $5 \times 10^{-7}$, it is clear that the higher-order multistep solver performs much better than the single step solver *ode23t*. This is most likely due to the lower (maximum) order of accuracy of *ode23t* as compared to *ode15s*. The increased tolerance very roughly doubles the solution time and number of steps for *ode15s*, while these increase by $\mathcal{O}\left(10\right)$ for *ode23t*.

## 6.3 Test Case 1

The results for the first test case will now be analysed in a some detail. For this analysis, the absolute tolerance used is $5 \times 10^{-5}$. Recall that Test Case 1 used the ramp-up and down input profile given in Figure 3. The response of the adaptive time step selection used by the solvers is clearly illustrated in Figures 8 and 9 and below.

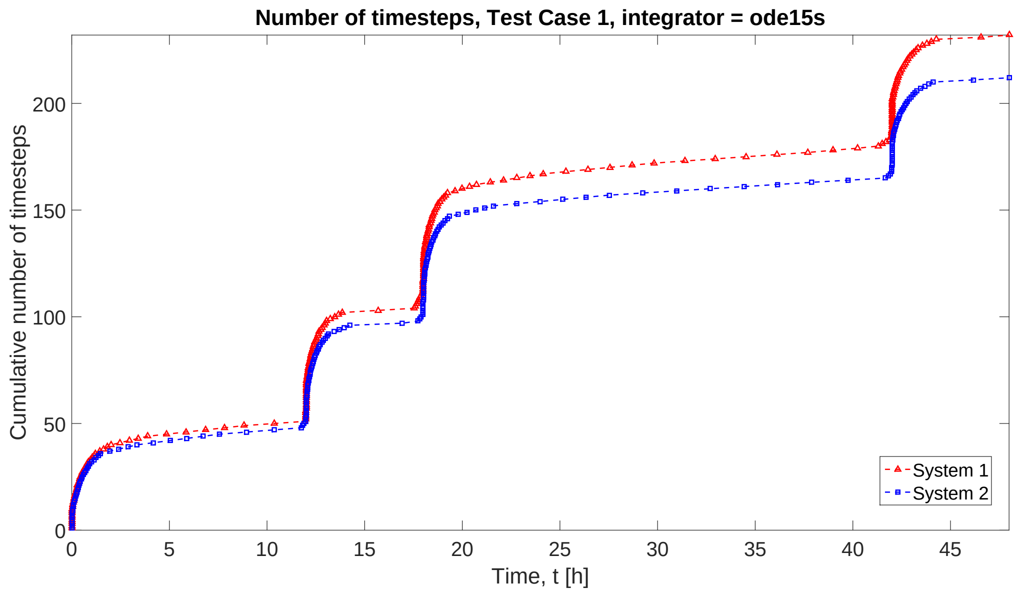


Figure 8: Timestep plot for ode15s, Test Case 1, both systems compared

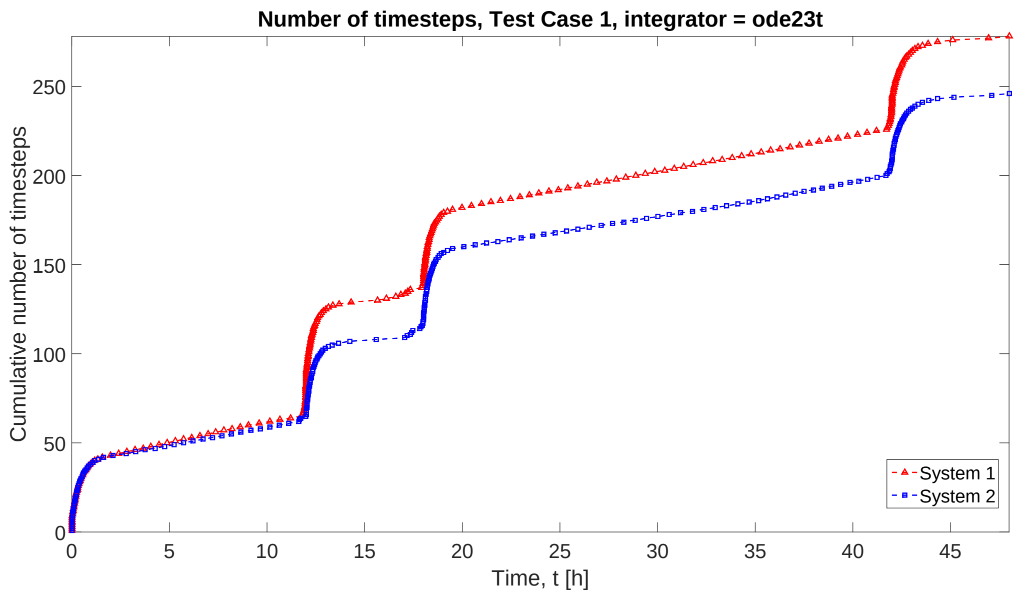


Figure 9: Timestep plot for ode23t, Test Case 1, both systems compared

Both solvers use a large number of timesteps in the initial few seconds. It is clear that the integrator takes many more timesteps near the non-differentiable steps in the solution function at $t = 12$, $t = 18$ and $t = 48$. The time stepping scheme used by *ode23t* requires a larger number of timesteps, which is shown to be due to the higher frequency of timesteps in between the input jumps. The routine *ode15s* is apparently able to solve the system with "smooth" (i.e. differentiable) input more efficiently at this tolerance.

For convenience, subsequent results will mainly be presented from the solver *oder15s* only, as the solvers produced nearly equivalent results and the numerical difference routine was faster as per Figure 5. Firstly, results for the composition-time space for both phases are presented in Figure 10. It is observed that the changes in the liquid phase composition are small relative to the vapour phase, where a much greater extent of vaporisation of propane is observed with increase temperature. It is noted that system dynamics are fast in that the system obtains steady-state nearly immediately after the input stabilizes.

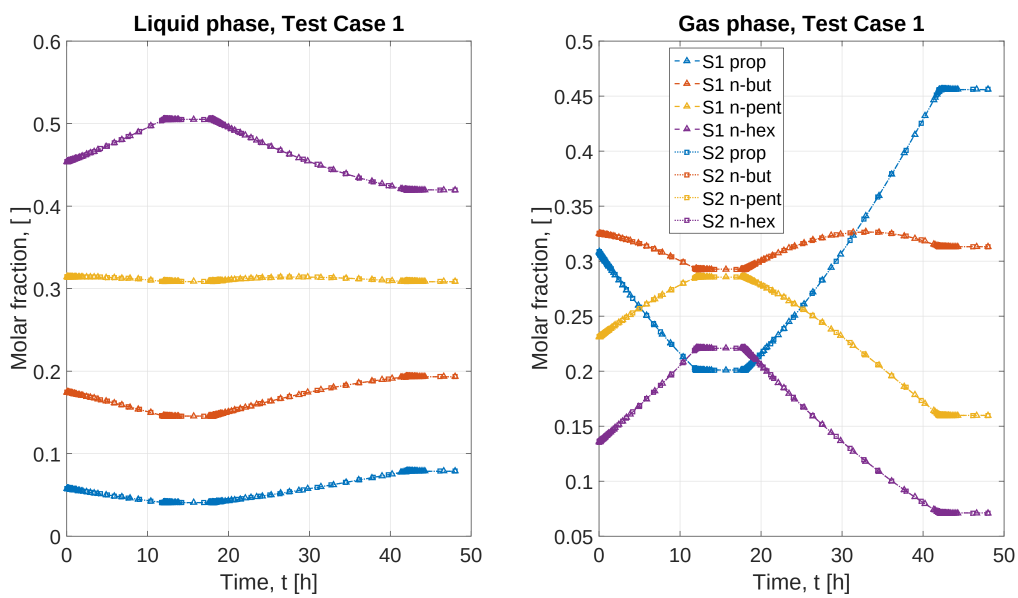


Figure 10: Time-composition plot solved with ode15s, Test Case 1, both systems compared

It is observed that the vapour fraction of the lightest and heaviest components, propane and hexane respectively, are most sensitive to changes in the input.

It is interesting to note that, on this metric, the behaviour of the two systems is nearly identical. Therefore, the additional equations included in the System 1 formulation do not appear to have an impact on the outflow composition under these conditions.

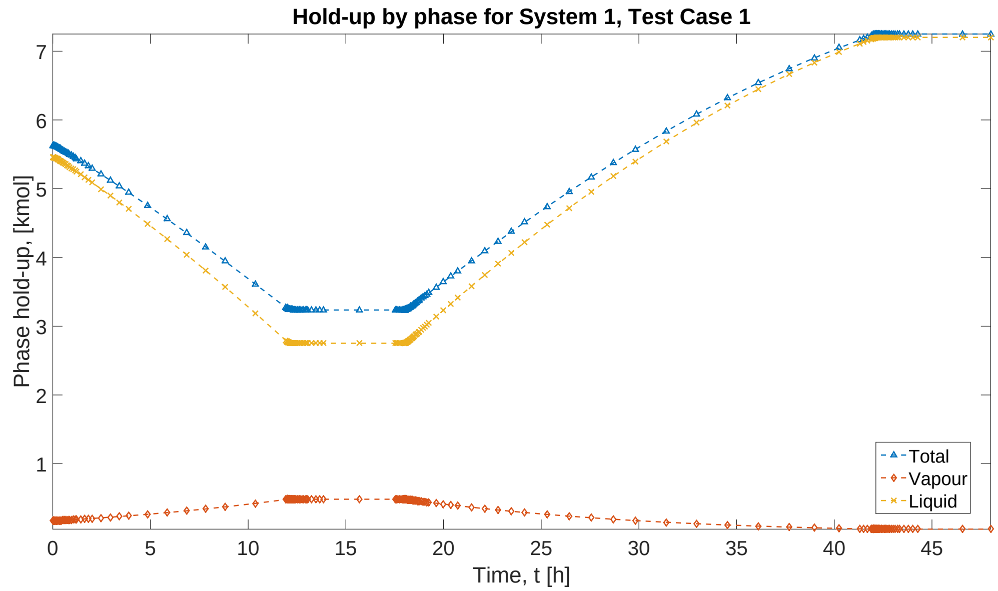


Figure 11: Hold-up fraction in vessel solved with ode15s, Test Case 1, System 1

Figures 11 and 12 show the additional information that is provided in the System 1 formulation. The red line in Figure 11 is the molar vapour hold-up in the vessel, which is not determined in System 2. This gives information about the relative abundance of vapour inside the drum as a function of time. From this figure alone, the assumption that this fraction is negligible seem reasonable.

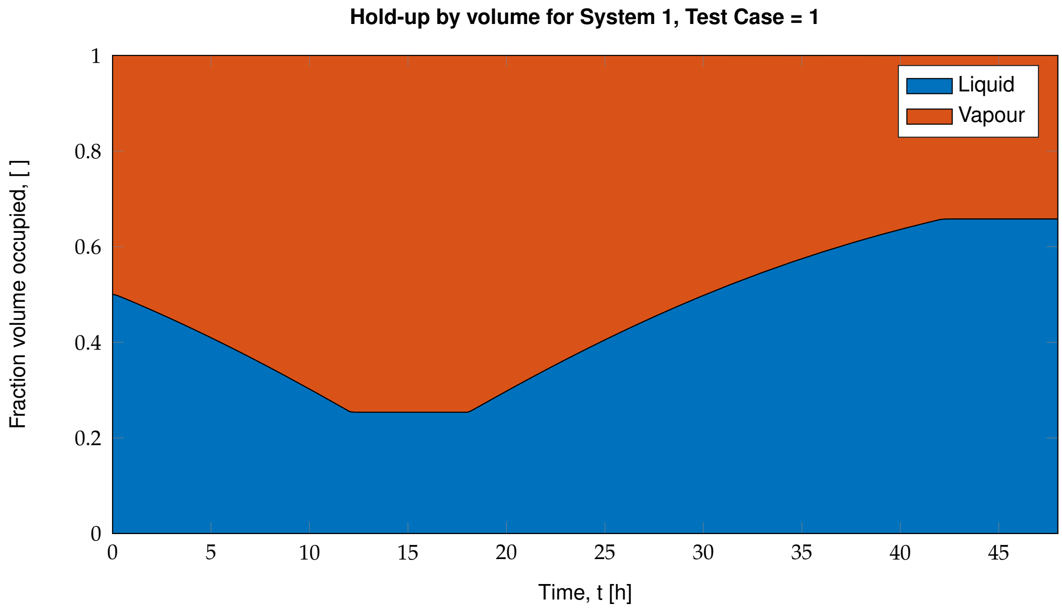


Figure 12: Volume fraction in vessel solved with ode15s, Test Case 1, System 1

However, as the density difference between vapour and liquid phases can be $\mathcal{O}\left(10^3\right)$, this small amount of vapour can be significant. From an operational standpoint, maintaining sufficient liquid inventory to avoid pumps running dry, or ensuring the vessel does not overflow, are important considerations. For example, if the liquid level is too high, it may escape out the vapour port in the top. Figure 12 illustrates the significant volume of vapour predicted despite the lower molar amount. Since System 2 does not divide the system inventory by phase, this information is not available.

The output criteria given in Section 5.7 are plotted below in Figures 13 and 14. From these, some interesting conclusions can be drawn. Firstly, the separation ratio for all species and the total flash ratio increase with temperature, which is a simple consequence of the Antoine Equation (5.2). The greater sensitivity of the propane vapour composition observed in Figure 10 is linked to the spike in the propane separation ratio.

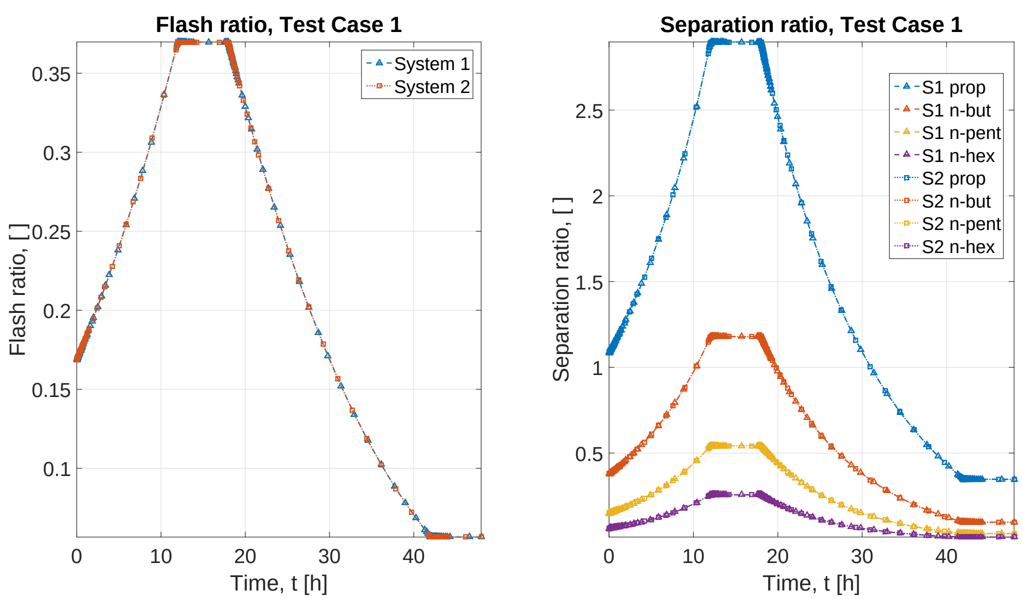


Figure 13: Flash ratio (L) and separation ratios (R) solved with ode15s, Test Case 1, both systems compared

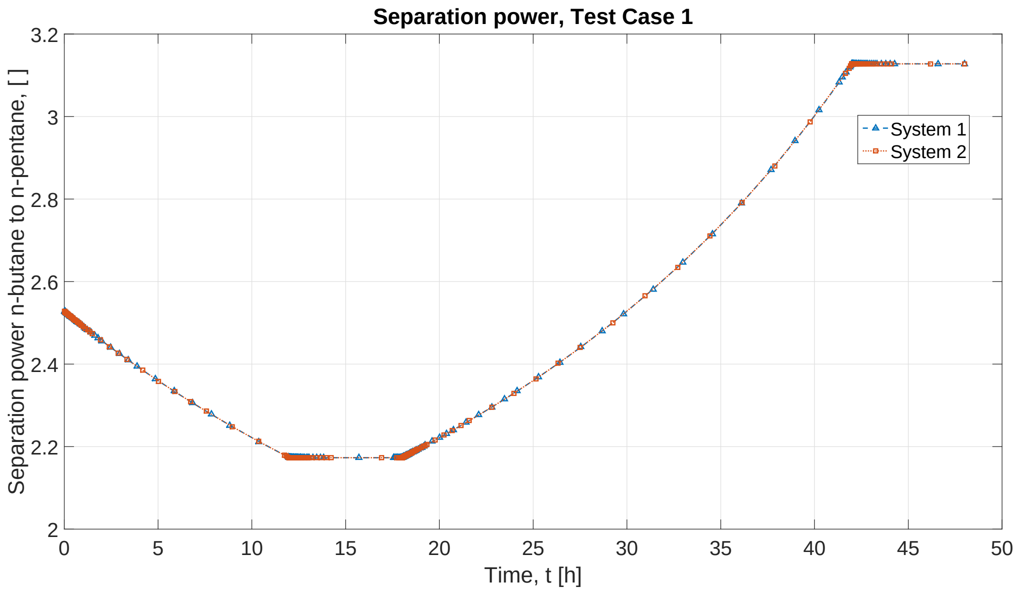


Figure 14: Separation power solved with ode15s, Test Case 1, both systems compared

The separation power is a measure of the relative separation of the middle or 'tie' components (as defined in Section 5.7). It is apparent from Figure 14 that the separation power is lower at higher temperature. This indicates a classical difficulty in separation - the trade-off between obtaining a cleaner (more pure) vapour output at low quantity or lower purity phase a higher flow rate. Clearly, this can only be decided based on operational concerns and in particular, what downstream processing is intended for each output.

Once again, the difference between the output metrics between the two systems is insignificant, which suggests that System 2 acts as an effective reduced order model to System 1 for these outputs. However, it is unable to provide the extra information about the phase split inside the vessel which is shown in Figures 11 and 12.

## 6.4 Test Case 2

The second test case was solved with the same absolute tolerance of $5 \times 10^{-5}$ as used previously. This test case uses a constant reference temperature and varying composition as per Figure 4, and an increasing net feed rate. The timestepping behaviour of both systems for the different solvers used is compared in Figures 15 and 16. Both of the varying inhomogeneities are smooth (as opposed to the previous test case) and hence the timestep plots do not show the same steep sections that are visible in Figures 8 and 9.

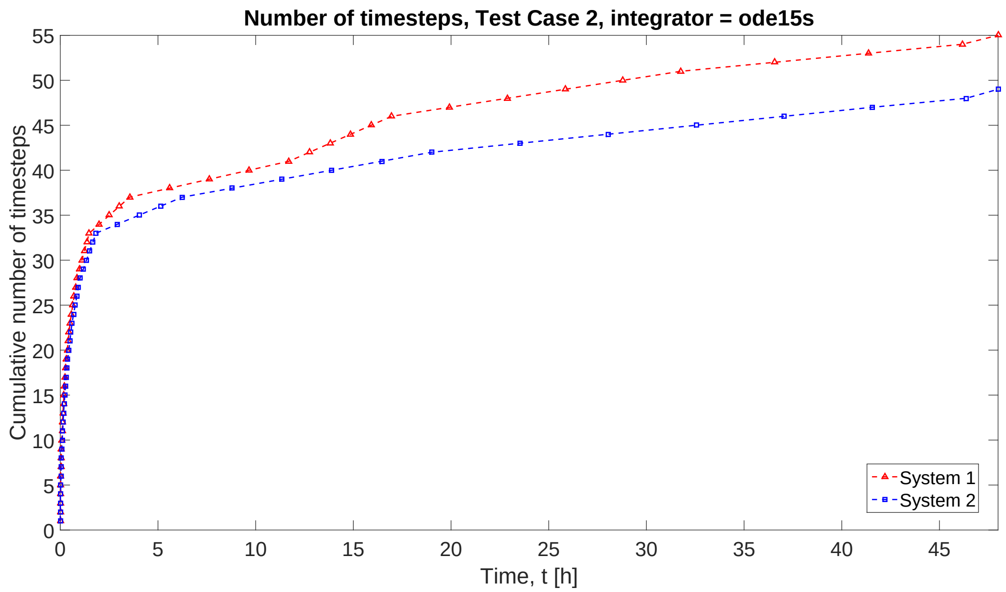


Figure 15: Timestep plot for ode15s, Test Case 2, both systems compared

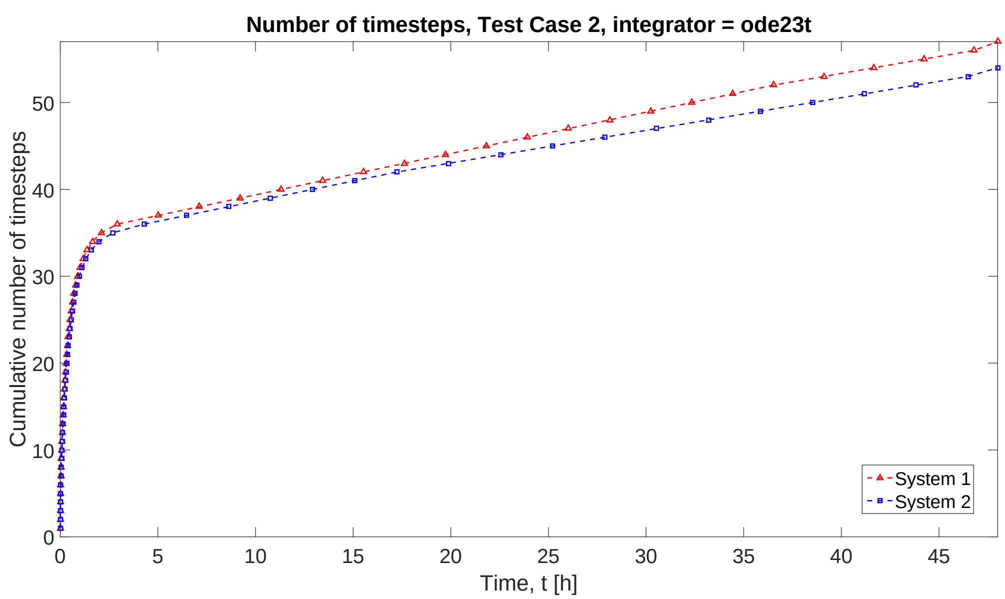


Figure 16: Timestep plot for ode23t, Test Case 2, both systems compared

Additionally, it is noted that the number of the timesteps taken for the same error tolerance is approximately five times fewer as compared with Test Case 1. Also, unlike the previous test case, the number of solution steps and the solution time is similar for both solvers and even both systems, which is consistent with Figures 5 and 6. This is attributable to the small size of the problem and the smooth data. Approximately half of the timesteps are taken in the initiation phase for both solvers.

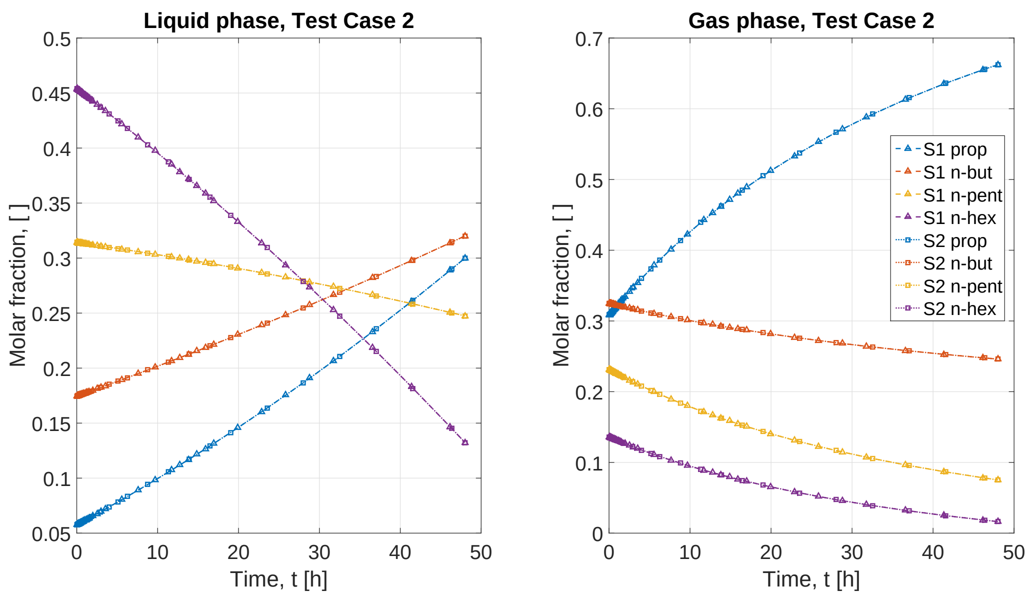


Figure 17: Time-composition plot solved with ode15s, Test Case 2, both systems compared

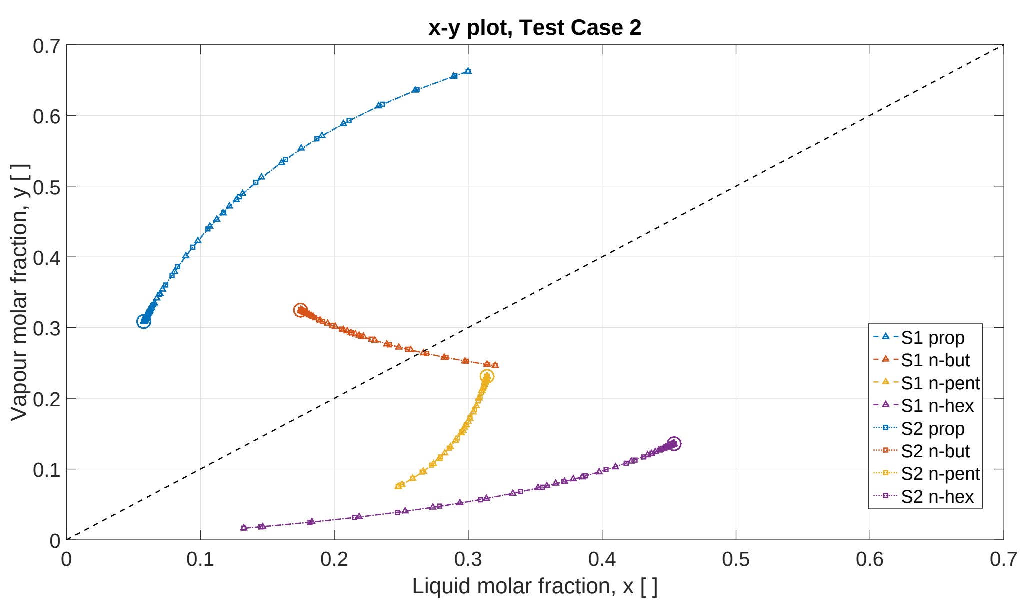


Figure 18: x-y phase plot solved with ode15s, Test Case 2, both systems compared, initial conditions marked with a circle

The results in phase composition show that both phases reflect the changing feed ratio, with decreasing n-hexane fraction in both phases. This is illustrated by Figure 17. Additionally, the equilibrium changes so that the fraction of vapour phase becomes increasingly dominated by the lightest species, propane. Figure 18 presents the time trajectories in the liquid-vapour ("x-y") composition space, with the initial-time conditions indicated by a circle. This is common format to display equilibrium conditions in distillation columns [22]. In particular, it is interesting to note that the trajectory for n-butane crosses the $y = x$ line, which indicates that the composition of this component is equal in both phases. This means that the equilibrium constant for this component, $K_{n-butane}$, is equal to unity at that time. This is due to the increasing pressure in the tank due to the increasing feed rate, and indicates a potential difficulty in selective recovery of this species.

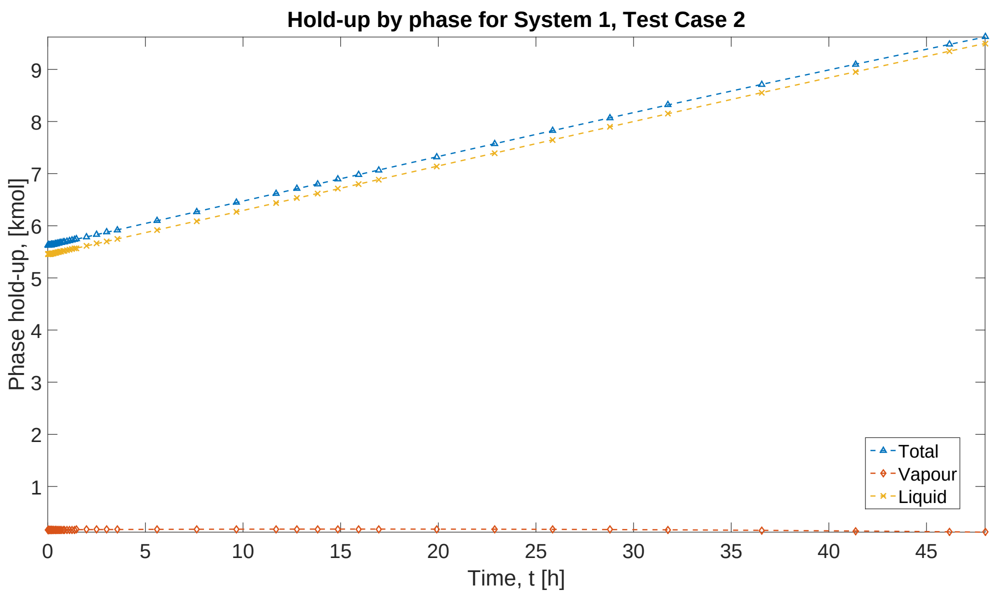


Figure 19: Hold-up fraction in vessel solved with ode15s, Test Case 2, System 1

Turning again to the extra information provided by System 1 only, it is observed from Figure 19 that the vapour fraction of the hold-up is negligible. It is also apparent that the increased feed rate leads to a higher total molar hold-up in the flash vessel over time. This can be clearly understood by considering the relative liquid-vapour volume split in Figure 20. As the feed rate increases and the inlet composition changes, vapour is displaced by liquid with a higher molar density. This leads to the net increase in hold-up, which increases from $\approx 5.5\,kmol$ to over $9.5\,kmol$.

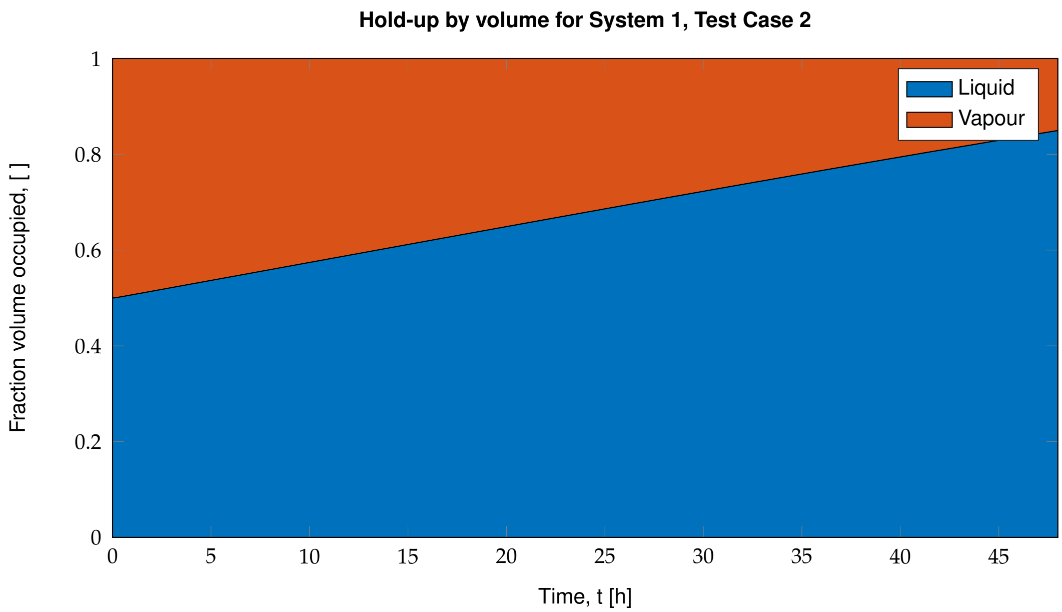


Figure 20: Volume fraction in vessel solved with ode15s, Test Case 2, System 1

Two important conclusions can be drawn from consideration of the phase outflows and total molar hold-ups for the two systems, presented in the sub-plots of Figure 21 respectively. Firstly, it is observed that the vapour outflow rate $(V)$ more than doubles in response to the increasing feed rate and increasing prevalence of light components in the feed. There is a smaller relative increase in the liquid outflow, which is the opposite trend compared to the results in phase hold-up in the preceding figures.

Secondly, it is observed that, although System 2 does not keep track of the split between the phases in the vessel, it does provide a nearly identical description of the total molar hold-up with time.

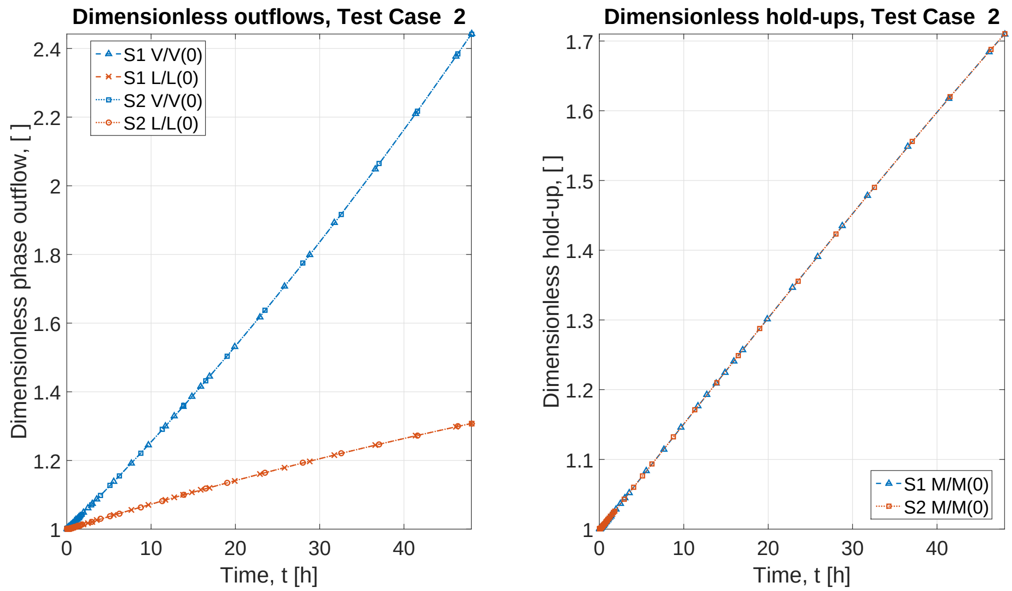


Figure 21: Phase outflows (L) and total hold-up (R) in vessel solved with ode15s, Test Case 2, both systems compared

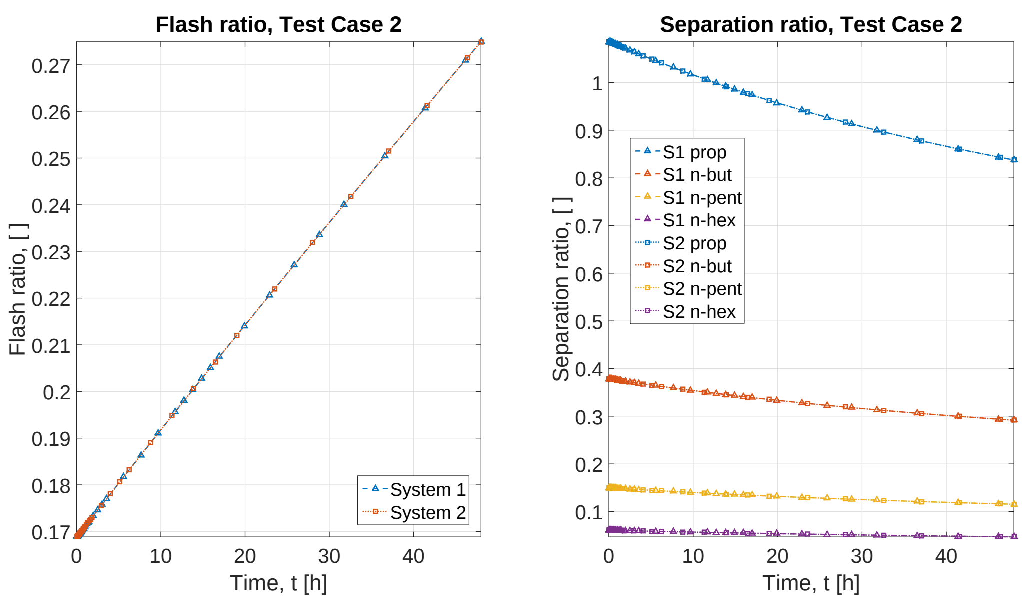


Figure 22: Flash ratio (L) and separation ratios (R) solved with ode15s, Test Case 2, both systems compared

The output metrics defined in Section 5.7 above for Test Case 2 are presented in Figures 22 and 23. There is a general decline in separation ratio for all components, which can be understood by considering that the vapour composition of all species except propane decreases, and the even though the increase in liquid outflow is proportionally smaller, the total liquid outflow still dominates. The flash ratio increases linearly with the changing feed conditions due to the increase in the vapour outflow rate observed in Figure 21.

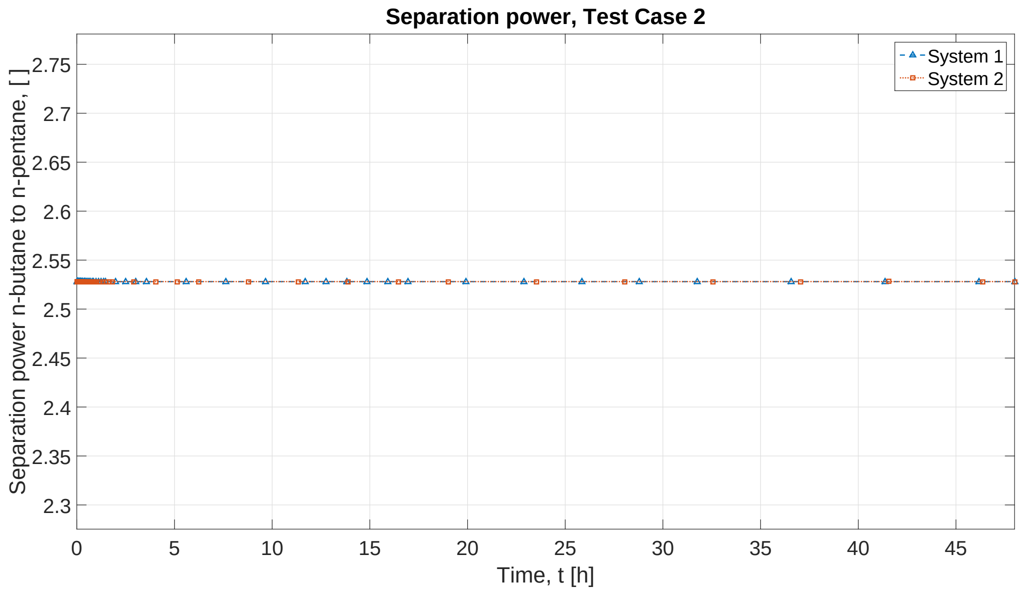


Figure 23: Separation power solved with ode15s, Test Case 2, both systems compared

By contrast, the separation power between the tie components n-butane and n-propane is not affected by the changing feed conditions at all. This is because it is fundamentally a function of the vapour-liquid equilibrium function used, and in this case, the simple structure of the model allows the pressure terms in Equation (5.3) to cancel. Hence, the output is a function of temperature only. This would not be the case if a more sophisticated model were used, for example a composition-dependent activity coefficient model.

Finally, as previously, the second system shows nearly identical output for the variables that are tracked, but does not provide information about the (rather interesting) liquid level behaviour in the vessel. Hence, it is a highly accurate reduced order model if this information is not needed, although the reduction in the number of equations is only order $\mathcal{O}(N_c)$ and hence the savings may be slim for a small number of components.

## 6.5 Test Case 3

The same inflow conditions used in Test Case 2 were paired with the control scheme given in Section 5.6 as Equation (5.9), using the same absolute tolerance $5 \times 10^{-5}$. A large increase in computational work was observed when the control was implemented, which was illustrated previously in Table 11. The timestepping behaviour of the solvers is given in more detail in Figures 24 and 25 below.

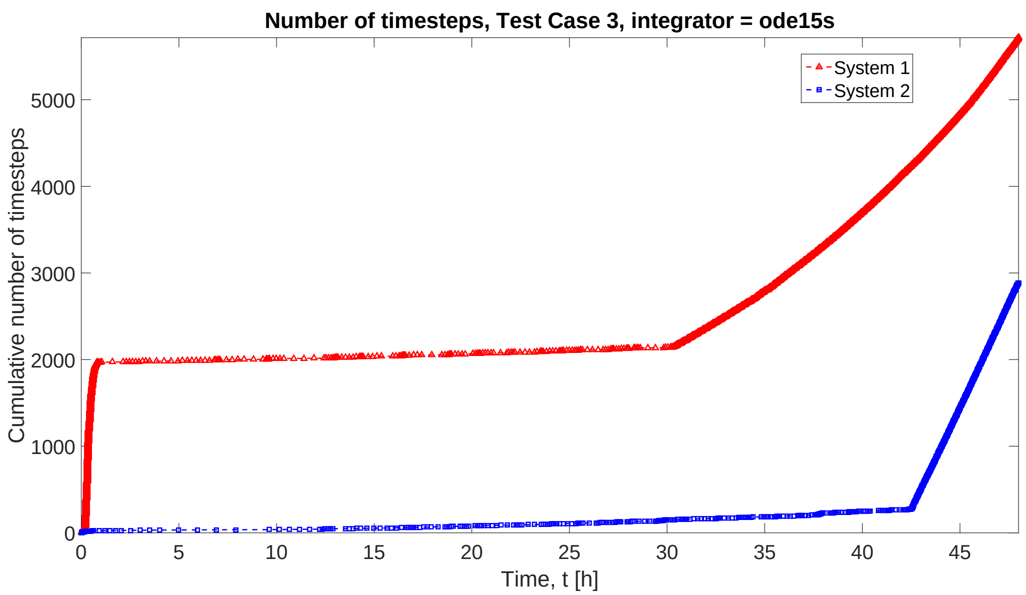


Figure 24: Timestep plot for ode15s, Test Case 3, both systems compared

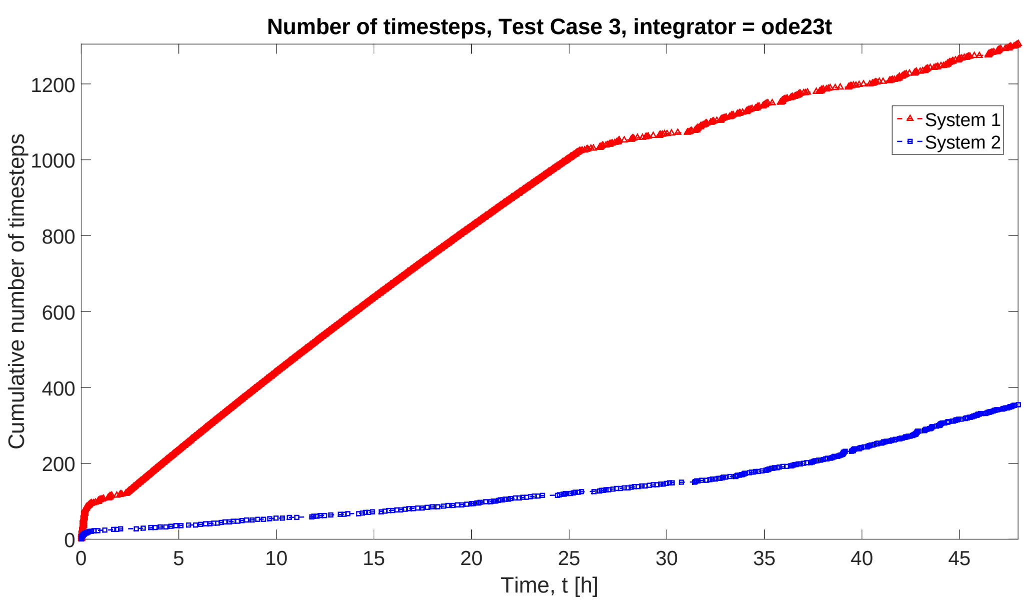


Figure 25: Timestep plot for ode23t, Test Case 3, both systems compared

Firstly, the number of steps taken by the solvers is far greater than in the uncontrolled case - compare Figure 24 with Figure 15 previously. As mentioned, this is likely due to the need to re-evaluate the Jacobian more frequently during calculation due to the large contribution of terms in $K(T, P)$ to the Jacobian. This is observed during Test Case 1 during the periods of temperature transition in Figures 8 and 9, where the small stepsize requirement during temperature changes is readily apparent. Unlike previous results, System 2 requires far fewer solution steps. This possibly also points to increased stiffness and greater coupling between the temperature and the other equations in the first system.

There is a very dense cluster of steps in the initial phase, particularly for the *ode15s* solution of system 1. Many more steps are required for the *ode15s* code in this case than the *ode23t* solver.

For simplicity, results are presented for *ode15s* and System 1 only. Again, the results from System 2 are effectively identical, but do not include information about the volume fractions inside the tank. The action taken by the controller is to increase the system temperature smoothly, with the simulated profile given in 26 below. This promotes vaporisation of the feed and hence counteracts the increasing liquid inflow rate.

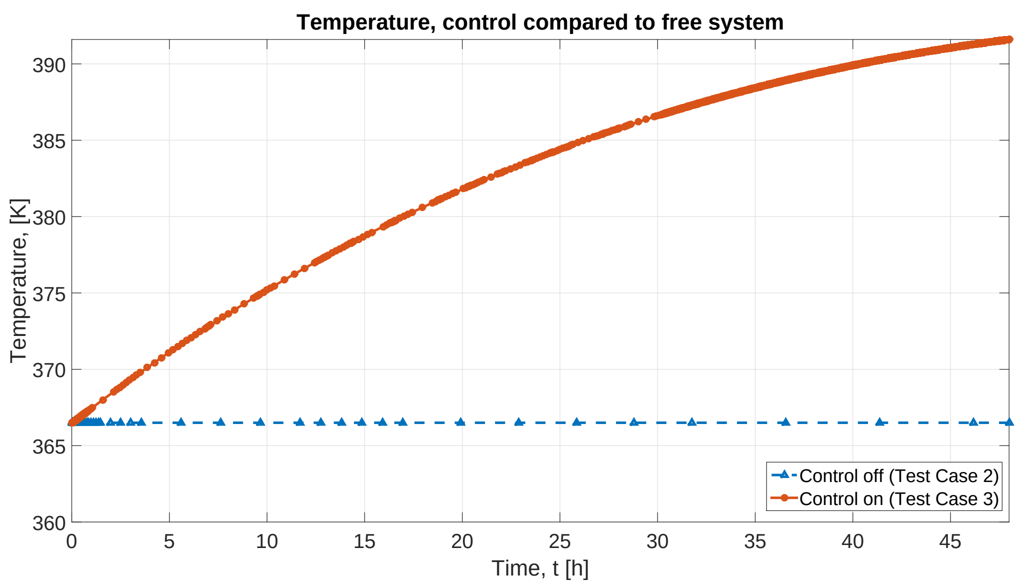


Figure 26: Control temperature profile solved with ode15s, Test Case 2 and 3 compared, System 1 only

The result of the control is observed in Figure 27 below, and it is apparent that the control action reduces the magnitude of the disturbance but settles in an offset position. This is expected for proportional-only control, and it is anticipated that the inclusion of an integral control term would be able to remove this offset.

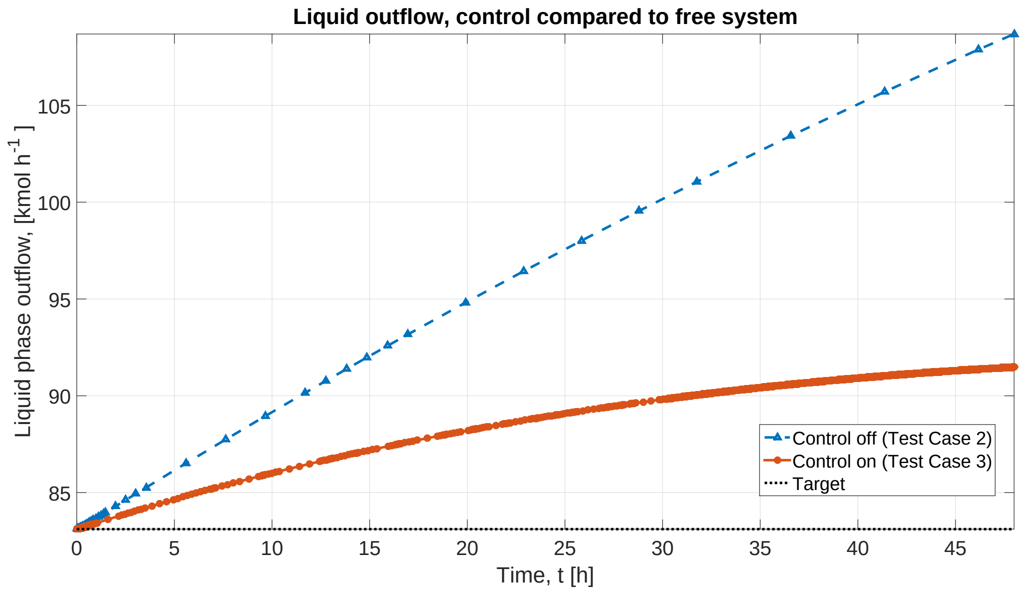


Figure 27: Liquid phase outflow solved with ode15s, Test Case 2 and 3 compared, System 1 only. Note the target line lies on the x-axis

The impact of the control action on the remaining state variables is also explored. Firstly, there is a substantial stabilising effect on the tank level in the simulation, which is good for operability purposes - compare Figure 28 below with Figure 20 above. It is clear that a much more even level is observed.

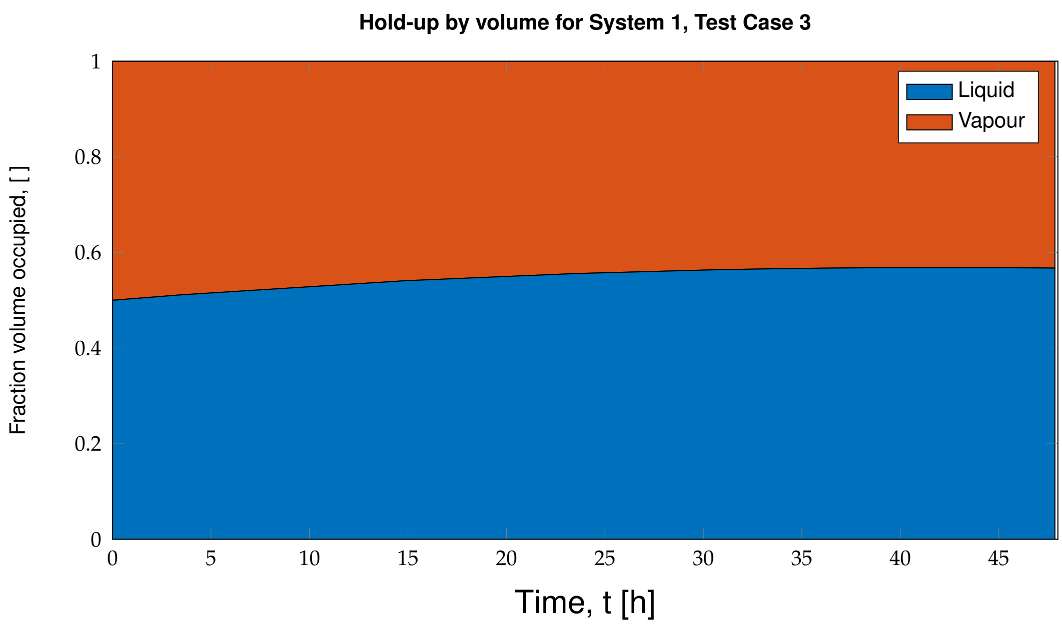


Figure 28: Volume fraction in vessel solved with ode15s, Test Case 3, System 1

Of course, the total feed is still increasing, and if the liquid outflow rate and tank volume are kept (relatively) flat, the vapour outflow rate must increase by a corresponding amount. This is observed in Figure 29 below, where the flash ratio in the presence of the control is seen to increase nearly twice as much in comparison to the free system.

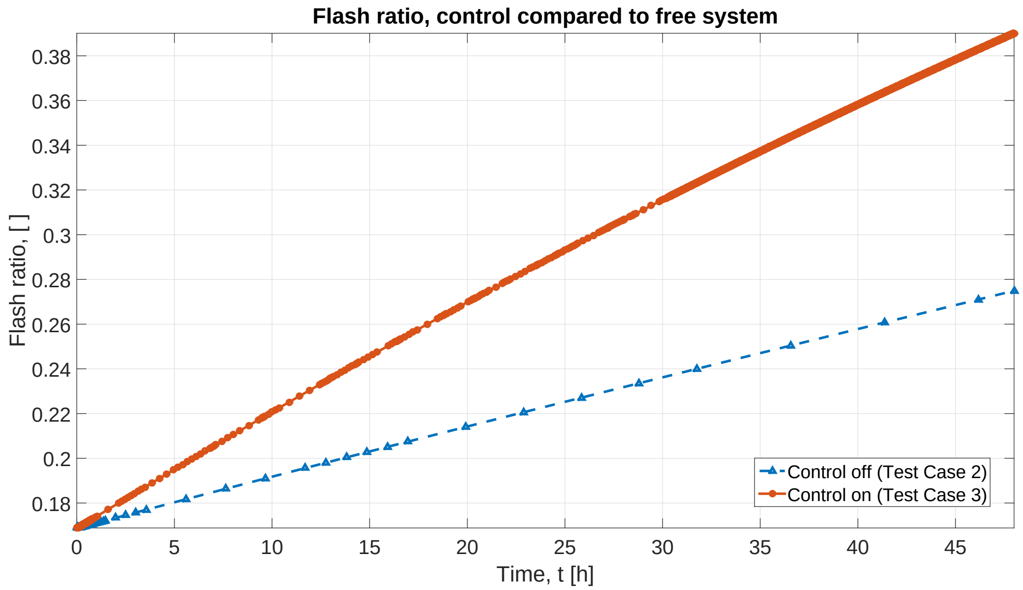


Figure 29: Flash ratio solved with ode15s, Test Case 2 and 3 compared, System 1 only

As observed in Figure 14, higher temperatures cause lower separation power between n-butane and n-pentane. Therefore, is is expected that this control action would result in lower separation power, which is indeed observed in Figure 30 below.

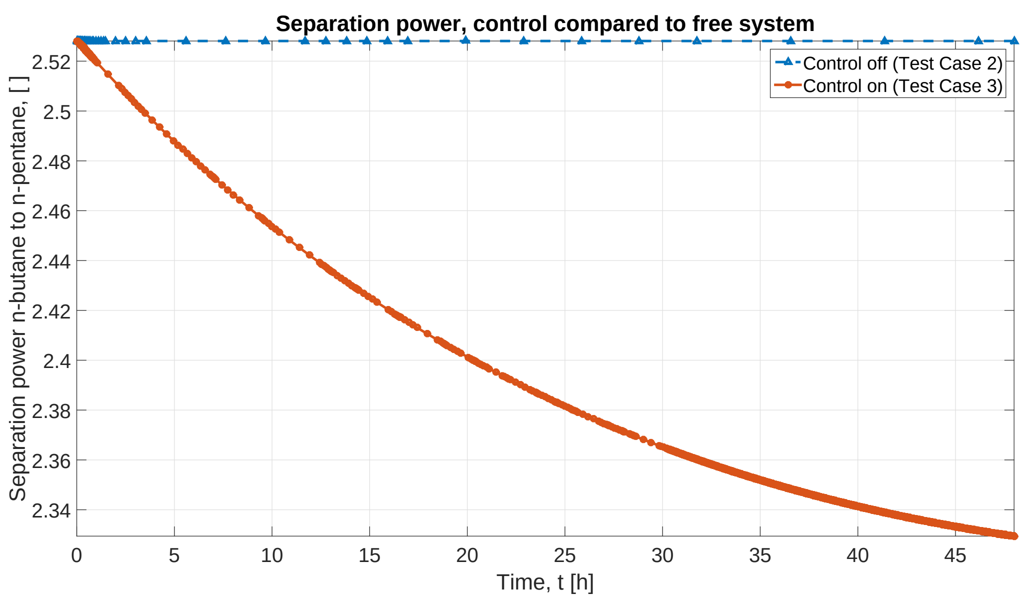


Figure 30: Separation power solved with ode15s, Test Case 2 and 3 compared, System 1 only

# 7 Conclusions and Outlook

This work has investigated two nonlinear dynamic flash models proposed in [5]. The first is a full description of an isothermal flash vessel in terms of a nonlinear DAE system, based on conservation principles supplemented with empirical relationships to describe multiphase behaviour and hydrodynamics. The second system is based on physical simplifications that result in a smaller system.

The models were analysed from a theoretical perspective using the strangeness index, as defined in Section 2.1. It is concluded that the index of the problems cannot be determined independently of the closure relations used, and explicit conditions on the systems being d-index 1 in terms of these relations are derived in Sections 3.2 and 4.2. The first system is strangeness free (analytically and numerically) under all physically likely scenarios.

The claims in the literature regarding the higher index behaviour of the second system are clearly resolved in the behaviour setting in Section 4.2. The confusion about the index of the second system stems from the choice of control and state variables. The second system is not d-index $1$ with the controls proposed in the source, but the system can be regularized by judicious choice of feedback control, specifically feedback with regard to the vapour outflow rate, or by choosing to control this variable directly. In this sense, this work provides an alternate interpretation of the models proposed in the literature in such a way that the resulting systems are both of d-index $1$. This successful analysis shows how a rigorous investigation of the equations in the behaviour setting can provide additional insight into the solution properties of the model.

A simple test problem is presented in Section 5, and was solved using two inbuilt Matlab® implicit integration routines. It was observed that the single-step *ode23t* solver preformed better than the multistep *ode15s* at crude error tolerance, but as the tolerance was decreased, the multistep solver was observed to be superior by a large margin. It is suggested that the desired accuracy be considered when selecting a solver, particularly in engineering contexts where the margin of uncertainty with regard to the physical data may be substantial, and a cruder integration tolerance is acceptable.

The second system appeared to be a very good reduced order model for the full system when considering the output metrics in Section 5.7, for all of the cases tested here. The smaller system requires approximately a quarter of the solution time. However, System 1 provides additional information in terms of the phase composition of the flash vessel with time, which may be of operational interest, and hence solving the larger system may be required.

A control test, using temperature to maintain constant liquid outflow during varying feed conditions was successfully implemented for both systems. The controlled variable remained at an offset due to the use of proportional only control, but this could be easily resolved by including integral terms. Implementation of a control scheme was seen to have a large impact on the solution time; this is attributed to the dependence of the Jacobian on the temperature.

The most logical extension to this work would be to include an energy balance equation, which allows for simulation of the (more physically relevant) adiabatic case, where the control is on the upstream temperature as opposed to that inside the vessel. This could also be extended to consider the delay in this type of control.

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# Appendices

## A System 1 Jacobian

In this section, the Jacobians needed for testing Hypothesis 1 for the first system of equations are derived and analysed. In order to investigate potential cases with higher-than-zero strangeness, the calculations are given for both $\mu = 0$ and $\mu = 1$.

The structure of the Jacobians can be visualised for the base case steady-state conditions derived in Section 5.5. While this does not give a fully general picture as the time-derivatives are all zero, and only simple closure models are applied, it allows the scaling and general structure of the initial matrix to be observed. The variable indices can be interpreted using Table 1 in Section 3.1. Whitespace in the figure means the value is zero.

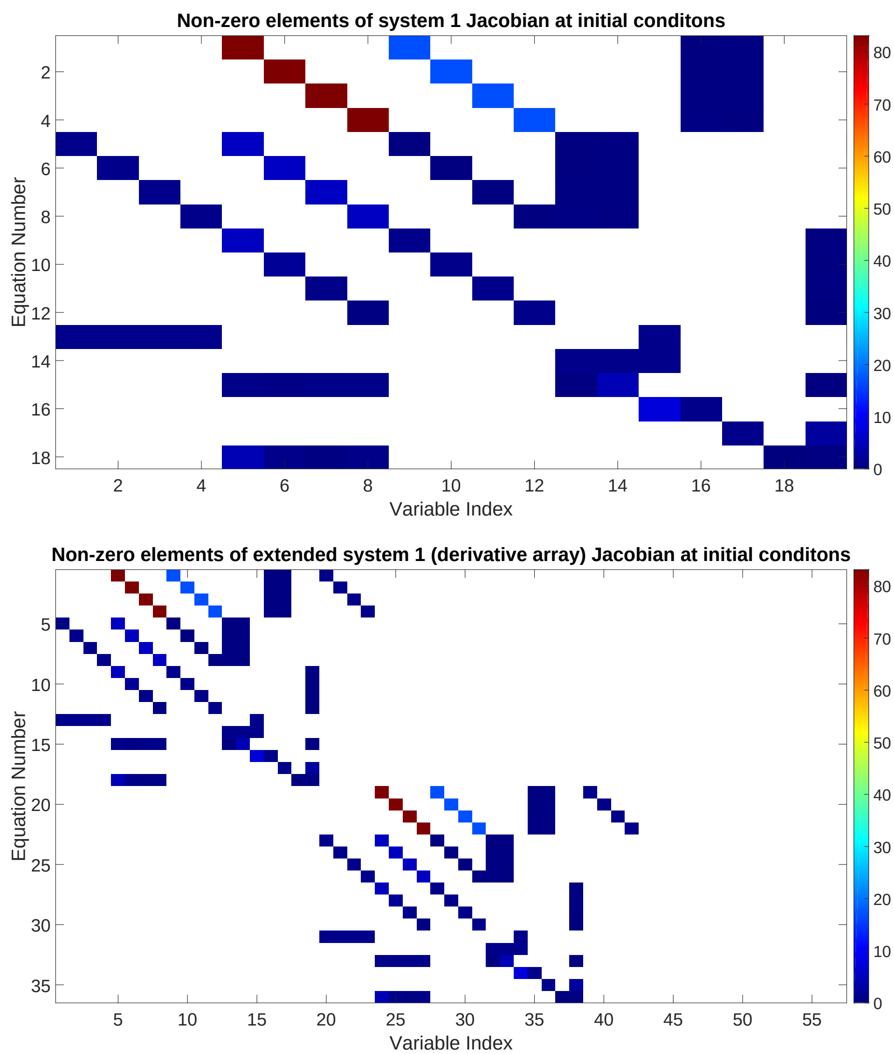



Figure 31: Jacobian of derivative array for system 1, $\mu = 0$ (top) and $\mu = 1$ (bottom) for sample problem at steady-state initial conditions.

## A.1 Time Derivative of System 1

In order to form the derivative array, the derivatives of the nonlinear DAE system given in (3.1-3.10) are needed. These are given as follows:

$$
\begin{aligned}
0 =& \ddot{z}_i - \dot{\phi}_i + \dot{z}_{(3N_c+4)} z_{(N_c+i)} + z_{(3N_c+4)} \dot{z}_{(N_c+i)} \\
& + \dot{z}_{(3N_c+5)} z_{(2N_c+i)} + z_{(3N_c+5)} \dot{z}_{(2N_c+i)} \quad i = 1, 2..N_c
\end{aligned} \tag{A.1}
$$

$$
\begin{aligned}
0 =& \dot{z}_i - \dot{z}_{(3N_c+1)} z_{(N_c+i)} - z_{(3N_c+1)} \dot{z}_{(N_c+i)} \\
& - \dot{z}_{(3N_c+2)} z_{(2N_c+i)} - z_{(3N_c+2)} \dot{z}_{(2N_c+i)} \quad i = 1, 2..N_c
\end{aligned} \tag{A.2}
$$

$$
\begin{aligned}
0 =& \dot{z}_{(2N_c+i)} - \left[ \frac{\partial K_i(\cdot)}{\partial z_{(3N_c+6)}} \dot{z}_{(3N_c+6)} + \frac{\partial K_i(\cdot)}{\partial z_{(3N_c+7)}} \dot{z}_{(3N_c+7)} \right] z_{(Nc+i)} \\
& - K_i(\cdot)\, \dot{z}_{(Nc+i)} \quad i = 1, 2..N_c
\end{aligned} \tag{A.3}
$$

$$
0 = \dot{z}_{(3N_c+3)} - \sum_{i=1}^{N_c} \dot{z}_i \tag{A.4}
$$

$$
0 = \dot{z}_{(3N_c+3)} - \dot{z}_{(3N_c+1)} - \dot{z}_{(3N_c+2)} \tag{A.5}
$$

$$
\begin{aligned}
0 =& \dot{\phi}_{(Nc+1)} - \dot{z}_{(3N_c+2)} \left( \rho_v(\cdot) \right)^{-1} \\
& + z_{(3N_c+2)} \left( \rho_v(\cdot) \right)^{-2} \left[ \sum_{i=2N_c+i}^{3N_c} \frac{\partial \rho_v(\cdot)}{\partial z_i} \dot{z}_i + \frac{\partial \rho_v(\cdot)}{\partial z_{(3N_c+6)}} \dot{z}_{(3N_c+6)} + \frac{\partial \rho_v(\cdot)}{\partial z_{(3N_c+7)}} \dot{z}_{(3N_c+7)} \right] \\
& - \dot{z}_{(3N_c+1)} \left( \rho_l(\cdot) \right)^{-1} \\
& + z_{(3N_c+1)} \left( \rho_l(\cdot) \right)^{-2} \left[ \sum_{i=N_c+1}^{2N_c} \left( \frac{\partial \rho_l(\cdot)}{d z_i} \dot{z}_i \right) + \frac{\partial \rho_l(\cdot)}{\partial z_{(3N_c+6)}} \dot{z}_{(3N_c+6)} + \frac{\partial \rho_l(\cdot)}{\partial z_{(3N_c+7)}} \dot{z}_{(3N_c+7)} \right]
\end{aligned} \tag{A.6}
$$

$$
0 = \dot{z}_{(3N_c+4)} - \left[ \frac{\partial \psi^L(\cdot)}{\partial z_{(3N_c+7)}} \dot{z}_{(3N_c+7)} + \frac{\partial \psi^L(\cdot)}{\partial z_{(3N_c+3)}} \dot{z}_{(3N_c+3)} \right] \tag{A.7}
$$

$$
0 = \dot{z}_{(3N_c+5)} - \left[ \frac{\partial \psi^V(\cdot)}{\partial z_{(3N_c+7)}} \dot{z}_{(3N_c+7)} + \frac{\partial \psi^V(\cdot)}{\partial \phi_{(N_c+2)}} \dot{\phi}_{(N_c+2)} \right] \tag{A.8}
$$

$$
0 = \sum_{i=1}^{N_c} \left[ \left( K_i(\cdot) - 1 \right) \dot{z}_{(Nc+i)} + \left( \frac{\partial K_i(\cdot)}{\partial z_{(3N_c+6)}} \dot{z}_{(3N_c+6)} + \frac{\partial K_i(\cdot)}{\partial z_{(3N_c+7)}} \dot{z}_{(3N_c+7)} \right) z_{(Nc+i)} \right] \tag{A.9}
$$

## A.2 Parameter Groups

For notational convenience, frequently used or complex expressions are grouped here, into a few broad categories. Most of the listed groups are used in forming the system Jacobian and in expressing the matrices that are needed to determine the rank of various blocks.

The parameters are loosely grouped as follows. $\beta$ denotes scalar groupings that occur frequently in the evaluation of the derivatives of the inflated system, but not directly in any final matrices. $\theta$ and $\xi$ denote shorthand for columns and rows respectively, where a single generating expression is given for the entire vector. $\alpha$ denotes scalar groups that appear as elements in the final matrices.

The expressions are as follows, first for $\beta$:

$$\beta_1 = \left[\sum_{j=N_c+1}^{2N_c}\left(\frac{\partial\rho_l(\cdot)}{\partial z_j}\dot{z}_j\right) + \frac{\partial\rho_l(\cdot)}{\partial z_{(3N_c+6)}}\dot{z}_{(3N_c+6)} + \frac{\partial\rho_l(\cdot)}{\partial z_{(3N_c+7)}}\dot{z}_{(3N_c+7)}\right]$$

$$\beta_2 = \left[\sum_{j=2N_c+1}^{3N_c}\left(\frac{\partial\rho_v(\cdot)}{\partial z_j}\dot{z}_j\right) + \frac{\partial\rho_v(\cdot)}{\partial z_{(3N_c+6)}}\dot{z}_{(3N_c+6)} + \frac{\partial\rho_v(\cdot)}{\partial z_{(3N_c+7)}}\dot{z}_{(3N_c+7)}\right]$$

The column vectors $\theta$ are given as:

$$\theta_{i,1} = \left[-z_{(Nc+i)}\frac{\partial K_i(\cdot)}{\partial z_{(3N_c+6)}}\right]$$

$$\theta_{i,2} = \left[-z_{(Nc+i)}\frac{\partial K_i(\cdot)}{\partial z_{(3N_c+7)}}\right]$$

$$\theta_{i,3} = -\left[\frac{\partial K_i(\cdot)}{\partial z_{(3N_c+6)}}\dot{z}_{(3N_c+6)} + \frac{\partial K_i(\cdot)}{\partial z_{(3N_c+7)}}\dot{z}_{(3N_c+7)}\right]$$

$$\theta_{i,4} = \left(-\left[\frac{\partial^2 K_i(\cdot)}{\partial z^2_{(3N_c+6)}}\dot{z}_{(3N_c+6)} + \frac{\partial^2 K_i(\cdot)}{\partial z_{(3N_c+7)}\partial z_{(3N_c+6)}}\dot{z}_{(3N_c+7)}\right]z_{(N_c+i)} - \frac{\partial K_i(\cdot)}{\partial z_{(3N_c+6)}}\dot{z}_{(N_c+i)}\right)$$

$$\theta_{i,5} = \left(-\left[\frac{\partial^2 K_i(\cdot)}{\partial z_{(3N_c+6)}\partial z_{(3N_c+7)}}\dot{z}_{(3N_c+6)} + \frac{\partial^2 K_i(\cdot)}{\partial z^2_{(3N_c+7)}}\dot{z}_{(3N_c+7)}\right]z_{(N_c+i)} - \frac{\partial K_i(\cdot)}{\partial z_{(3N_c+7)}}\dot{z}_{(N_c+i)}\right)$$

$$\theta_{i,6} = \frac{z_{(N_c+i)}}{z_{(3N_c+1)}}K_i(\cdot)$$

$$\theta_{i,7} = \frac{z_{(2N_c+i)}}{z_{(3N_c+1)}}K_i(\cdot)$$

$$\theta_{i,8} = \left(1 + \frac{z_{(3N_c+2)}K_i(\cdot)}{z_{(3N_c+1)}}\right)^{-1}$$

$$\theta_{9,i} = z_{(N_c+i)} - z_{(2N_c+i)} + z_{(3N_c+2)}\left(\rho_v^{-1} - \rho_l^{-1}\right)\left[\theta_{i,2}\frac{\alpha_3}{\alpha_3\alpha_{41} - \alpha_4\alpha_{40}} - \theta_{i,1}\frac{\alpha_4}{\alpha_3\alpha_{41} - \alpha_4\alpha_{40}}\right]$$

The row vectors $\xi$ are given as:

$$\xi_{1,i} = \left[z_{(3N_c+1)}\rho_l^{-2}(\cdot)\frac{\partial \rho_l(\cdot)}{\partial z_{(N_c+i)}}\right]$$

$$\xi_{2,i} = \left[z_{(3N_c+2)}\rho_v^{-2}(\cdot)\frac{\partial \rho_v(\cdot)}{\partial z_{(2N_c+i)}}\right]$$

$$\tilde{\xi}_{3,i} = \dot{z}_{(3N_c+1)}\rho_l^{-2}(\cdot)\frac{\partial \rho_l(\cdot)}{\partial z_{(N_c+i)}} - 2z_{(3N_c+1)}\rho_l^{-3}(\cdot)\frac{\partial \rho_l(\cdot)}{\partial z_{(N_c+i)}}\beta_1$$

$$\hat{\xi}_{3,i} = z_{(3N_c+1)}\rho_l^{-2}(\cdot)\left[\sum_{j=N_c+1}^{2N_c}\left(\frac{\partial^2 \rho_l(\cdot)}{\partial z_{(N_c+i)}\partial z_j}\dot{z}_j\right) + \frac{\partial^2 \rho_l(\cdot)}{\partial z_{(N_c+i)}\partial z_{(3N_c+6)}}\dot{z}_{(3N_c+6)}\right.$$
$$\left. + \frac{\partial^2 \rho_l(\cdot)}{\partial z_{(N_c+i)}\partial z_{(3N_c+7)}}\dot{z}_{(3N_c+7)}\right]$$

$$\xi_{3,i} = \tilde{\xi}_{3,i} + \hat{\xi}_{3,i}$$

$$\xi_{4,i} = \left(\frac{\partial K_i(\cdot)}{\partial z_{(3N_c+6)}}\dot{z}_{(3N_c+6)} + \frac{\partial K_i(\cdot)}{\partial z_{(3N_c+7)}}\dot{z}_{(3N_c+7)}\right)$$

$$\tilde{\xi}_{5,i} = \dot{z}_{(3N_c+2)}\rho_v^{-2}(\cdot)\frac{\partial \rho_v(\cdot)}{\partial z_{(2N_c+i)}} - 2z_{(3N_c+2)}\rho_v^{-3}(\cdot)\frac{\partial \rho_v(\cdot)}{\partial z_{(2N_c+i)}}$$

$$\hat{\xi}_{5,i} = z_{(3N_c+2)}\rho_v^{-2}(\cdot)\left[\sum_{j=2N_c+1}^{3N_c}\left(\frac{\partial^2 \rho_v(\cdot)}{\partial z_{(2N_c+i)}\partial z_j}\dot{z}_j\right) + \frac{\partial^2 \rho_v(\cdot)}{\partial z_{(2N_c+i)}\partial z_{(3N_c+6)}}\dot{z}_{(3N_c+6)}\right.$$
$$\left. + \frac{\partial^2 \rho_v(\cdot)}{\partial z_{(2N_c+i)}\partial z_{(3N_c+7)}}\dot{z}_{(3N_c+7)}\right]$$

$$\xi_{5,i} = \tilde{\xi}_{5,i} + \hat{\xi}_{5,i}$$

$$\xi_{7,i} = K_i(\cdot) - 1$$

$$\xi_{9,i} = -z_{(3N_c+4)} + K_i(\cdot)\, z_{(3N_c+5)}$$

$$\xi_{10,i} = \xi_{1,i} + K_i(\cdot)\,\xi_{2,i}$$

$$\xi_{11,i} = \frac{z_{(3N_c+2)}}{z_{(3N_c+1)}}\xi_{10,i}$$

$$\xi_{12,i} = \frac{z_{(3N_c+2)}}{z_{(3N_c+1)}}\xi_{7,i}$$

$$\xi_{13,i} = -\left(z_{(3N_c+1)} + K_i z_{(3N_c+2)}\right)$$

$$\xi_{14,i} = (\xi_{1,i} + K_i\xi_{2,i})$$

$$\xi_{15,i} = \begin{cases} \left(\alpha_{41} - \frac{\alpha_4\alpha_{40}}{\alpha_3}\right)^{-1}\left(-\xi_{10}x_i - \left(\rho_v^{-1} - \rho_l^{-1}\right) + \frac{\alpha_{40}}{\alpha_3}\xi_7 x_i\right) & i \neq N_c \\ \left(\alpha_{41} - \frac{\alpha_4\alpha_{40}}{\alpha_3}\right)^{-1}\left(-\xi_{10}x_i + \rho_v^{-1} + \frac{\alpha_{40}}{\alpha_3}\xi_7 x_i\right) & i = N_c \end{cases}$$

$$\xi_{16,i} = (-\xi_7 x_i - \alpha_4\xi_{15,i})\left(\frac{1}{\alpha_3}\right)$$

$$\xi_{17,i} = \frac{\partial \psi^V}{\partial z_{(3N_c+7)}}\xi_{15,i}$$

$$\xi_{18,i} = \begin{cases} \frac{\partial \psi^L}{\partial z_{(3N_c+7)}} \xi_{15,i} & i \neq N_c \\ \frac{\partial \psi^L}{\partial z_{(3N_c+7)}} \xi_{15,i} + \frac{\partial \psi^L}{\partial z_{(3N_c+3)}} & i = N_c \end{cases}$$

Finally, the parameters $\alpha$ are given as:

$$\alpha_1 = \left[ z_{(3N_c+2)} \rho_v^{-2}(\cdot) \frac{\partial \rho_v(\cdot)}{\partial z_{(3N_c+6)}} + z_{(3N_c+1)} \rho_l^{-2}(\cdot) \frac{\partial \rho_l(\cdot)}{\partial z_{3N_c+6}} \right]$$

$$\alpha_2 = \left[ z_{(3N_c+2)} \rho_v^{-2}(\cdot) \frac{\partial \rho_l(\cdot)}{\partial z_{(3N_c+7)}} + z_{(3N_c+1)} \rho_l^{-2}(\cdot) \frac{\partial \rho_l(\cdot)}{\partial z_{(3N_c+7)}} \right]$$

$$\alpha_3 = \left[ \sum_{i=1}^{N_c} \left( \frac{\partial K_i(\cdot)}{\partial z_{(3N_{c+6})}} z_{(Nc+i)} \right) \right]$$

$$\alpha_4 = \left[ \sum_{i=1}^{N_c} \left( \frac{\partial K_i(\cdot)}{\partial z_{(3N_{c+7})}} z_{(Nc+i)} \right) \right]$$

$$\alpha_5 = \rho_l^{-2}(\cdot) \left[ \sum_{j=N_c+1}^{2N_c} \left( \frac{\partial \rho_l(\cdot)}{\partial z_j} \dot{z}_j \right) + \frac{\partial \rho_l(\cdot)}{\partial z_{(3N_c+6)}} \dot{z}_{(3N_c+6)} + \frac{\partial \rho_l(\cdot)}{\partial z_{(3N_c+7)}} \dot{z}_{(3N_c+7)} \right]$$

$$\alpha_6 = \rho_v^{-2}(\cdot) \left[ \sum_{j=2N_c+1}^{3N_c} \left( \frac{\partial \rho_v(\cdot)}{\partial z_j} \dot{z}_j \right) + \frac{\partial \rho_v(\cdot)}{\partial z_{(3N_c+6)}} \dot{z}_{(3N_c+6)} + \frac{\partial \rho_v(\cdot)}{\partial z_{(3N_c+7)}} \dot{z}_{(3N_c+7)} \right]$$

$$\begin{aligned} \tilde{\alpha}_7 = \Bigg[ & \dot{z}_{(3N_c+1)} \rho_l^{-2}(\cdot) \frac{\partial \rho_l(\cdot)}{\partial z_{(3N_c+6)}} - 2 z_{(3N_c+1)} \rho_l^{-3}(\cdot) \frac{\partial \rho_l(\cdot)}{\partial z_{(3N_c+6)}} \beta_1 \\ & + z_{(3N_c+1)} \rho_l^{-2}(\cdot) \Bigg[ \sum_{j=N_c+1}^{2N_c} \left( \frac{\partial^2 \rho_l(\cdot)}{\partial z_{(3N_c+6)} \partial z_j} \dot{z}_j \right) \\ & + \frac{\partial^2 \rho_l(\cdot)}{\partial z_{(3N_c+6)}^2} \dot{z}_{(3N_c+6)} + \frac{\partial^2 \rho_l(\cdot)}{\partial z_{(3N_c+6)} \partial z_{(3N_c+7)}} \dot{z}_{(3N_c+7)} \Bigg] \Bigg] \end{aligned}$$

$$\begin{aligned} \hat{\alpha}_7 = \Bigg[ & \dot{z}_{(3N_c+2)} \rho_v^{-2}(\cdot) \frac{\partial \rho_v(\cdot)}{\partial z_{(3N_c+6)}} - 2 z_{(3N_c+2)} \rho_v^{-3}(\cdot) \frac{\partial \rho_v(\cdot)}{\partial z_{(3N_c+6)}} \beta_2 \\ & + z_{(3N_c+2)} \rho_v^{-2}(\cdot) \Bigg[ \sum_{j=2N_c+1}^{3N_c} \left( \frac{\partial^2 \rho_v(\cdot)}{\partial z_{(3N_c+6)} \partial z_j} \dot{z}_j \right) + \frac{\partial^2 \rho_v(\cdot)}{\partial z_{(3N_c+6)}^2} \dot{z}_{(3N_c+6)} + \frac{\partial^2 \rho_v(\cdot)}{\partial z_{(3N_c+6)} \partial z_{(3N_c+7)}} \dot{z}_{(3N_c+7)} \Bigg] \Bigg] \end{aligned}$$

$$\alpha_7 = [\tilde{\alpha}_7 + \hat{\alpha}_7]$$

$$\begin{aligned} \tilde{\alpha}_8 = \Bigg[ & \dot{z}_{(3N_c+1)} \rho_l^{-2}(\cdot) \frac{\partial \rho_l(\cdot)}{\partial z_{(3N_c+7)}} - 2 z_{(3N_c+1)} \rho_l^{-3}(\cdot) \frac{\partial \rho_l(\cdot)}{\partial z_{(3N_c+7)}} \beta_1 \\ & + z_{(3N_c+1)} \rho_l^{-2}(\cdot) \Bigg[ \sum_{j=N_c+1}^{2N_c} \left( \frac{\partial^2 \rho_l(\cdot)}{\partial z_{(3N_c+7)} \partial z_j} \dot{z}_j \right) + \frac{\partial^2 \rho_l(\cdot)}{\partial z_{(3N_c+7)} \partial z_{(3N_c+6)}} \dot{z}_{(3N_c+6)} + \frac{\partial^2 \rho_l(\cdot)}{\partial z_{(3N_c+7)}^2} \dot{z}_{(3N_c+7)} \Bigg] \Bigg] \end{aligned}$$

$$\begin{aligned} \hat{\alpha}_8 = \Bigg[ & \dot{z}_{(3N_c+2)} \rho_v^{-2}(\cdot) \frac{\partial \rho_v(\cdot)}{\partial z_{(3N_c+7)}} - 2 z_{(3N_c+2)} \rho_v^{-3}(\cdot) \frac{\partial \rho_v(\cdot)}{\partial z_{(3N_c+7)}} \beta_2 \\ & + z_{(3N_c+2)} \rho_v^{-2}(\cdot) \Bigg[ \sum_{j=2N_c+1}^{3N_c} \left( \frac{\partial^2 \rho_v(\cdot)}{\partial z_{(3N_c+7)} \partial z_j} \dot{z}_j \right) + \frac{\partial^2 \rho_v(\cdot)}{\partial z_{(3N_c+7)} \partial z_{(3N_c+6)}} \dot{z}_{(3N_c+6)} + \frac{\partial^2 \rho_v(\cdot)}{\partial z_{(3N_c+7)}^2} \dot{z}_{(3N_c+7)} \Bigg] \Bigg] \end{aligned}$$

$$\alpha_8 = [\tilde{\alpha}_8 + \hat{\alpha}_8]$$

$$\alpha_9 = -\left[\frac{\partial^2 \psi_L(\cdot)}{\partial z_{(3N_c+3)} \partial z_{(3N_c+7)}} \dot{z}_{(3N_c+7)} + \frac{\partial^2 \psi_L(\cdot)}{\partial z^2_{(3N_c+3)}} \dot{z}_{(3N_c+3)}\right]$$

$$\alpha_{10} = -\left[\frac{\partial^2 \psi_L(\cdot)}{\partial z^2_{(3N_c+7)}} \dot{z}_{(3N_c+7)} + \frac{\partial^2 \psi_L(\cdot)}{\partial z_{(3N_c+7)} \partial z_{(3N_c+3)}} \dot{z}_{(3N_c+3)}\right]$$

$$\alpha_{11} = -\left[\frac{\partial^2 \psi_V(\cdot)}{\partial z^2_{(3N_c+7)}} \dot{z}_{(3N_c+7)} + \frac{\partial^2 \psi_V(\cdot)}{\partial z_{(3N_c+7)} \partial \phi_{(N_c+2)}} \dot{\phi}_{(N_c+2)}\right]$$

$$\alpha_{12} = \sum_{i=1}^{Nc} \left[\frac{\partial K_i(\cdot)}{\partial z_{(3N_c+6)}} \dot{z}_{(N_c+i)} + \left(\frac{\partial^2 K_i(\cdot)}{\partial z^2_{(3N_c+6)}} \dot{z}_{(3N_c+6)} + \frac{\partial^2 K_i(\cdot)}{\partial z_{(3N_c+6)} \partial z_{(3N_c+7)}} \dot{z}_{(3N_c+7)}\right) z_{(N_c+i)}\right]$$

$$\alpha_{13} = \sum_{i=1}^{Nc} \left[\frac{\partial K_i(\cdot)}{\partial z_{(3N_c+7)}} \dot{z}_{(N_c+i)} + \left(\frac{\partial^2 K_i(\cdot)}{\partial z_{(3N_c+7)} \partial z_{(3N_c+6)}} \dot{z}_{(3N_c+6)} + \frac{\partial^2 K_i(\cdot)}{\partial z^2_{(3N_c+7)}} \dot{z}_{(3N_c+7)}\right) z_{(N_c+i)}\right]$$

$$\alpha_{14} = \left[z_{(3N_c+1)} \rho_l^{-2}(\cdot) \frac{\partial \rho_l(\cdot)}{\partial z_{(3N_c+6)}} + z_{(3N_c+2)} \rho_v^{-2}(\cdot) \frac{\partial \rho_v(\cdot)}{\partial z_{(3N_c+6)}}\right] = \alpha_1$$

$$\alpha_{15} = \left[z_{(3N_c+1)} \rho_l^{-2}(\cdot) \frac{\partial \rho_l(\cdot)}{\partial z_{(3N_c+7)}} + z_{(3N_c+2)} \rho_v^{-2}(\cdot) \frac{\partial \rho_v(\cdot)}{\partial z_{(3N_c+7)}}\right] = \alpha_2$$

$$\alpha_{16} = \sum_{i=1}^{N_c} \left[\frac{\partial K_i(\cdot)}{\partial z_{(3N_c+6)}} z_{(N_c+i)}\right] = \alpha_3$$

$$\alpha_{17} = \sum_{i=1}^{N_c} \left[\frac{\partial K_i(\cdot)}{\partial z_{(3N_c+7)}} z_{(N_c+i)}\right] = \alpha_4$$

$$\alpha_{18} = \left(-z_{(3N_c+2)} \sum_{i=1}^{N_c} \theta_{i,1}\right)$$

$$\alpha_{19} = \left(-z_{(3N_c+2)} \sum_{i=1}^{N_c} \theta_{i,2}\right)$$

$$\alpha_{20} = \alpha_1 + \sum_{i=1}^{N_c} \theta_{i,1} \xi_{2,i}$$

$$\alpha_{21} = \alpha_2 + \sum_{i=1}^{N_c} \theta_{i,2} \xi_{2,i}$$

$$\alpha_{22} = \sum_{i=1}^{N_c} \frac{\xi_{10,i} z_{(N_c+i)}}{\xi_{13,i}} - \rho_l^{-1}(\cdot)$$

$$\alpha_{23} = \sum_{i=1}^{N_c} \frac{\xi_{10,i} z_{(2N_c+i)}}{\xi_{13,i}} - \rho_v^{-1}(\cdot)$$

$$\alpha_{24} = -z_{(3N_c+2)} \sum_{i=1}^{N_c} \frac{\xi_{10,i} \theta_{i,1}}{\xi_{13,i}} + \alpha_1$$

$$\alpha_{25} = -z_{(3N_c+2)} \sum_{i=1}^{N_c} \frac{\xi_{10,i} \theta_{i,2}}{\xi_{13,i}} + \alpha_2$$

$$\alpha_{26} = \sum_{i=1}^{N_c} \frac{\xi_{7,i} z_{(N_c+i)}}{\xi_{13,i}}$$

$$\alpha_{27} = \sum_{i=1}^{N_c} \frac{\xi_{7,i} z_{(2N_c+i)}}{\xi_{13,i}}$$

$$\alpha_{28} = -z_{(3N_c+2)} \sum_{i=1}^{N_c} \frac{\xi_{7,i}\theta_{i,1}}{\xi_{13,i}} + \alpha_3$$

$$\alpha_{29} = -z_{(3N_c+2)} \sum_{i=1}^{N_c} \frac{\xi_{7,i}\theta_{i,2}}{\xi_{13,i}} + \alpha_4$$

$$\bar{\alpha}_{30} = -\sum_{i=1}^{N_c} \frac{z_{(N_c+i)}}{z_{(3N_c+1)}} \xi_{10,i} - \rho_l^{-1}(\cdot)$$

$$\bar{\alpha}_{31} = -\sum_{i=1}^{N_c} \frac{z_{(2N_c+i)}}{z_{(3N_c+1)}} \xi_{10,i} - \rho_v^{-1}(\cdot)$$

$$\bar{\alpha}_{32} = -\sum_{i=1}^{N_c} \frac{z_{(N_c+i)}}{z_{(3N_c+1)}} (\xi_{7,i})$$

$$\bar{\alpha}_{33} = -\sum_{i=1}^{N_c} \frac{z_{(2N_c+i)}}{z_{(3N_c+1)}} (\xi_{7,i})$$

$$\bar{\alpha}_{34} = \alpha_{14} - \sum_{i=1}^{N_c} \xi_{2,i}\theta_{i,1}$$

$$\bar{\alpha}_{35} = \alpha_{15} - \sum_{i=1}^{N_c} \xi_{2,i}\theta_{i,2}$$

$$\tilde{\alpha}_{30} = \sum_{i=1}^{N_c} \xi_{11,i}\theta_{i,8}\theta_{i,6}$$

$$\tilde{\alpha}_{31} = \sum_{i=1}^{N_c} \xi_{11,i}\theta_{i,8}\theta_{i,7}$$

$$\tilde{\alpha}_{32} = \sum_{i=1}^{N_c} \xi_{12,i}\theta_{i,8}\theta_{i,6}$$

$$\tilde{\alpha}_{33} = \sum_{i=1}^{N_c} \xi_{12,i}\theta_{i,8}\theta_{i,7}$$

$$\tilde{\alpha}_{34} = \sum_{i=1}^{N_c} \xi_{11,i}\theta_{i,8}\theta_{i,1}$$

$$\tilde{\alpha}_{35} = \sum_{i=1}^{N_c} \xi_{11,i}\theta_{i,8}\theta_{i,2}$$

$$\alpha_{30} = \bar{\alpha}_{30} + \tilde{\alpha}_{30}$$
$$\alpha_{31} = \bar{\alpha}_{31} + \tilde{\alpha}_{31}$$
$$\alpha_{32} = \bar{\alpha}_{32} + \tilde{\alpha}_{32}$$
$$\alpha_{33} = \bar{\alpha}_{33} + \tilde{\alpha}_{33}$$
$$\alpha_{34} = \bar{\alpha}_{34} + \tilde{\alpha}_{34}$$
$$\alpha_{35} = \bar{\alpha}_{35} + \tilde{\alpha}_{35}$$

$$\alpha_{36} = \sum_{i=1}^{N_c} \xi_{12,i}\theta_{i,8}\theta_{i,1} + \alpha_3$$

$$\alpha_{37} = \sum_{i=1}^{N_c} \xi_{12,i}\theta_{i,8}\theta_{i,2} + \alpha_4$$

$$\alpha_{38} = z_{(3N_c+2)} \sum_{i=1}^{N_c} \theta_{i,1} = -z_{(3N_c+2)}\alpha_3$$

$$\alpha_{39} = z_{(3N_c+2)} \sum_{i=1}^{N_c} \theta_{i,2} = -z_{(3N_c+2)}\alpha_4$$

$$\alpha_{40} = \alpha_1 - \left(\sum_{i=1}^{N_c} \xi_{2,i}\theta_{i,1}\right)$$

$$\alpha_{41} = \alpha_2 - \left(\sum_{i=1}^{N_c} \xi_{2,i}\theta_{i,2}\right)$$

## A.3 Jacobian of the Derivative Array for System 1

The Jacobian of the derivative array is constructed in the following way:

$$\mathcal{F}_1|_{z,\dot{z},\ddot{z}} = \begin{bmatrix} F|_z & F|_{\dot{z}} & F|_{\ddot{z}} \\ \dot{F}|_z & \dot{F}|_{\dot{z}} & \dot{F}|_{\ddot{z}} \end{bmatrix}$$

$$F|_z = \frac{\partial}{\partial z_i} F\left(t, z, \dot{z}\right) = \begin{bmatrix} J_{1,1} & J_{1,2} & J_{1,3} & J_{1,4} \\ J_{2,1} & J_{2,2} & J_{2,3} & J_{2,4} \\ J_{3,1} & J_{3,2} & J_{3,3} & J_{3,4} \\ J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4} \end{bmatrix} \in \mathbb{R}^{3N_c+6\times 3N_c+7}$$

$$F|_{\dot{z}} = \frac{\partial}{\partial \dot{z}_i} F\left(t, z, \dot{z}\right) = \begin{bmatrix} J_{1,5} & J_{1,6} & J_{1,7} & J_{1,8} \\ J_{2,5} & J_{2,6} & J_{2,7} & J_{2,8} \\ J_{3,5} & J_{3,6} & J_{3,7} & J_{3,8} \\ J_{4,5} & J_{4,6} & J_{4,7} & J_{4,8} \end{bmatrix} \in \mathbb{R}^{3N_c+6\times 3N_c+7}$$

$$F|_{\ddot{z}} = \frac{\partial}{\partial \ddot{z}_i} F\left(t, z, \dot{z}\right) = \begin{bmatrix} J_{1,9} & J_{1,10} & J_{1,11} & J_{1,12} \\ J_{2,5} & J_{2,10} & J_{2,11} & J_{2,12} \\ J_{3,5} & J_{3,10} & J_{3,11} & J_{3,12} \\ J_{4,5} & J_{4,10} & J_{4,11} & J_{4,12} \end{bmatrix} \in \mathbb{R}^{3N_c+6\times 3N_c+7}$$

$$\dot{F}|_z = \frac{\partial}{\partial z_i} \frac{dF}{dt}\left(t, z, \dot{z}\right) = \begin{bmatrix} J_{5,1} & J_{5,2} & J_{5,3} & J_{5,4} \\ J_{6,1} & J_{6,2} & J_{6,3} & J_{6,4} \\ J_{7,1} & J_{7,2} & J_{7,3} & J_{7,4} \\ J_{8,1} & J_{8,2} & J_{8,3} & J_{8,4} \end{bmatrix} \in \mathbb{R}^{3N+6\times 3N_c+7}$$

$$\dot{F}|_{\dot{z}} = \frac{\partial}{\partial \dot{z}_i} \frac{dF}{dt}\left(t, z, \dot{z}\right) = \begin{bmatrix} J_{5,5} & J_{5,6} & J_{5,7} & J_{5,8} \\ J_{6,5} & J_{6,6} & J_{6,7} & J_{6,8} \\ J_{7,5} & J_{7,6} & J_{7,7} & J_{7,8} \\ J_{8,5} & J_{8,6} & J_{8,7} & J_{8,8} \end{bmatrix} \in \mathbb{R}^{3N_c+6\times 3N_c+7}$$

$$\dot{F}|_{\ddot{z}} = \frac{\partial}{\partial \ddot{z}_i} \frac{dF}{dt}\left(t, z, \dot{z}\right) = \begin{bmatrix} J_{5,9} & J_{5,10} & J_{5,11} & J_{5,12} \\ J_{6,9} & J_{6,10} & J_{6,11} & J_{6,12} \\ J_{7,9} & J_{7,10} & J_{7,11} & J_{7,12} \\ J_{8,9} & J_{8,10} & J_{8,11} & J_{8,12} \end{bmatrix} \in \mathbb{R}^{3N_c+6\times 3N_c+7}$$

$$J_{1,1} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{1,2} = \begin{bmatrix} z_{(3N_c+4)} & 0 & \cdots & & 0 \\ 0 & z_{(3N_c+4)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & z_{(3N_c+4)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{1,3} = \begin{bmatrix} z_{(3N_c+5)} & 0 & \cdots & & 0 \\ 0 & z_{(3N_c+5)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & z_{(3N_c+5)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{1,4} = \begin{bmatrix} 0 & 0 & 0 & z_{(N_c+1)} & z_{(2N_c+1)} & 0 & 0 \\ \vdots & \vdots & \vdots & z_{(N_c+2)} & z_{(2N_c+2)} & \vdots & \vdots \\ & & & \vdots & \vdots & & \\ 0 & 0 & 0 & z_{(2N_c)} & z_{(3N_c)} & 0 & 0 \end{bmatrix} \in \mathbb{R}^{N_c \times 7}$$

$$J_{1,5} = I_{N_c} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{1,6} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{1,7} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{1,8} = 0 \in \mathbb{R}^{N_c \times 7}$$

$$J_{1,9} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{1,10} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{1,11} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{1,12} = 0 \in \mathbb{R}^{N_c \times 7}$$

$$J_{2,1} = I_{N_c} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{2,2} = \begin{bmatrix} -z_{(3N_c+1)} & 0 & \cdots & & 0 \\ 0 & -z_{(3N_c+1)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & -z_{(3N_c+1)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{2,3} = \begin{bmatrix} -z_{(3N_c+2)} & 0 & \cdots & & 0 \\ 0 & -z_{(3N_c+2)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & -z_{(3N_c+2)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{2,4} = \begin{bmatrix} -z_{(N_c+1)} & -z_{(2N_c+1)} & 0 & 0 & 0 & 0 & 0 \\ -z_{(N_c+2)} & -z_{(2N_c+2)} & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & & & & & \\ -z_{(2N_c)} & -z_{(3N_c)} & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{N_c \times 7}$$

$$J_{2,5} = 0 \in \mathbb{R}^{N_c \times N_c}$$
$$J_{2,6} = 0 \in \mathbb{R}^{N_c \times N_c}$$
$$J_{2,7} = 0 \in \mathbb{R}^{N_c \times N_c}$$
$$J_{2,8} = 0 \in \mathbb{R}^{N_c \times 7}$$
$$J_{2,9} = 0 \in \mathbb{R}^{N_c \times N_c}$$
$$J_{2,10} = 0 \in \mathbb{R}^{N_c \times N_c}$$
$$J_{2,11} = 0 \in \mathbb{R}^{N_c \times N_c}$$
$$J_{2,12} = 0 \in \mathbb{R}^{N_c \times 7}$$

$$J_{3,1} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{3,2} = \begin{bmatrix} -K_1(\cdot) & 0 & \cdots & & 0 \\ 0 & -K_2(\cdot) & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & -K_{N_c}(\cdot) \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{3,3} = I_{N_c} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{3,4} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \theta_{1,1} & \theta_{1,2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \theta_{2,1} & \theta_{2,2} \\ & & & & & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \theta_{N_c,1} & \theta_{N_c,2} \end{bmatrix} \in \mathbb{R}^{N_c \times 7}$$

$$J_{3,5} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{3,6} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{3,7} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{3,8} = 0 \in \mathbb{R}^{N_c \times 7}$$

$$J_{3,9} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{3,10} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{3,11} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{3,12} = 0 \in \mathbb{R}^{N_c \times 7}$$

$$J_{4,1} = \begin{bmatrix} -1 & \cdots & & -1 \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \end{bmatrix} \in \mathbb{R}^{6\times N_c}$$

$$J_{4,2} = \begin{bmatrix} 0 & \cdots & & & 0 \\ 0 & \cdots & & & 0 \\ \xi_{1,1} & \xi_{1,2} & & & \xi_{1,N_c} \\ 0 & \cdots & & & 0 \\ 0 & \cdots & & & 0 \\ \xi_{7,1} & \xi_{7,2} & \cdots & & \xi_{7,N_c} \end{bmatrix} \in \mathbb{R}^{6\times N_c}$$

$$J_{4,3} = \begin{bmatrix} 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{2,1} & \xi_{2,2} & & \xi_{2,N_c} \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \end{bmatrix} \in \mathbb{R}^{6\times N_c}$$

$$J_{4,4} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ -\rho_l^{-1}(\cdot) & -\rho_v^{-1}(\cdot) & 0 & 0 & 0 & \alpha_1 & \alpha_2 \\ 0 & 0 & -\frac{\partial\psi^L}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial\psi^L}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial\psi^V}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 0 & \alpha_3 & \alpha_4 \end{bmatrix} \in \mathbb{R}^{6\times 7}$$

$$J_{4,5} = 0 \in \mathbb{R}^{6\times N_c}$$

$$J_{4,6} = 0 \in \mathbb{R}^{6\times N_c}$$

$$J_{4,7} = 0 \in \mathbb{R}^{6\times N_c}$$

$$J_{4,8} = 0 \in \mathbb{R}^{6\times 7}$$

$$J_{4,9} = 0 \in \mathbb{R}^{6\times N_c}$$

$$J_{4,10} = 0 \in \mathbb{R}^{6\times N_c}$$

$$J_{4,11} = 0 \in \mathbb{R}^{6\times N_c}$$

$$J_{4,12} = 0 \in \mathbb{R}^{6\times 7}$$

$$J_{5,1} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,2} = \begin{bmatrix} \dot{z}_{(3N_c+4)} & 0 & \cdots & & 0 \\ 0 & \dot{z}_{(3N_c+4)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & \dot{z}_{(3N_c+4)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,3} = \begin{bmatrix} \dot{z}_{(3N_c+5)} & 0 & \cdots & & 0 \\ 0 & \dot{z}_{(3N_c+5)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & \dot{z}_{(3N_c+5)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,4} = \begin{bmatrix} 0 & 0 & 0 & \dot{z}_{(N_c+1)} & \dot{z}_{(2N_c+1)} & 0 & 0 \\ \vdots & \vdots & \vdots & \dot{z}_{(N_c+2)} & \dot{z}_{(2N_c+2)} & \vdots & \vdots \\ & & & \vdots & \vdots & & \\ 0 & 0 & 0 & \dot{z}_{(2N_c)} & \dot{z}_{(3N_c)} & 0 & 0 \end{bmatrix} \in \mathbb{R}^{N_c \times 7}$$

$$J_{5,5} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,6} = \begin{bmatrix} z_{(3N_c+4)} & 0 & \cdots & & 0 \\ 0 & z_{(3N_c+4)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & z_{(3N_c+4)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,7} = \begin{bmatrix} z_{(3N_c+5)} & 0 & \cdots & & 0 \\ 0 & z_{(3N_c+5)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & z_{(3N_c+5)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,8} = \begin{bmatrix} 0 & 0 & 0 & z_{(N_c+1)} & z_{(2N_c+1)} & 0 & 0 \\ \vdots & \vdots & \vdots & z_{(N_c+2)} & z_{(2N_c+2)} & \vdots & \vdots \\ & & & \vdots & \vdots & & \\ 0 & 0 & 0 & z_{(2N_c)} & z_{(3N_c)} & 0 & 0 \end{bmatrix} \in \mathbb{R}^{N_c \times 7}$$

$$J_{5,9} = I_{N_c} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,10} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,11} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,12} = 0 \in \mathbb{R}^{N_c \times 7}$$

$$J_{6,1} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{6,2} = \begin{bmatrix} -\dot{z}_{(3N_c+1)} & 0 & \cdots & & 0 \\ 0 & -\dot{z}_{(3N_c+1)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & -\dot{z}_{(3N_c+1)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{6,3} = \begin{bmatrix} -\dot{z}_{(3N_c+2)} & 0 & \cdots & & 0 \\ 0 & -\dot{z}_{(3N_c+2)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & -\dot{z}_{(3N_c+2)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{6,4} = \begin{bmatrix} -\dot{z}_{(N_c+1)} & -\dot{z}_{(2N_c+1)} & 0 & 0 & 0 & 0 & 0 \\ -\dot{z}_{(N_c+2)} & -\dot{z}_{(2N_c+2)} & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & & & & & \\ -\dot{z}_{(2N_c)} & -\dot{z}_{(3N_c)} & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{N_c \times 7}$$

$$J_{6,5} = I_{N_c} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{6,6} = \begin{bmatrix} -z_{(3N_c+1)} & 0 & \cdots & & 0 \\ 0 & -z_{(3N_c+1)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & -z_{(3N_c+1)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{6,7} = \begin{bmatrix} -z_{(3N_c+2)} & 0 & \cdots & & 0 \\ 0 & -z_{(3N_c+2)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & -z_{(3N_c+2)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{6,8} = \begin{bmatrix} -z_{(N_c+1)} & -z_{(2N_c+1)} & 0 & 0 & 0 & 0 & 0 \\ -z_{(N_c+2)} & -z_{(2N_c+2)} & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & & & & & \\ -z_{(2N_c)} & -z_{(3N_c)} & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{N_c \times 7}$$

$$J_{6,9} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{6,10} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{6,11} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{6,12} = 0 \in \mathbb{R}^{N_c \times 7}$$

$$J_{7,1} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{7,2} = \begin{bmatrix} \theta_{1,3} & 0 & \cdots & & 0 \\ 0 & \theta_{2,3} & & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & \theta_{N_c,3} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{7,3} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{7,4} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \theta_{1,4} & \theta_{1,5} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \theta_{2,4} & \theta_{2,5} \\ & & & & & \vdots & \vdots \\ & & & & & & \\ 0 & 0 & 0 & 0 & 0 & \theta_{N_c,4} & \theta_{N_c,5} \end{bmatrix} \in \mathbb{R}^{N_c \times 7}$$

$$J_{7,5} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{7,6} = \begin{bmatrix} -K_1(\cdot) & 0 & \cdots & & 0 \\ 0 & -K_2(\cdot) & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & -K_{N_c}(\cdot) \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{7,7} = I_{N_C} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{7,8} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \theta_{1,1} & \theta_{1,2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \theta_{2,1} & \theta_{2,2} \\ & & & & & \vdots & \vdots \\ & & & & & & \\ 0 & 0 & 0 & 0 & 0 & \theta_{N_c,1} & \theta_{N_c,2} \end{bmatrix} \in \mathbb{R}^{N_c \times 7}$$

$$J_{7,9} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{7,10} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{7,11} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{7,12} = 0 \in \mathbb{R}^{N_c \times 7}$$

$$J_{8,1} = 0 \in \mathbb{R}^{6\times N_c}$$

$$J_{8,2} = \begin{bmatrix} 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{3,1} & \xi_{3,2} & \cdots & \xi_{3,N_c} \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{4,1} & \xi_{4,2} & \cdots & \xi_{4,N_c} \end{bmatrix} \in \mathbb{R}^{6\times N_c}$$

$$J_{8,3} = \begin{bmatrix} 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{5,1} & \xi_{5,2} & \cdots & \xi_{5,N_c} \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \end{bmatrix} \in \mathbb{R}^{6\times N_c}$$

$$J_{8,4} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \alpha_5 & \alpha_6 & 0 & 0 & 0 & \alpha_7 & \alpha_8 \\ 0 & 0 & \alpha_9 & 0 & 0 & 0 & \alpha_{10} \\ 0 & 0 & 0 & 0 & 0 & 0 & \alpha_{11} \\ 0 & 0 & 0 & 0 & 0 & \alpha_{12} & \alpha_{13} \end{bmatrix} \in \mathbb{R}^{6\times 7}$$

$$J_{8,5} = \begin{bmatrix} -1 & \cdots & -1 \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \end{bmatrix} \in \mathbb{R}^{6\times N_c}$$

$$J_{8,6} = \begin{bmatrix} 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{1,1} & \xi_{1,2} & \cdots & \xi_{1,Nc} \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{7,1} & \xi_{7,2} & \cdots & \xi_{7,Nc} \end{bmatrix} \in \mathbb{R}^{6\times N_c}$$

$$J_{8,7} = \begin{bmatrix} 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{2,1} & \xi_{2,2} & \cdots & \xi_{2,Nc} \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \end{bmatrix} \in \mathbb{R}^{6\times N_c}$$

$$J_{8,8} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ -\rho_l^{-1}(\cdot) & -\rho_v^{-1}(\cdot) & 0 & 0 & 0 & \alpha_{14} & \alpha_{15} \\ 0 & 0 & -\frac{\partial \psi_L(\cdot)}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial \psi_L(\cdot)}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial \psi_V(\cdot)}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 0 & \alpha_{16} & \alpha_{17} \end{bmatrix} \in \mathbb{R}^{6\times 7}$$

$$J_{8,9} = 0 \in \mathbb{R}^{6\times N_c}$$

$$J_{8,10} = 0 \in \mathbb{R}^{6\times N_c}$$

$$J_{8,11} = 0 \in \mathbb{R}^{6\times N_c}$$
$$J_{8,12} = 0 \in \mathbb{R}^{6\times 7}$$

The total Jacobian is given as:

$$\mathcal{F}_1|_{z,\dot{z},\ddot{z}} = \begin{bmatrix} 0 & J_{1,2} & J_{1,3} & J_{1,4} & I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ I_{N_C} & J_{2,2} & J_{2,3} & J_{2,4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & J_{5,2} & J_{5,3} & J_{5,4} & 0 & J_{5,6} & J_{5,7} & J_{5,8} & I_{N_c} & 0 & 0 & 0 \\ 0 & J_{6,2} & J_{6,3} & J_{6,4} & I_{N_c} & J_{6,6} & J_{6,7} & J_{6,8} & 0 & 0 & 0 & 0 \\ 0 & J_{7,2} & 0 & J_{7,4} & 0 & J_{7,6} & I_{N_C} & J_{7,8} & 0 & 0 & 0 & 0 \\ J_{8,1} & J_{8,2} & J_{8,3} & J_{8,4} & J_{8,5} & J_{8,6} & J_{8,7} & J_{8,8} & 0 & 0 & 0 & 0 \end{bmatrix} \qquad \begin{matrix} (N_c) \\ (N_c) \\ (N_c) \\ (6) \\ (N_c) \\ (N_c) \\ (N_c) \\ (6) \end{matrix} \tag{A.10}$$

## A.4 Ranks of System 1 Jacobian Elements

### A.4.1 Case $\mu = 0$

In order to test Hypothesis 1, the ranks of the matrices $\mathcal{F}_0|_{z,\dot{z}} = F|_{z,\dot{z}}$ and $\mathcal{F}_0|_{\dot{z}}$ must be determined.

$$
\begin{array}{cc}
\mathcal{F}_0|_{z,\dot{z}} = \begin{bmatrix} 0 & J_{1,2} & J_{1,3} & J_{1,4} & I_{N_c} & 0 & 0 & 0 \\ I_{N_C} & J_{2,2} & J_{2,3} & J_{2,4} & 0 & 0 & 0 & 0 \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} & 0 & 0 & 0 & 0 \\ J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4} & 0 & 0 & 0 & 0 \end{bmatrix} & \begin{array}{c} (N_c) \\ (N_c) \\ (N_c) \\ (6) \end{array}
\end{array}
$$

$$
\text{rank} \begin{bmatrix} 0 & J_{1,2} & J_{1,3} & J_{1,4} & I_{N_c} \\ I_{N_C} & J_{2,2} & J_{2,3} & J_{2,4} & 0 \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} & 0 \\ J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4} & 0 \end{bmatrix}
$$

$$
= \text{rank} \begin{bmatrix} 0 & J_{1,2} & J_{1,3} & J_{1,4} & I_{N_c} \\ I_{N_C} & (J_{2,2} - J_{2,3}J_{3,2}) & 0 & (J_{2,4} - J_{2,3}J_{3,4}) & 0 \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} & 0 \\ 0 & (J_{4,2} - J_{4,1}J_{2,2}) & (J_{4,3} - J_{4,1}J_{2,3}) & (J_{4,4} - J_{4,1}J_{2,4}) & 0 \end{bmatrix} \begin{array}{c} \\ R_2 - J_{2,3}R_3 \\ \\ R_4 - J_{4,1}R_2 \end{array}
$$

Define the following notation:

$$
\begin{aligned}
J^*_{4,2} &= J_{4,2} - J_{4,1}J_{2,2} \\
J^*_{4,3} &= J_{4,3} - J_{4,1}J_{2,3} \\
J^*_{4,4} &= J_{4,4} - J_{4,1}J_{2,4} \\
J^{**}_{4,2} &= J^*_{4,2} - J^*_{4,3}J_{3,2} \\
J^{**}_{4,4} &= J^*_{4,4} - J^*_{4,3}J_{3,4}
\end{aligned}
$$

Which gives:

$$
\text{rank} \begin{bmatrix} 0 & J_{1,2} & J_{1,3} & J_{1,4} & I_{N_c} \\ I_{N_C} & (J_{2,2} - J_{2,3}J_{3,2}) & 0 & (J_{2,4} - J_{2,3}J_{3,4}) & 0 \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} & 0 \\ 0 & J^*_{4,2} & J^*_{4,3} & J^*_{4,4} & 0 \end{bmatrix}
$$

$$
= \text{rank} \begin{bmatrix} 0 & 0 & 0 & 0 & I_{N_c} \\ I_{N_C} & 0 & 0 & 0 & 0 \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} & 0 \\ 0 & J^{**}_{4,2} & 0 & J^{**}_{4,4} & 0 \end{bmatrix} \begin{array}{c} \text{eliminate} \\ \text{eliminate} \\ \\ R_4 - J^*_{4,3}R_3 \end{array} = \text{rank} \begin{bmatrix} 0 & 0 & 0 & 0 & I_{N_c} \\ I_{N_C} & 0 & 0 & 0 & 0 \\ 0 & 0 & I_{N_c} & 0 & 0 \\ 0 & J^{**}_{4,2} & 0 & J^{**}_{4,4} & 0 \end{bmatrix} \begin{array}{c} \\ \\ \text{eliminate} \\ \\ \end{array}
$$

This is simplified as follows:

$$\text{rank}\left[\mathcal{F}_0|_{z,\dot{z}}\right] = 3N_c + \text{rank}\left[\begin{array}{cc} J_{4,2}^{**} & J_{4,4}^{**} \end{array}\right]$$

In order to investigate the matrix rank, the following ingredients are needed:

$$J_{4,2}^{*} = \begin{bmatrix} -z_{(3N_c+1)} & \cdots & & -z_{(3N_c+1)} \\ 0 & \cdots & & 0 \\ \xi_{1,1} & \xi_{1,2} & & \xi_{1,N_c} \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{7,1} & \xi_{7,2} & \cdots & \xi_{7,N_c} \end{bmatrix} \in \mathbb{R}^{6\times N_c}$$

$$J_{4,3}^{*} = \begin{bmatrix} -z_{(3N_c+2)} & \cdots & -z_{(3N_c+2)} \\ 0 & \cdots & 0 \\ \xi_{2,1} & \xi_{2,2} & \xi_{2,N_c} \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \end{bmatrix} \in \mathbb{R}^{6\times N_c}$$

$$J_{4,2}^{**} = \begin{bmatrix} \xi_{13,1} & \cdots & \xi_{13,N_c} \\ 0 & \cdots & 0 \\ \xi_{10,1} & \cdots & \xi_{10,N_c} \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ \xi_{7,1} & \cdots & \xi_{7,N_c} \end{bmatrix} \in \mathbb{R}^{6\times N_c}$$

$$J_{4,4}^{*} = \begin{bmatrix} -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ -\rho_l^{-1}(\cdot) & -\rho_v^{-1}(\cdot) & 0 & 0 & 0 & \alpha_1 & \alpha_2 \\ 0 & 0 & -\frac{\partial\psi^L}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial\psi^L}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial\psi^V}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 0 & \alpha_3 & \alpha_4 \end{bmatrix} \in \mathbb{R}^{6\times 7}$$

$$J_{4,4}^{**} = \begin{bmatrix} -1 & -1 & 1 & 0 & 0 & -\alpha_{18} & -\alpha_{19} \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ -\rho_l^{-1}(\cdot) & -\rho_v^{-1}(\cdot) & 0 & 0 & 0 & \alpha_{20} & \alpha_{21} \\ 0 & 0 & -\frac{\partial\psi^L}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial\psi^L}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial\psi^V}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 0 & \alpha_3 & \alpha_4 \end{bmatrix} \in \mathbb{R}^{6\times 7}$$

Note that on a solution manifold, $\sum_{i=N_c+1}^{2N_c} z_i = \sum_{i=2N_C+1}^{3N_c} z_i = 1$. Putting these together, under Assumptions 3.1 and 3.2, it follows that:

$$\text{rank}\left[\begin{array}{cc} J_{4,2}^{**} & J_{4,4}^{**} \end{array}\right] = \text{rank}\begin{array}{l}\begin{bmatrix} \xi_{13,1} & \cdots & \xi_{13,N_c} & 0 & 0 & 0 & 0 & 0 & -\alpha_{18} & -\alpha_{19} \\ 0 & \cdots & 0 & -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ \xi_{10,1} & \cdots & \xi_{10,N_c} & -\rho_l^{-1}(\cdot) & -\rho_v^{-1}(\cdot) & 0 & 0 & 0 & \alpha_{20} & \alpha_{21} \\ 0 & \cdots & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \xi_{7,1} & \cdots & \xi_{7,N_c} & 0 & 0 & 0 & 0 & 0 & \alpha_3 & \alpha_4 \end{bmatrix}\end{array}\begin{array}{l} R_1 - R_2 \\ \\ \\ \text{eliminate} \\ \text{eliminate} \\ \\ \end{array}$$

$$
= \text{rank} \left[ \begin{matrix} \xi_{13,1} & \cdots & \xi_{13,N_c} & 0 & 0 & 0 & 0 & 0 & -\alpha_{18} & -\alpha_{19} \\ 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ \xi_{10,1} & \cdots & \xi_{10,N_c} & -\rho_l^{-1}(\cdot) & -\rho_v^{-1}(\cdot) & 0 & 0 & 0 & \alpha_{20} & \alpha_{21} \\ 0 & \cdots & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \xi_{7,1} & \cdots & \xi_{7,N_c} & 0 & 0 & 0 & 0 & 0 & \alpha_3 & \alpha_4 \end{matrix} \right] \begin{matrix} \\ \text{eliminate} \\ \\ \\ \\ \\ \end{matrix}
$$

$$
= 3 + \text{rank} \left[ \begin{matrix} \xi_{13,1} & \cdots & \xi_{13,N_c} & 0 & 0 & -z_{(3N_c+2)}\alpha_3 & -z_{(3N_c+2)}\alpha_4 \\ \xi_{10,1} & \cdots & \xi_{10,N_c} & -\rho_l^{-1}(\cdot) & -\rho_v^{-1}(\cdot) & \alpha_{20} & \alpha_{21} \\ \xi_{7,1} & \cdots & \xi_{7,N_c} & 0 & 0 & \alpha_3 & \alpha_4 \end{matrix} \right]
$$

$$
= 6
$$

Which further gives:

$$
\text{rank}\left(\mathcal{F}_0|_{z,\dot{z}}\right) = 3N_c + 6
$$

For $\mathcal{F}_0|_{\dot{z}}$, the calculation is trivial:

$$
\mathcal{F}_0|_{\dot{z}} = \left[ \begin{matrix} I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{matrix} \right] \qquad \begin{matrix} (N_c) \\ (N_c) \\ (N_c) \\ (6) \end{matrix}
$$

$$
\text{rank}\left(\mathcal{F}_0|_{\dot{z}}\right) = N_c
$$

### A.4.2 Case $\mu = 1$

The ranks of the matrices $\mathcal{F}_1|_{z,\dot{z},\ddot{z}}$ and $\mathcal{F}_1|_{\dot{z},\ddot{z}}$ must be determined. Beginning with the form of the Jacobian given previously as (A.10). The first step is to swap columns and perform row operations:

$$
\text{rank} \left[ \begin{matrix} 0 & D_{1,2} & D_{1,3} & J_{1,4} & I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ I_{N_C} & D_{2,2} & D_{2,3} & J_{2,4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & J_{5,2} & J_{5,3} & J_{5,4} & 0 & D_{5,6} & D_{5,7} & J_{5,8} & I_{N_c} & 0 & 0 & 0 \\ 0 & J_{6,2} & J_{6,3} & J_{6,4} & I_{N_c} & D_{6,6} & D_{6,7} & J_{6,8} & 0 & 0 & 0 & 0 \\ 0 & J_{7,2} & 0 & J_{7,4} & 0 & D_{7,6} & I_{N_C} & J_{7,8} & 0 & 0 & 0 & 0 \\ 0 & J_{8,2} & J_{8,3} & J_{8,4} & J_{8,5} & J_{8,6} & J_{8,7} & J_{8,8} & 0 & 0 & 0 & 0 \end{matrix} \right]
$$

$$
= \text{rank} \left[ \begin{matrix} I_{N_c} & 0 & D_{1,3} & J_{1,4} & 0 & 0 & 0 & 0 & D_{1,2} \\ 0 & I_{N_C} & D_{2,3} & J_{2,4} & 0 & 0 & 0 & 0 & D_{2,2} \\ 0 & 0 & I_{N_c} & J_{3,4} & 0 & 0 & 0 & 0 & J_{3,2} \\ 0 & J_{4,1} & J_{4,3} & J_{4,4} & 0 & 0 & 0 & 0 & J_{4,2} \\ 0 & 0 & J_{5,3} & J_{5,4} & I_{N_c} & D_{5,6} & D_{5,7} & J_{5,8} & J_{5,2} \\ I_{N_c} & 0 & J_{6,3} & J_{6,4} & 0 & D_{6,6} & D_{6,7} & J_{6,8} & J_{6,2} \\ 0 & 0 & 0 & J_{7,4} & 0 & D_{7,6} & I_{N_C} & J_{7,8} & J_{7,2} \\ J_{8,5} & 0 & J_{8,3} & J_{8,4} & 0 & J_{8,6} & J_{8,7} & J_{8,8} & J_{8,2} \end{matrix} \right]
$$

$$
\text{rank} \left[ \begin{matrix} I_{N_c} & 0 & D_{1,3} & J_{1,4} & 0 & 0 & 0 & 0 & D_{1,2} \\ 0 & I_{N_C} & D_{2,3} & J_{2,4} & 0 & 0 & 0 & 0 & D_{2,2} \\ 0 & 0 & I_{N_c} & J_{3,4} & 0 & 0 & 0 & 0 & J_{3,2} \\ 0 & J_{4,1} & J_{4,3} & J_{4,4} & 0 & 0 & 0 & 0 & J_{4,2} \\ 0 & 0 & J_{5,3} & J_{5,4} & I_{N_c} & D_{5,6} & D_{5,7} & J_{5,8} & J_{5,2} \\ I_{N_c} & 0 & J_{6,3} & J_{6,4} & 0 & D_{6,6} & D_{6,7} & J_{6,8} & J_{6,2} \\ 0 & 0 & 0 & J_{7,4} & 0 & D_{7,6} & I_{N_C} & J_{7,8} & J_{7,2} \\ J_{8,5} & 0 & J_{8,3} & J_{8,4} & 0 & J_{8,6} & J_{8,7} & J_{8,8} & J_{8,2} \end{matrix} \right]
$$

$$
= \text{rank} \left[ \begin{matrix} I_{N_c} & 0 & 0 & (J_{1,4} - D_{1,3}J_{3,4}) & 0 & 0 & 0 & 0 & (D_{1,2} - D_{1,3}J_{3,2}) \\ 0 & I_{N_C} & 0 & (J_{2,4} - D_{2,3}J_{3,4}) & 0 & 0 & 0 & 0 & (D_{2,2} - D_{2,3}J_{3,2}) \\ 0 & 0 & I_{N_c} & J_{3,4} & 0 & 0 & 0 & 0 & J_{3,2} \\ 0 & J_{4,1} & J_{4,3} & J_{4,4} & 0 & 0 & 0 & 0 & J_{4,2} \\ 0 & 0 & J_{5,3} & J_{5,4} & I_{N_c} & D_{5,6} & D_{5,7} & J_{5,8} & J_{5,2} \\ 0 & 0 & (J_{6,3} - D_{1,3}) & (J_{6,4} - J_{1,4}) & 0 & D_{6,6} & D_{6,7} & J_{6,8} & (J_{6,2} - D_{1,2}) \\ 0 & 0 & 0 & J_{7,4} & 0 & D_{7,6} & I_{N_C} & J_{7,8} & J_{7,2} \\ 0 & 0 & (J_{8,3} - J_{8,5}D_{1,3}) & (J_{8,4} - J_{8,5}J_{1,4}) & 0 & J_{8,6} & J_{8,7} & J_{8,8} & (J_{8,2} - J_{8,5}D_{1,2}) \end{matrix} \right] \begin{matrix} R_1 - D_{1,3}R_3 \\ R_2 - D_{2,3}R_3 \\ \\ \\ \\ R_6 - R_1 \\ \\ R_8 - J_{8,5}R_1 \end{matrix}
$$

$$
=\text{rank}\begin{bmatrix}
I_{N_c} & 0 & 0 & (J_{1,4}-D_{1,3}J_{3,4}) & 0 & 0 & 0 & 0 & (D_{1,2}-D_{1,3}J_{3,2}) \\
0 & I_{N_C} & 0 & (J_{2,4}-D_{2,3}J_{3,4}) & 0 & 0 & 0 & 0 & (D_{2,2}-D_{2,3}J_{3,2}) \\
0 & 0 & I_{N_c} & J_{3,4} & 0 & 0 & 0 & 0 & J_{3,2} \\
0 & 0 & J_{4,3} & (J_{4,4}-J_{4,1}\left(J_{2,4}-D_{2,3}J_{3,4}\right)) & 0 & 0 & 0 & 0 & (J_{4,2}-J_{4,1}\left(D_{2,2}-D_{2,3}J_{3,2}\right)) \\
0 & 0 & J_{5,3} & J_{5,4} & I_{N_c} & D_{5,6} & D_{5,7} & J_{5,8} & J_{5,2} \\
0 & 0 & (J_{6,3}-D_{1,3}) & (J_{6,4}-J_{1,4}) & 0 & D_{6,6} & D_{6,7} & J_{6,8} & (J_{6,2}-D_{1,2}) \\
0 & 0 & 0 & J_{7,4} & 0 & D_{7,6} & I_{N_C} & J_{7,8} & J_{7,2} \\
0 & 0 & (J_{8,3}-J_{8,5}D_{1,3}) & (J_{8,4}-J_{8,5}J_{1,4}) & 0 & J_{8,6} & J_{8,7} & J_{8,8} & (J_{8,2}-J_{8,5}D_{1,2})
\end{bmatrix}
\begin{matrix} \\ \\ \\ R_4-J_{41}R_2 \\ \\ \\ \\ \\ \end{matrix}
$$

$$
=\text{rank}\begin{bmatrix}
I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & I_{N_C} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & I_{N_c} & J_{3,4} & 0 & 0 & 0 & 0 & J_{3,2} \\
0 & 0 & J_{4,3} & (J_{4,4}-J_{4,1}\left(J_{2,4}-D_{2,3}J_{3,4}\right)) & 0 & 0 & 0 & 0 & (J_{4,2}-J_{4,1}\left(D_{2,2}-D_{2,3}J_{3,2}\right)) \\
0 & 0 & J_{5,3} & J_{5,4} & I_{N_c} & D_{5,6} & D_{5,7} & J_{5,8} & J_{5,2} \\
0 & 0 & (J_{6,3}-D_{1,3}) & (J_{6,4}-J_{1,4}) & 0 & D_{6,6} & D_{6,7} & J_{6,8} & (J_{6,2}-D_{1,2}) \\
0 & 0 & 0 & J_{7,4} & 0 & D_{7,6} & I_{N_C} & J_{7,8} & J_{7,2} \\
0 & 0 & (J_{8,3}-J_{8,5}D_{1,3}) & (J_{8,4}-J_{8,5}J_{1,4}) & 0 & J_{8,6} & J_{8,7} & J_{8,8} & (J_{8,2}-J_{8,5}D_{1,2})
\end{bmatrix}
\begin{matrix} \text{Eliminate} \\ \text{Eliminate} \\ \\ \\ \\ \\ \\ \\ \end{matrix}
$$

Define some convenient matrices to condense the typography:

$$
\begin{aligned}
J^*_{4,4} &= J_{4,4} - J_{4,1}\left(J_{2,4} - D_{2,3}J_{3,4}\right) \\
J^*_{4,2} &= J_{4,2} - J_{4,1}\left(D_{2,2} - D_{2,3}J_{3,2}\right) \\
J^*_{6,3} &= J_{6,3} - D_{1,3} \\
J^*_{6,4} &= J_{6,4} - J_{1,4} \\
J^*_{8,3} &= J_{8,3} - J_{8,5}D_{1,3} \\
J^*_{8,4} &= J_{8,4} - J_{8,5}J_{1,4} \\
J^*_{8,2} &= J_{8,2} - J_{8,5}D_{1,2} \\
J^*_{6,2} &= J_{6,2} - D_{1,2}
\end{aligned}
$$

$$
\text{rank}\begin{bmatrix}
I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & I_{N_C} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & I_{N_c} & J_{3,4} & 0 & 0 & 0 & 0 & J_{3,2} \\
0 & 0 & J_{4,3} & J^*_{4,4} & 0 & 0 & 0 & 0 & J^*_{4,2} \\
0 & 0 & J_{5,3} & J_{5,4} & I_{N_c} & D_{5,6} & D_{5,7} & J_{5,8} & J_{5,2} \\
0 & 0 & J^*_{6,3} & J^*_{6,4} & 0 & D_{6,6} & D_{6,7} & J_{6,8} & J^*_{6,2} \\
0 & 0 & 0 & J_{7,4} & 0 & D_{7,6} & I_{N_C} & J_{7,8} & J_{7,2} \\
0 & 0 & J^*_{8,3} & J^*_{8,4} & 0 & J_{8,6} & J_{8,7} & J_{8,8} & J^*_{8,2}
\end{bmatrix}
$$

$$
=\text{rank}\begin{bmatrix}
I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & I_{N_C} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & I_{N_c} & J_{3,4} & 0 & 0 & 0 & 0 & J_{3,2} \\
0 & 0 & 0 & \left(J^*_{4,4}-J_{4,3}J_{3,4}\right) & 0 & 0 & 0 & 0 & \left(J^*_{4,2}-J_{4,3}J_{3,2}\right) \\
0 & 0 & 0 & (J_{5,4}-J_{5,3}J_{3,4}) & I_{N_c} & D_{5,6} & D_{5,7} & J_{5,8} & (J_{5,2}-J_{5,3}J_{3,2}) \\
0 & 0 & 0 & \left(J^*_{6,4}-J^*_{6,3}J_{3,4}\right) & 0 & D_{6,6} & D_{6,7} & J_{6,8} & \left(J^*_{6,2}-J^*_{6,3}J_{3,2}\right) \\
0 & 0 & 0 & J_{7,4} & 0 & D_{7,6} & I_{N_C} & J_{7,8} & J_{7,2} \\
0 & 0 & 0 & \left(J^*_{8,4}-J^*_{8,3}J_{3,4}\right) & 0 & J_{8,6} & J_{8,7} & J_{8,8} & \left(J^*_{8,2}-J^*_{8,3}J_{3,2}\right)
\end{bmatrix}
\begin{matrix} \\ \\ \\ R_4-J_{4,3}R_3 \\ R_5-J_{5,3}R_3 \\ R_6-J^*_{6,3}R_3 \\ \\ R_8-J^*_{8,3}R_3 \end{matrix}
$$

More groups can be defined:

$$
\begin{aligned}
J^{**}_{4,4} &= J^*_{4,4} - J_{4,3}J_{3,4} \\
J^*_{5,4} &= J_{5,4} - J_{5,3}J_{3,4} \\
J^{**}_{6,4} &= J^*_{6,4} - J^*_{6,3}J_{3,4}
\end{aligned}
$$

$$
\begin{aligned}
J_{8,4}^{**} &= J_{8,4}^{*} - J_{8,3}^{*}J_{3,4}\\
J_{4,2}^{**} &= J_{4,2}^{*} - J_{4,3}J_{3,2}\\
J_{5,2}^{*} &= J_{5,2} - J_{5,3}J_{3,2}\\
J_{6,2}^{**} &= J_{6,2}^{*} - J_{6,3}^{*}J_{3,2}\\
J_{8,2}^{**} &= J_{8,2}^{*} - J_{8,3}^{*}J_{3,2}\\
J_{6,4}^{***} &= J_{6,4}^{**} - D_{6,7}J_{7,4}\\
D_{6,6}^{*} &= D_{6,6} - D_{6,7}D_{7,6}\\
J_{6,8}^{*} &= J_{6,8} - D_{6,7}J_{7,8}\\
J_{6,2}^{***} &= J_{6,2}^{**} - D_{6,7}J_{7,2}\\
J_{8,4}^{***} &= J_{8,4}^{**} - J_{8,7}J_{7,4}\\
J_{8,6}^{*} &= J_{8,6} - J_{8,7}D_{7,6}\\
J_{8,8}^{*} &= J_{8,8} - J_{8,7}J_{7,8}\\
J_{8,2}^{***} &= J_{8,2}^{**} - J_{8,7}J_{7,2}
\end{aligned}
$$

$$
\text{rank}\begin{bmatrix}
I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & I_{N_C} & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & I_{N_c} & J_{3,4} & 0 & 0 & 0 & 0 & J_{3,2}\\
0 & 0 & 0 & J_{4,4}^{**} & 0 & 0 & 0 & 0 & J_{4,2}^{**}\\
0 & 0 & 0 & J_{5,4}^{*} & I_{N_c} & D_{5,6} & D_{5,7} & J_{5,8} & J_{5,2}^{*}\\
0 & 0 & 0 & J_{6,4}^{**} & 0 & D_{6,6} & D_{6,7} & J_{6,8} & J_{6,2}^{**}\\
0 & 0 & 0 & J_{7,4} & 0 & D_{7,6} & I_{N_C} & J_{7,8} & J_{7,2}\\
0 & 0 & 0 & J_{8,4}^{**} & 0 & J_{8,6} & J_{8,7} & J_{8,8} & J_{8,2}^{**}
\end{bmatrix}
$$

$$
=\text{rank}\begin{bmatrix}
I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & I_{N_C} & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & J_{4,4}^{**} & 0 & 0 & 0 & 0 & J_{4,2}^{**}\\
0 & 0 & 0 & 0 & I_{N_c} & 0 & 0 & 0 & 0\\
0 & 0 & 0 & \left(J_{6,4}^{**} - D_{6,7}J_{7,4}\right) & 0 & (D_{6,6} - D_{6,7}D_{7,6}) & 0 & (J_{6,8} - D_{6,7}J_{7,8}) & \left(J_{6,2}^{**} - D_{6,7}J_{7,2}\right)\\
0 & 0 & 0 & J_{7,4} & 0 & D_{7,6} & I_{N_C} & J_{7,8} & J_{7,2}\\
0 & 0 & 0 & \left(J_{8,4}^{**} - J_{8,7}J_{7,4}\right) & 0 & (J_{8,6} - J_{8,7}D_{7,6}) & 0 & (J_{8,8} - J_{8,7}J_{7,8}) & \left(J_{8,2}^{**} - J_{8,7}J_{7,2}\right)
\end{bmatrix}
\begin{array}{c}
\\
\\
\\
\text{Eliminate}\\
\text{Eliminate}\\
R_6 - D_{6,7}R_7\\
\\
R_8 - J_{8,7}R_7
\end{array}
$$

$$
\text{rank}\begin{bmatrix}
I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & I_{N_C} & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & J_{4,4}^{**} & 0 & 0 & 0 & 0 & J_{4,2}^{**}\\
0 & 0 & 0 & 0 & I_{N_c} & 0 & 0 & 0 & 0\\
0 & 0 & 0 & J_{6,4}^{***} & 0 & D_{6,6}^{*} & 0 & J_{6,8}^{*} & J_{6,2}^{***}\\
0 & 0 & 0 & J_{7,4} & 0 & D_{7,6} & I_{N_C} & J_{7,8} & J_{7,2}\\
0 & 0 & 0 & J_{8,4}^{***} & 0 & J_{8,6}^{*} & 0 & J_{8,8}^{*} & J_{8,2}^{***}
\end{bmatrix}
$$

$$
=\text{rank}\begin{bmatrix}
I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & I_{N_C} & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & J_{4,4}^{**} & 0 & 0 & 0 & 0 & J_{4,2}^{**}\\
0 & 0 & 0 & 0 & I_{N_c} & 0 & 0 & 0 & 0\\
0 & 0 & 0 & J_{6,4}^{***} & 0 & D_{6,6}^{*} & 0 & J_{6,8}^{*} & J_{6,2}^{***}\\
0 & 0 & 0 & 0 & 0 & 0 & I_{N_C} & 0 & 0\\
0 & 0 & 0 & J_{8,4}^{***} & 0 & J_{8,6}^{*} & 0 & J_{8,8}^{*} & J_{8,2}^{***}
\end{bmatrix}
\begin{array}{c}
\\
\\
\\
\\
\\
\\
\text{Eliminate}\\
\\
\end{array}
$$

$$
=5N_c + \text{rank}\begin{bmatrix}
J_{4,4}^{**} & 0 & 0 & J_{4,2}^{**}\\
J_{6,4}^{***} & D_{6,6}^{*} & J_{6,8}^{*} & J_{6,2}^{***}\\
J_{8,4}^{***} & J_{8,6}^{*} & J_{8,8}^{*} & J_{8,2}^{***}
\end{bmatrix}
$$

Note that $D^{*}_{6,6}$is a diagonal matrix assumed non-zero and hence:

$$\text{rank}\begin{bmatrix} J^{**}_{4,4} & 0 & 0 & J^{**}_{4,2} \\ J^{***}_{6,4} & D^{*}_{6,6} & J^{*}_{6,8} & J^{***}_{6,2} \\ J^{***}_{8,4} & J^{*}_{8,6} & J^{*}_{8,8} & J^{***}_{8,2} \end{bmatrix} = \text{rank}\begin{bmatrix} J^{**}_{4,4} & 0 & 0 & J^{**}_{4,2} \\ D^{*-1}_{6,6}J^{***}_{6,4} & I_{Nc} & D^{*-1}_{6,6}J^{*}_{6,8} & D^{*-1}_{6,6}J^{***}_{6,2} \\ J^{***}_{8,4} & J^{*}_{8,6} & J^{*}_{8,8} & J^{***}_{8,2} \end{bmatrix}$$

$$\text{rank}\begin{bmatrix} J^{**}_{4,4} & 0 & 0 & J^{**}_{4,2} \\ D^{*-1}_{6,6}J^{***}_{6,4} & I_{Nc} & D^{*-1}_{6,6}J^{*}_{6,8} & D^{*-1}_{6,6}J^{***}_{6,2} \\ J^{***}_{8,4} & J^{*}_{8,6} & J^{*}_{8,8} & J^{***}_{8,2} \end{bmatrix}$$

$$=\text{rank}\begin{bmatrix} J^{**}_{4,4} & 0 & 0 & J^{**}_{4,2} \\ D^{*-1}_{6,6}J^{***}_{6,4} & I_{Nc} & D^{*-1}_{6,6}J^{*}_{6,8} & D^{*-1}_{6,6}J^{***}_{6,2} \\ \left(J^{***}_{8,4} - J^{*}_{8,6}D^{*-1}_{6,6}J^{***}_{6,4}\right) & 0 & \left(J^{*}_{8,8} - J^{*}_{8,6}D^{*-1}_{6,6}J^{*}_{6,8}\right) & \left(J^{***}_{8,2} - J^{*}_{8,6}D^{*-1}_{6,6}J^{***}_{6,2}\right) \end{bmatrix} \quad R_3 - J^{*}_{8,6}R_2$$

Some final groups are required:

$$\begin{aligned} J^{(4*)}_{8,4} &= J^{***}_{8,4} - J^{*}_{8,6}D^{*-1}_{6,6}J^{***}_{6,4} \\ J^{**}_{8,8} &= J^{*}_{8,8} - J^{*}_{8,6}D^{*-1}_{6,6}J^{*}_{6,8} \\ J^{(4*)}_{8.2} &= J^{***}_{8,2} - J^{*}_{8,6}D^{*-1}_{6,6}J^{***}_{6,2} \end{aligned}$$

$$\text{rank}\begin{bmatrix} J^{**}_{4,4} & 0 & 0 & J^{**}_{4,2} \\ D^{*-1}_{6,6}J^{***}_{6,4} & I_{Nc} & D^{*-1}_{6,6}J^{*}_{6,8} & D^{*-1}_{6,6}J^{***}_{6,2} \\ J^{(4*)}_{8,4} & 0 & J^{**}_{8,8} & J^{(4*)}_{8.2} \end{bmatrix} =\text{rank}\begin{bmatrix} J^{**}_{4,4} & 0 & 0 & J^{**}_{4,2} \\ 0 & I_{Nc} & 0 & 0 \\ J^{(4*)}_{8,4} & 0 & J^{**}_{8,8} & J^{(4*)}_{8.2} \end{bmatrix} \qquad \text{Eliminate}$$

$$=N_c + \text{rank}\begin{bmatrix} J^{**}_{4,4} & 0 & J^{**}_{4,2} \\ J^{(4*)}_{8,4} & J^{**}_{8,8} & J^{(4*)}_{8.2} \end{bmatrix}$$

To determine $J^{**}_{4,4}$ explicitly requires the following:

$$J^{**}_{4,4} = J^{*}_{4,4} - J_{4,3}J_{3,4} = J_{4,4} - J_{4,1}\left(J_{2,4} - D_{2,3}J_{34}\right) - J_{4,3}J_{3,4}$$

Term-wise, these matrix products are given by:

$$D_{2,3}J_{34} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \left(-z_{(3N_c+2)}\theta_{1,1}\right) & \left(-z_{(3N_c+2)}\theta_{1,2}\right) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \left(-z_{(3N_c+2)}\theta_{2,1}\right) & \left(-z_{(3N_c+2)}\theta_{2,2}\right) \\ & & & & & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \left(-z_{(3N_c+2)}\theta_{N_c,1}\right) & \left(-z_{(3N_c+2)}\theta_{N_c,2}\right) \end{bmatrix} \in \mathbb{R}^{N_c\times 7}$$

$$J_{2,4} - D_{2,3}J_{34} = \begin{bmatrix} -z_{(N_c+1)} & -z_{(2N_c+1)} & 0 & 0 & 0 & \left(-z_{(3N_c+2)}\theta_{1,1}\right) & \left(-z_{(3N_c+2)}\theta_{1,2}\right) \\ -z_{(N_c+2)} & -z_{(2N_c+2)} & \vdots & \vdots & \vdots & \left(-z_{(3N_c+2)}\theta_{2,1}\right) & \left(-z_{(3N_c+2)}\theta_{2,2}\right) \\ \vdots & \vdots & & & & \vdots & \vdots \\ -z_{(2N_c)} & -z_{(3N_c)} & 0 & 0 & 0 & \left(-z_{(3N_c+2)}\theta_{N_c,1}\right) & \left(-z_{(3N_c+2)}\theta_{N_c,2}\right) \end{bmatrix} \in \mathbb{R}^{N_c\times 7}$$

$$J_{41}\left(J_{2,4} - D_{2,3}J_{34}\right) = \begin{bmatrix} \left(\sum_{i=N_c+1}^{2N_c} z_i\right) & \left(\sum_{i=2N_C+1}^{3N_c} z_i\right) & 0 & 0 & 0 & \left(z_{(3N_c+2)}\sum_{i=1}^{N_c}\theta_{i,1}\right) & \left(z_{(3N_c+2)}\sum_{i=1}^{N_c}\theta_{i,2}\right) \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

On the solution manifold $\sum_{i=N_c+1}^{2N_c} z_i = \sum_{i=2N_C+1}^{3N_c} z_i = 1$. Now, recall groups for $\alpha_{18}$ to $\alpha_{21}$:

$$J_{4,4}^{**} = \begin{bmatrix} -1 & -1 & 1 & 1 & 1 & \alpha_{18} & \alpha_{19} \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ -\rho_l^{-1}(\cdot) & -\rho_v^{-1}(\cdot) & 0 & 0 & 0 & \alpha_{20} & \alpha_{21} \\ 0 & 0 & -\frac{\partial\psi^L}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial\psi^L}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial\psi^V}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 0 & \alpha_3 & \alpha_4 \end{bmatrix} \in \mathbb{R}^{6\times 7}$$

Now to determine $J_{4,2}^{**}$:

$$J_{4,2}^{**} = J_{4,2}^{*} - J_{4,3}J_{3,2} = J_{4,2} - J_{4,1}\left(D_{2,2} - D_{2,3}J_{3,2}\right) - J_{4,3}J_{3,2}$$

Once again, the intermediate matrices are:

$$J_{2,3}J_{3,2} = \begin{bmatrix} z_{(3N_c+2)}K_1(\cdot) & 0 & \cdots & & 0 \\ 0 & z_{(3N_c+2)}K_2(\cdot) & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & z_{(3N_c+2)}K_{N_c}(\cdot) \end{bmatrix} \in \mathbb{R}^{N_c\times N_c}$$

$$J_{2,2} - J_{2,3}J_{3,2} = \begin{bmatrix} \xi_{13,1} & 0 & \cdots & & 0 \\ 0 & \xi_{13,2} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & \xi_{13,N_c} \end{bmatrix} \in \mathbb{R}^{N_c\times N_c}$$

$$J_{4,1}\left(J_{2,2} - J_{2,3}J_{3,2}\right) = \begin{bmatrix} -\xi_{13,1} & \cdots & -\xi_{13,N_c} \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \end{bmatrix} \in \mathbb{R}^{6\times N_c}$$

$$J_{4,3}J_{3,2} = \begin{bmatrix} 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ -K_1(\cdot)\,\xi_{2,1} & -K_2(\cdot)\,\xi_{2,2} & & -K_{N_c}(\cdot)\,\xi_{2,N_c} \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \end{bmatrix} \in \mathbb{R}^{6\times N_c}$$

Which gives:

$$\begin{aligned} J_{4,2}^{**} &= J_{4,2} - J_{4,1}\left(J_{2,2} - J_{2,3}J_{3,2}\right) - J_{4,3}J_{3,2} \\ &= \begin{bmatrix} \xi_{9,1} & \xi_{9,2} & & \xi_{9,N_c} \\ 0 & \cdots & & 0 \\ \xi_{10,1} & \xi_{10,2} & & \xi_{10,N_c} \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{7,1} & & \cdots & \xi_{7,N_c} \end{bmatrix} \in \mathbb{R}^{6\times N_c} \end{aligned}$$

This gives the rank of the block row:

$$\text{rank}\begin{bmatrix} J_{4,4}^{**} & J_{4,2}^{**} \end{bmatrix}$$

$$=\text{rank}\begin{bmatrix} \xi_{13,1} & \xi_{13,2} & & \xi_{13,N_c} & -1 & -1 & 1 & 1 & 1 & \alpha_{18} & \alpha_{19} \\ 0 & \cdots & & 0 & -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ \xi_{10,1} & \xi_{10,2} & & \xi_{10,N_c} & -\rho_l^{-1}(\cdot) & -\rho_v^{-1}(\cdot) & 0 & 0 & 0 & \alpha_{20} & \alpha_{21} \\ 0 & \cdots & & 0 & 0 & 0 & -\frac{\partial\psi^L}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial\psi^L}{\partial z_{(3N_c+7)}} \\ 0 & \cdots & & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial\psi^V}{\partial z_{(3N_c+7)}} \\ \xi_{7,1} & & \cdots & \xi_{7,N_c} & 0 & 0 & 0 & 0 & 0 & \alpha_3 & \alpha_4 \end{bmatrix}$$

$$=3+\text{rank}\begin{bmatrix} \xi_{13,1} & \xi_{13,2} & & \xi_{13,N_c} & 0 & 0 & \alpha_{18} & \alpha_{19} \\ \xi_{10,1} & \xi_{10,2} & & \xi_{10,N_c} & -\rho_l^{-1}(\cdot) & -\rho_v^{-1}(\cdot) & \alpha_{20} & \alpha_{21} \\ \xi_{7,1} & & \cdots & \xi_{7,N_c} & 0 & 0 & \alpha_3 & \alpha_4 \end{bmatrix}$$

Under the assumptions for physical systems (see Assumption 3.1), it holds that $\rho_v, \rho_l \neq 0$ and $\xi_{13,i} \neq 0 \,\forall i = 1, 2..., Nc$, and therefore the rank dependency of the above is on the following block:

$$\begin{aligned} &\text{rank}\begin{bmatrix} \xi_{13,1} & \xi_{13,2} & \cdots & \xi_{13,N_c} & \alpha_{18} & \alpha_{19} \\ \xi_{7,1} & xi_{7,2} & \cdots & \xi_{7,N_c} & \alpha_3 & \alpha_4 \end{bmatrix} \\ &= 1+\text{rank}\begin{bmatrix} \xi_{7,1} & xi_{7,2} & \cdots & \xi_{7,N_c} & \alpha_3 & \alpha_4 \end{bmatrix} \end{aligned} \tag{A.11}$$

This row is non-zero under Assumption 3.2. Now consider:

$$J_{8,8}^{**} = J_{8,8} - J_{8,7}J_{7,8} - (J_{8,6} - J_{8,7}D_{7,6})\,(D_{6,6} - D_{6,7}D_{7,6})^{-1}\,(J_{6,8} - D_{6,7}J_{7,8})$$

$$J_{8,6} - J_{8,7}D_{7,6} = \begin{bmatrix} 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{10,1} & \xi_{10,2} & \cdots & \xi_{10,N_c} \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{7,1} & \xi_{7,2} & \cdots & \xi_{7,Nc} \end{bmatrix} \in \mathbb{R}^{6\times N_c}$$

$$D_{6,6} - D_{6,7}D_{7,6} = \begin{bmatrix} \xi_{13,1} & 0 & \cdots & & 0 \\ 0 & \xi_{13,2} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & \xi_{13,N_c} \end{bmatrix} \in \mathbb{R}^{N_c\times N_c}$$

$$J_{6,8} - D_{6,7}J_{7,8} = \begin{bmatrix} -z_{(N_c+1)} & -z_{(2N_c+1)} & 0 & 0 & 0 & z_{(3N_c+2)}\theta_{1,1} & z_{(3N_c+2)}\theta_{1,2} \\ -z_{(N_c+2)} & -z_{(2N_c+2)} & \vdots & \vdots & \vdots & z_{(3N_c+2)}\theta_{2,1} & z_{(3N_c+2)}\theta_{2,2} \\ \vdots & \vdots & & & & \vdots & \vdots \\ -z_{(2N_c)} & -z_{(3N_c)} & 0 & 0 & 0 & z_{(3N_c+2)}\theta_{N_c,1} & z_{(3N_c+2)}\theta_{N_c,2} \end{bmatrix} \in \mathbb{R}^{N_c\times 7}$$

Putting these together gives the result:

$$(J_{8,6} - J_{8,7}D_{7,6})\,(D_{6,6} - D_{6,7}D_{7,6})^{-1}\,(J_{6,8} - D_{6,7}J_{7,8}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \alpha_{22} & \alpha_{23} & 0 & 0 & 0 & \tilde{\alpha}_{24} & \tilde{\alpha}_{25} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \alpha_{26} & \alpha_{27} & 0 & 0 & 0 & \alpha_{28} & \alpha_{29} \end{bmatrix} \in \mathbb{R}^{6\times 7}$$

$$J_{8,7}J_{7,8} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \bar{\alpha}_{24} & \bar{\alpha}_{25} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{6\times 7}$$

Finally, the matrix $J^{**}_{8,8}$ can be formed:

$$J^{**}_{8,8} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ -\rho_l^{-1}(\cdot) - \alpha_{22} & -\rho_v^{-1}(\cdot) - \alpha_{23} & 0 & 0 & 0 & \alpha_{14} - \alpha_{24} & \alpha_{15} - \alpha_{25} \\ 0 & 0 & -\frac{\partial \psi_L(\cdot)}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial \psi^L(\cdot)}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial \psi^V(\cdot)}{\partial z_{(3N_c+7)}} \\ -\alpha_{26} & -\alpha_{27} & 0 & 0 & 0 & (\alpha_{16} - \alpha_{28}) & (\alpha_{17} - \alpha_{29}) \end{bmatrix} \in \mathbb{R}^{6\times 7}$$

In detail:

$$\begin{aligned} \text{rank}\left[J^{**}_{8,8}\right] &= \text{rank} \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ \alpha_{22} & \alpha_{23} & 0 & 0 & 0 & \alpha_{24} & \alpha_{25} \\ 0 & 0 & -\frac{\partial \psi_L(\cdot)}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial \psi_L(\cdot)}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial \psi_V(\cdot)}{\partial z_{(3N_c+7)}} \\ \alpha_{26} & \alpha_{27} & 0 & 0 & 0 & \alpha_{28} & \alpha_{29} \end{bmatrix} \\ &= \text{rank} \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ \alpha_{22} & \alpha_{23} & 0 & 0 & 0 & \alpha_{24} & \alpha_{25} \\ 0 & 0 & -\frac{\partial \psi_L(\cdot)}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial \psi_L(\cdot)}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial \psi_V(\cdot)}{\partial z_{(3N_c+7)}} \\ \alpha_{26} & \alpha_{27} & 0 & 0 & 0 & \alpha_{28} & \alpha_{29} \end{bmatrix} \\ &= \text{rank} \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ \alpha_{22} & \alpha_{23} & 0 & 0 & 0 & \alpha_{24} & \alpha_{25} \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \alpha_{26} & \alpha_{27} & 0 & 0 & 0 & \alpha_{28} & \alpha_{29} \end{bmatrix} \qquad \begin{array}{c} R_2 - R_1 \\ \\ \\ \text{eliminate} \end{array} \\ &= 4 + \text{rank} \begin{bmatrix} \alpha_{24} & \alpha_{25} \\ \alpha_{28} & \alpha_{29} \end{bmatrix} \end{aligned}$$

Term-wise:

$$\alpha_{24} = -z_{(3N_c+2)} \sum_{i=1}^{N_c} \frac{\xi_{10,i}\theta_{i,1}}{\xi_{13,i}} + \alpha_1$$

$$\alpha_{25} = -z_{(3N_c+2)} \sum_{i=1}^{N_c} \frac{\xi_{10,i}\theta_{i,2}}{\xi_{13,i}} + \alpha_2$$
$$\alpha_{28} = -z_{(3N_c+2)} \sum_{i=1}^{N_c} \frac{\xi_{7,i}\theta_{i,1}}{\xi_{13,i}} + \alpha_3$$
$$\alpha_{29} = -z_{(3N_c+2)} \sum_{i=1}^{N_c} \frac{\xi_{7,i}\theta_{i,2}}{\xi_{13,i}} + \alpha_4$$

This block is non-singular only under Assumptions 3.2 and 3.1. This implies that:

$$\text{rank}\begin{bmatrix} J_{4,4}^{**} & 0 & J_{4,2}^{**} \\ J_{8,4}^{(4*)} & J_{8,8}^{**} & J_{8.2}^{(4*)} \end{bmatrix} = 12$$

This condition applies even if $\alpha_3$ and $\alpha_4$ are zero, as the additional rows in $J_{4,2}^{*,*}$, in particular $\xi_{7,i}$, allow the top block row to maintain full row rank. This further gives:

$$\text{rank}\left(\mathcal{F}_1|_{z,\dot{z},\ddot{z}}\right) = 6N_c + 12 \tag{A.12}$$

It still remains to determine rank $\left(\mathcal{F}_1|_{\dot{z},\ddot{z}}\right)$:

$$\begin{aligned}
\text{rank}\left(\mathcal{F}_1|_{\dot{z},\ddot{z}}\right) = &\text{rank} \begin{array}{c} \begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & J_{5,6} & J_{5,7} & J_{5,8} & I_{N_c} & 0 & 0 & 0 \\ I_{N_c} & J_{6,6} & J_{6,7} & J_{6,8} & 0 & 0 & 0 & 0 \\ 0 & J_{7,6} & I_{N_C} & J_{7,8} & 0 & 0 & 0 & 0 \\ J_{8,5} & J_{8,6} & J_{8,7} & J_{8,8} & 0 & 0 & 0 & 0 \end{bmatrix} \end{array} \begin{array}{c} (N_c) \\ (N_c) \\ (N_c) \\ (6) \\ (N_c) \\ (N_c) \\ (N_c) \\ (6) \end{array} \\
= &\text{rank} \begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 \\ 0 & I_{N_c} & J_{5,7} & J_{5,8} & J_{5,6} \\ I_{N_c} & 0 & J_{6,7} & J_{6,8} & J_{6,6} \\ 0 & 0 & I_{N_C} & J_{7,8} & J_{7,6} \\ J_{8,5} & 0 & J_{8,7} & J_{8,8} & J_{8,6} \end{bmatrix} \\
= &\text{rank} \begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 \\ 0 & I_{N_c} & J_{5,6} & J_{5,7} & J_{5,8} \\ I_{N_c} & 0 & J_{6,6} & J_{6,7} & J_{6,8} \\ 0 & 0 & J_{7,6} & I_{N_C} & J_{7,8} \\ J_{8,5} & 0 & J_{8,6} & J_{8,7} & J_{8,8} \end{bmatrix}
\end{aligned}$$

Once again, elementary row operations allow the rank to determined:

$$\text{rank} \begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 \\ 0 & I_{N_c} & J_{5,6} & J_{5,7} & J_{5,8} \\ I_{N_c} & 0 & J_{6,6} & J_{6,7} & J_{6,8} \\ 0 & 0 & J_{7,6} & I_{N_C} & J_{7,8} \\ J_{8,5} & 0 & J_{8,6} & J_{8,7} & J_{8,8} \end{bmatrix}$$

$$
=\text{rank}\begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 \\ 0 & I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & J_{6,6} & J_{6,7} & J_{6,8} \\ 0 & 0 & J_{7,6} & I_{N_C} & J_{7,8} \\ 0 & 0 & (J_{8,6} - J_{8,7}J_{7,6}) & 0 & (J_{8,8} - J_{8,7}J_{7,8}) \end{bmatrix} \qquad \begin{array}{c} \text{eliminate} \\ \\ R_6 - R_1 \\ \\ R_8 - J_{8,5}R_1 - J_{8,7}R_7 \end{array}
$$

Define the following groupings, noting that, since they are not used outside this proof, they are not defined in the groupings list and do not correspond to those used elsewhere:

$$
\begin{aligned} J^*_{8,6} &= J_{8,6} - J_{8,7}J_{7,6} \\ J^*_{8,8} &= J_{8,8} - J_{8,7}J_{7,8} \end{aligned}
$$

Note that $J_{6,6}$ is a non-zero diagonal matrix under the stated assumptions and therefore the inverse, $J^{-1}_{6,6}$, exists. Then:

$$
\text{rank}\begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 \\ 0 & I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & J_{6,6} & J_{6,7} & J_{6,8} \\ 0 & 0 & J_{7,6} & I_{N_C} & J_{7,8} \\ 0 & 0 & J^*_{8,6} & 0 & J^*_{8,8} \end{bmatrix}
$$

$$
=\text{rank}\begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 \\ 0 & I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & I_{Nc} & J^{-1}_{6,6}J_{6,7} & J^{-1}_{6,6}J_{6,8} \\ 0 & 0 & J_{7,6} & I_{N_C} & J_{7,8} \\ 0 & 0 & J^*_{8,6} & 0 & J^*_{8,8} \end{bmatrix}
$$

$$
=\text{rank}\begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 \\ 0 & I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & I_{Nc} & J^{-1}_{6,6}J_{6,7} & J^{-1}_{6,6}J_{6,8} \\ 0 & 0 & 0 & \left(I_{N_C} - J_{7,6}J^{-1}_{6,6}J_{6.7}\right) & \left(J_{7,8} - J_{7,6}J^{-1}_{6,6}J_{6,8}\right) \\ 0 & 0 & 0 & -J^*_{8,6}J^{-1}_{6,6}J_{6.7} & \left(J^*_{8,8} - J^*_{8,6}J^{-1}_{6,6}J_{6,8}\right) \end{bmatrix} \qquad \begin{array}{c} \\ \\ \\ R_4 - J_{7,6}R_3 \\ R_5 - J^*_{8,6}R_3 \end{array}
$$

Further note the $J_{7,6}$ and $J_{6,7}$ are non-zero diagonal matrices, and therefore $\left(I_{N_C} - J_{7,6}J^{-1}_{6,6}J_{6.7}\right)^{-1}$ exists as a diagonal matrix with elements $\theta_{i,8} := \left(1 + \frac{z_{(3N_c+2)}K_i(\cdot)}{z_{(3N_c+1)}}\right)^{-1}$. The elements are guaranteed to be non-zero as $\frac{z_{(3N_c+2)}K_i(\cdot)}{z_{(3N_c+1)}} > 0 \quad \forall i \in \{1, ..N_c\}$ under natural physical assumptions (being equivalent to $\frac{M_v K_i}{M_l}$), as given in Assumption 3.1. Therefore:

$$
\text{rank}\begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 \\ 0 & I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & I_{Nc} & J^{-1}_{6,6}J_{6,7} & J^{-1}_{6,6}J_{6,8} \\ 0 & 0 & 0 & \left(I_{N_C} - J_{7,6}J^{-1}_{6,6}J_{6,7}\right) & \left(J_{7,8} - J_{7,6}J^{-1}_{6,6}J_{6,8}\right) \\ 0 & 0 & 0 & -J^*_{8,6}J^{-1}_{6,6}J_{6.7} & \left(J^*_{8,8} - J^*_{8,6}J^{-1}_{6,6}J_{6,8}\right) \end{bmatrix}
$$

$$
=\text{rank}\begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 \\ 0 & I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & I_{Nc} & 0 & 0 \\ 0 & 0 & 0 & I_{Nc} & \left(I_{N_C} - J_{7,6}J_{6,6}^{-1}J_{6,7}\right)^{-1}\left(J_{7,8} - J_{7,6}J_{6,6}^{-1}J_{6,8}\right) \\ 0 & 0 & 0 & -J_{8,6}^{*}J_{6,6}^{-1}J_{6.7} & \left(J_{8,8}^{*} - J_{8,6}^{*}J_{6,6}^{-1}J_{6,8}\right) \end{bmatrix} \text{ eliminate}
$$

Now define:

$$
J_{8,8}^{**} = \left(J_{8,8}^{*} - J_{8,6}^{*}J_{6,6}^{-1}J_{6,8}\right) + J_{8,6}^{*}J_{6,6}^{-1}J_{6,7}\left(I_{N_C} - J_{7,6}J_{6,6}^{-1}J_{6.7}\right)^{-1}\left(J_{7,8} - J_{7,6}J_{6,6}^{-1}J_{6,8}\right)
$$

Such that:

$$
\begin{aligned}
&\text{rank}\begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 \\ 0 & I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & I_{Nc} & 0 & 0 \\ 0 & 0 & 0 & I_{Nc} & \left(I_{N_C} - J_{7,6}J_{6,6}^{-1}J_{6.7}\right)^{-1}\left(J_{7,8} - J_{7,6}J_{6,6}^{-1}J_{6,8}\right) \\ 0 & 0 & 0 & -J_{8,6}^{*}J_{6,6}^{-1}J_{6.7} & \left(J_{8,8}^{*} - J_{8,6}^{*}J_{6,6}^{-1}J_{6,8}\right) \end{bmatrix} \\
=&\text{rank}\begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 \\ 0 & I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & I_{Nc} & 0 & 0 \\ 0 & 0 & 0 & I_{Nc} & \left(I_{N_C} - J_{7,6}J_{6,6}^{-1}J_{6,7}\right)\left(J_{7,8} - J_{7,6}J_{6,6}^{-1}J_{6,8}\right) \\ 0 & 0 & 0 & 0 & J_{8,8}^{**} \end{bmatrix} \quad \begin{matrix} \\ \\ 0 \\ 0 \\ R_5 + J_{8,6}^{*}J_{6,6}^{-1}J_{6.7}R_4 \end{matrix} \\
=&\text{rank}\begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 \\ 0 & I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & I_{Nc} & 0 & 0 \\ 0 & 0 & 0 & I_{Nc} & 0 \\ 0 & 0 & 0 & 0 & J_{8,8}^{**} \end{bmatrix} \text{ eliminate} \\
=&4N_c + \text{rank } \left[J_{8,8}^{**}\right]
\end{aligned}
$$

Hence, it remains to evaluate $J_{8,8}^{**}$. Step-by-step:

$$
J_{8,6}^{*} = \begin{bmatrix} 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{10,1} & \xi_{10,2} & \cdots & \xi_{10,N_c} \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{7,1} & \xi_{7,2} & \cdots & \xi_{7,Nc} \end{bmatrix} \in \mathbb{R}^{6\times N_c}
$$

$$
J_{8,8}^{*} - J_{8,6}^{*}J_{6,6}^{-1}J_{6,8} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ \bar{\alpha}_{30} & \bar{\alpha}_{31} & 0 & 0 & 0 & \bar{\alpha}_{34} & \bar{\alpha}_{35} \\ 0 & 0 & -\frac{\partial\psi^L(\cdot)}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial\psi^L(\cdot)}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial\psi^V(\cdot)}{\partial z_{(3N_c+7)}} \\ \bar{\alpha}_{32} & \bar{\alpha}_{33} & 0 & 0 & 0 & \alpha_{16} & \alpha_{17} \end{bmatrix} \in \mathbb{R}^{6\times 7}
$$

$$
J_{7,8} - J_{7,6}J_{6,6}^{-1}J_{6,8} = \begin{bmatrix} \theta_{1,6} & \theta_{1,7} & 0 & 0 & 0 & \theta_{1,1} & \theta_{1,2} \\ \theta_{2,6} & \theta_{2,7} & \vdots & \vdots & \vdots & \theta_{2,1} & \theta_{2,2} \\ \vdots & \vdots & & & & \vdots & \vdots \\ & & & & & & \\ \theta_{N_c,6} & \theta_{N_c,7} & 0 & 0 & 0 & \theta_{N_c,1} & \theta_{N_c,2} \end{bmatrix} \in \mathbb{R}^{N_c \times 7}
$$

$$
\left(I_{N_C} - J_{7,6}J_{6,6}^{-1}J_{6.7}\right)^{-1} = \begin{bmatrix} \theta_{1,8} & 0 & \cdots & & 0 \\ 0 & \theta_{2,8} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & \theta_{N_c,8} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}
$$

$$
J_{8,6}^{*}J_{6,6}^{-1}J_{6,7} = \begin{bmatrix} 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{11,1} & \xi_{11,2} & \cdots & \xi_{11,N_c} \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{12,1} & \xi_{12,2} & \cdots & \xi_{12,Nc} \end{bmatrix} \in \mathbb{R}^{6 \times N_c}
$$

and finally:

$$
J_{8,8}^{**} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ \alpha_{30} & \alpha_{31} & 0 & 0 & 0 & \alpha_{34} & \alpha_{35} \\ 0 & 0 & -\frac{\partial \psi_L(\cdot)}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial \psi_L(\cdot)}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial \psi_V(\cdot)}{\partial z_{(3N_c+7)}} \\ \alpha_{32} & \alpha_{33} & 0 & 0 & 0 & \alpha_{36} & \alpha_{37} \end{bmatrix} \in \mathbb{R}^{6 \times 7}
$$

In detail:

$$
\begin{aligned}
&\text{rank} \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ \alpha_{30} & \alpha_{31} & 0 & 0 & 0 & \alpha_{34} & \alpha_{35} \\ 0 & 0 & -\frac{\partial \psi_L(\cdot)}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial \psi_L(\cdot)}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial \psi_V(\cdot)}{\partial z_{(3N_c+7)}} \\ \alpha_{32} & \alpha_{33} & 0 & 0 & 0 & \alpha_{36} & \alpha_{37} \end{bmatrix} \\
&= 2 + \text{rank} \begin{bmatrix} -1 & -1 & 0 & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{34} & \alpha_{35} \\ \alpha_{32} & \alpha_{33} & \alpha_{36} & \alpha_{37} \end{bmatrix} \\
&= 2 + \text{rank} \begin{bmatrix} -1 & -1 & 0 & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{34} & \alpha_{35} \\ \alpha_{32} & \alpha_{33} & \alpha_{36} & \alpha_{37} \end{bmatrix} \\
&= 3 + \text{rank} \begin{bmatrix} (\alpha_{31} - \alpha_{30}) & \alpha_{34} & \alpha_{35} \\ (\alpha_{33} - \alpha_{32}) & \alpha_{36} & \alpha_{37} \end{bmatrix}
\end{aligned} \tag{A.13}
$$

This matrix has full rank on the condition that this block is full rank.

Looking term by term:

$$
\begin{aligned}
(\alpha_{31}-\alpha_{30}) &= (\bar{\alpha}_{31}+\tilde{\alpha}_{31})-(\bar{\alpha}_{30}+\tilde{\alpha}_{30})\\
&= \left(\sum_{i=1}^{N_c}\xi_{11,i}\theta_{i,8}\theta_{i,7}-\sum_{i=1}^{N_c}\frac{z_{(2N_c+i)}}{z_{(3N_c+1)}}\xi_{10,i}-\rho_v^{-1}(\cdot)\right)\\
&- \left(\sum_{i=1}^{N_c}\xi_{11,i}\theta_{i,8}\theta_{i,6}-\sum_{i=1}^{N_c}\frac{z_{(N_c+i)}}{z_{(3N_c+1)}}\xi_{10,i}-\rho_l^{-1}(\cdot)\right)\\
&= \left(\sum_{i=1}^{N_c}\xi_{11,i}\theta_{i,8}\left(\theta_{i,7}-\theta_{i,6}\right)+\sum_{i=1}^{N_c}\frac{\xi_{10,i}\left(z_{(N_c+i)}-z_{(2N_c+i)}\right)}{z_{(3N_c+1)}}\right)+\left(\rho_l^{-1}(\cdot)-\rho_v^{-1}(\cdot)\right)\\
&= \left(\sum_{i=1}^{N_c}\xi_{11,i}\theta_{i,8}\frac{K_i\left(\cdot\right)}{z_{(3N_c+1)}}\left(z_{(2N_c+i)}-z_{(N_c+i)}\right)+\sum_{i=1}^{N_c}\frac{\xi_{10,i}\left(z_{(N_c+i)}-z_{(2N_c+i)}\right)}{z_{(3N_c+1)}}\right)\\
&+ \left(\rho_l^{-1}(\cdot)-\rho_v^{-1}(\cdot)\right)\\
&= \sum_{i=1}^{N_c}\frac{\xi_{11,i}\theta_{i,8}K_i\left(\cdot\right)+\xi_{10,i}}{z_{(3N_c+1)}}\left(z_{(2N_c+i)}-z_{(N_c+i)}\right)+\left(\rho_l^{-1}(\cdot)-\rho_v^{-1}(\cdot)\right)\\
&= \frac{1}{z_{(3N_c+1)}}\sum_{i=1}^{N_c}\left(\frac{K_i\left(\cdot\right)z_{(3N_c+2)}}{z_{(3N_c+1)}+K_i\left(\cdot\right)z_{(3N_c+2)}}+1\right)\left(\xi_{1,i}+K_i\left(\cdot\right)\xi_{2,i}\right)\left(z_{(2N_c+i)}-z_{(N_c+i)}\right)\\
&+ \left(\rho_l^{-1}(\cdot)-\rho_v^{-1}(\cdot)\right)
\end{aligned}
$$

The first term of the sum is guaranteed to be non-zero under the natural physical assumptions if $z_{(2N_c+i)} \neq z_{(N_c+i)}$ for all $i$. However, since on a solution manifold $K_i = \frac{z_{(2N_c+i)}}{z_{(N_c+i)}}$, this condition is equivalent to $K_i \neq 1$ , which is implied if Assumption 3.2 holds but $\alpha_3 = \alpha_4 = 0$ (from point 1). Once again, the inverse density difference should prevent this term from being close to 0 numerically for a realistic physical case. Terms $\xi_{1,i}$ and $\xi_{2,i}$ are related to the derivatives of the densities with respect to composition.

$$
\begin{aligned}
\alpha_{34} &= \alpha_1-\sum_{i=1}^{N_c}\xi_{2,i}\theta_{i,1}\\
\alpha_{35} &= \alpha_2-\sum_{i=1}^{N_c}\xi_{2,i}\theta_{i,2}
\end{aligned}
$$

The first entry in the final row is:

$$
\begin{aligned}
(\alpha_{33}-\alpha_{32}) &= (\bar{\alpha}_{33}+\tilde{\alpha}_{33})-(\bar{\alpha}_{32}+\tilde{\alpha}_{32})\\
&= \left(\sum_{i=1}^{N_c}\xi_{12,i}\theta_{i,8}\theta_{i,7}-\sum_{i=1}^{N_c}\frac{z_{(2N_c+i)}}{z_{(3N_c+1)}}\xi_{7,i}\right)-\left(\sum_{i=1}^{N_c}\xi_{12,i}\theta_{i,8}\theta_{i,6}-\sum_{i=1}^{N_c}\frac{z_{(N_c+i)}}{z_{(3N_c+1)}}\xi_{7,i}\right)\\
&= \left(\sum_{i=1}^{N_c}\xi_{12,i}\theta_{i,8}\left(\theta_{i,7}-\theta_{i,6}\right)+\sum_{i=1}^{N_c}\frac{\xi_{7,i}\left(z_{(N_c+i)}-z_{(2N_c+i)}\right)}{z_{(3N_c+1)}}\right)
\end{aligned}
$$

$$
\begin{aligned}
&= \left( \sum_{i=1}^{N_c} \xi_{12,i}\theta_{i,8} \frac{K_i\left(\cdot\right)}{z_{(3N_c+1)}} \left( z_{(2N_c+i)} - z_{(N_c+i)} \right) + \sum_{i=1}^{N_c} \frac{\xi_{7,i}\left( z_{(N_c+i)} - z_{(2N_c+i)} \right)}{z_{(3N_c+1)}} \right) \\
&= \sum_{i=1}^{N_c} \frac{\xi_{12,i}\theta_{i,8}K_i\left(\cdot\right) + \xi_{7,i}}{z_{(3N_c+1)}} \left( z_{(2N_c+i)} - z_{(N_c+i)} \right) \\
&= \frac{1}{z_{(3N_c+1)}} \sum_{i=1}^{N_c} \left( \frac{K_i\left(\cdot\right) z_{(3N_c+2)}}{z_{(3N_c+1)} + K_i\left(\cdot\right) z_{(3N_c+2)}} + 1 \right) \left(K_i\left(\cdot\right) - 1\right) \left( z_{(2N_c+i)} - z_{(N_c+i)} \right)
\end{aligned}
$$

The remaining terms in the final row are as follows:

$$
\begin{aligned}
\alpha_{36} &= \sum_{i=1}^{N_c} \xi_{12,i}\theta_{i,8}\theta_{i,1} + \alpha_3 \\
\alpha_{37} &= \sum_{i=1}^{N_c} \xi_{12,i}\theta_{i,8}\theta_{i,1} + \alpha_4
\end{aligned}
$$

If Assumption 3.2 holds, there are two limiting cases. If $K_i \neq 1$ but $\alpha_3 = \alpha_4 = 0, \implies \theta_{i,1} = \theta_{i,2} = 0 \; \forall i$ , the block in question has the following structure:

$$
\text{rank} \begin{bmatrix} (\alpha_{31} - \alpha_{30}) & \alpha_{34} & \alpha_{35} \\ (\alpha_{33} - \alpha_{32}) & \alpha_{36} & \alpha_{37} \end{bmatrix} = \text{rank} \begin{bmatrix} (\alpha_{31} - \alpha_{30}) & \alpha_1 & \alpha_2 \\ (\alpha_{33} - \alpha_{32}) & 0 & 0 \end{bmatrix}
$$

Here, $\alpha_1$ and $\alpha_2$ depend on the partial derivatives of the phase densities with respect to temperature and pressure ($z_{(3N_c+6)}$ and $z_{(3N_c+7)}$ respectively). Alternatively, if 3.2 holds with $K_i = 1$ but $\alpha_3, \alpha_4 \neq 0$ , the block in question has the following structure:

$$
\text{rank} \begin{bmatrix} (\alpha_{31} - \alpha_{30}) & \alpha_{34} & \alpha_{35} \\ (\alpha_{33} - \alpha_{32}) & \alpha_{36} & \alpha_{37} \end{bmatrix} = \text{rank} \begin{bmatrix} \left(\rho_l^{-1}(\cdot) - \rho_v^{-1}(\cdot)\right) & \alpha_{34} & \alpha_{35} \\ 0 & \alpha_{36} & \alpha_{37} \end{bmatrix}
$$

However, if neither condition holds, then the block will be rank deficient and the hypothesis will not be satisfied for $\mu = 1$ .

$$
\text{rank}\left(\mathcal{F}_1|_{\dot{z},\ddot{z}}\right) = 4N_c + 6 \tag{A.14}
$$

## A.5 System 1 Reduced Order Projection Matrices

### A.5.1 Case $\mu = 0$

Recall the expression for $\mathcal{F}_0|_{\dot{z}}$:

$$\mathcal{F}_0|_{\dot{z}} = \begin{array}{c} \begin{bmatrix} I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{array} \begin{array}{c} (N_c) \\ (N_c) \\ (N_c) \\ (6) \end{array} \in \mathbb{R}^{3N_c+6\times 3N_c+7}$$

A candidate for the matrix $Z_2$ is as follows:

$$Z_2 = \begin{bmatrix} 0 & 0 & 0 \\ I_{N_c} & 0 & 0 \\ 0 & I_{N_c} & 0 \\ 0 & 0 & I_6 \end{bmatrix} \begin{array}{c} (N_c) \\ (N_c) \\ (N_c) \\ (6) \end{array} \in \mathbb{R}^{3N_c+12\times 2Nc+6}$$

This satisfies Condition 1:

$$\begin{aligned} Z_2^T \mathcal{F}_0|_{\dot{z}} &= \begin{bmatrix} 0 & I_{Nc} & 0 & 0 \\ 0 & 0 & I_{N_c} & 0 \\ 0 & 0 & 0 & I_6 \end{bmatrix} \begin{bmatrix} I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{array}{c} (N_c) \\ (N_c) \\ (N_c) \\ (6) \end{array} \\ &= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{2Nc+6\times 3N_c+7} \end{aligned}$$

And Condition 2:

$$\begin{aligned} Z_2^T \mathcal{F}_0|_{z} &= \begin{bmatrix} 0 & I_{Nc} & 0 & 0 \\ 0 & 0 & I_{N_c} & 0 \\ 0 & 0 & 0 & I_6 \end{bmatrix} \begin{bmatrix} 0 & J_{1,2} & J_{1,3} & J_{1,4} \\ I_{N_c} & J_{2,2} & J_{2,3} & J_{2,4} \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} \\ J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4} \end{bmatrix} \begin{array}{c} (N_c) \\ (N_c) \\ (N_c) \\ (6) \end{array} \\ &= \begin{bmatrix} I_{N_c} & J_{2,2} & J_{2,3} & J_{2,4} \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} \\ J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4} \end{bmatrix} \in \mathbb{R}^{2Nc+6\times 3N_c+7} \end{aligned}$$

It remains to verify that this matrix is point-wise full rank. For convenience, define:

$$\begin{aligned} J_{4,3}^* &= (J_{4,3} - J_{4,1}J_{2,3}) \\ J_{4,2}^* &= J_{4,2} - J_{4,1}J_{2,2} - J_{4,3}^*J_{3,2} \\ J_{4,4}^* &= J_{4,4} - J_{4,1}J_{2,4} - J_{4,3}^*J_{3,4} \end{aligned}$$

$$\begin{aligned} &\text{rank} \begin{bmatrix} I_{N_c} & J_{2,2} & J_{2,3} & J_{2,4} \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} \\ J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4} \end{bmatrix} \\ &= \text{rank} \begin{bmatrix} I_{N_c} & (J_{2,2} - J_{2,3}J_{3,2}) & 0 & (J_{2,4} - J_{2,3}J_{3,4}) \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} \\ 0 & (J_{4,2} - J_{4,1}J_{2,2}) & (J_{4,3} - J_{4,1}J_{2,3}) & (J_{4,4} - J_{4,1}J_{2,4}) \end{bmatrix} \begin{array}{c} R_1 - J_{2,3}R_2 \\ \\ R_4 - J_{4,1}R_1 \end{array} \end{aligned}$$

$$
\begin{aligned}
&= \text{rank}\begin{bmatrix} I_{N_c} & (J_{2,2}-J_{2,3}J_{3,2}) & 0 & (J_{2,4}-J_{2,3}J_{3,4}) \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} \\ 0 & \left(J_{4,2}-J_{4,1}J_{2,2}-J^*_{4,3}J_{3,2}\right) & 0 & \left(J_{4,4}-J_{4,1}J_{2,4}-J^*_{4,3}J_{3,4}\right) \end{bmatrix} \quad R_3 - J^*_{4,3}R_2 \\
&= \text{rank}\begin{bmatrix} I_{N_c} & (J_{2,2}-J_{2,3}J_{3,2}) & 0 & (J_{2,4}-J_{2,3}J_{3,4}) \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} \\ 0 & J^*_{4,2} & 0 & J^*_{4,4} \end{bmatrix} \\
&= \text{rank}\begin{bmatrix} I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & I_{N_c} & 0 \\ 0 & J^*_{4,2} & 0 & J^*_{4,4} \end{bmatrix} \quad \begin{matrix}\text{eliminate} \\ \text{eliminate} \\ \phantom{x}\end{matrix} \\
&= 2N_c + \text{rank}\begin{bmatrix} J^*_{4,2} & J^*_{4,4} \end{bmatrix}
\end{aligned}
$$

Now, to investigate this matrix in more detail, the following expressions are needed:

$$
J^*_{4,3} = \begin{bmatrix} -z_{(3N_c+2)} & \cdots & -z_{(3N_c+2)} \\ 0 & \cdots & 0 \\ \xi_{2,1} & \xi_{2,2} & \xi_{2,N_c} \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \end{bmatrix} \in \mathbb{R}^{6\times N_c}
$$

$$
J^*_{4,2} = \begin{bmatrix} \xi_{13,1} & \xi_{13,2} & \cdots & \xi_{13,N_c} \\ 0 & \cdots & & 0 \\ \xi_{10,1} & \xi_{10,2} & \cdots & \xi_{10,N_c} \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{7,1} & \xi_{7,2} & \cdots & \xi_{7,N_c} \end{bmatrix} \in \mathbb{R}^{6\times N_c}
$$

$$
\begin{aligned}
J_{4,1}J_{2,4} &= \begin{bmatrix} \left(\sum_{i=N_c+1}^{2N_c} z_i\right) & \left(\sum_{i=2N_C+1}^{3N_c} z_i\right) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{6\times 7}
\end{aligned}
$$

Note that on a solution manifold, $\sum_{i=N_c+1}^{2N_c} z_i = \sum_{i=2N_C+1}^{3N_c} z_i = 1$.

$$
J^*_{4,4} = \begin{bmatrix} -1 & -1 & 1 & 0 & 0 & \alpha_{38} & \alpha_{39} \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ -\rho_l^{-1}(\cdot) & -\rho_v^{-1}(\cdot) & 0 & 0 & 0 & \alpha_{40} & \alpha_{41} \\ 0 & 0 & -\frac{\partial\psi^L}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial\psi^L}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial\psi^V}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 0 & \alpha_3 & \alpha_4 \end{bmatrix} \in \mathbb{R}^{6\times 7}
$$

The matrix $\begin{bmatrix} J^*_{4,2} & J^*_{4,4} \end{bmatrix}$ is then given by:

$$\begin{bmatrix} \xi_{13,1} & \xi_{13,2} & \cdots & \xi_{13,N_c} & -1 & -1 & 1 & 0 & 0 & -z_{(3N_c+2)}\alpha_3 & -z_{(3N_c+2)}\alpha_4 \\ 0 & \cdots & & 0 & -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ \xi_{10,1} & \xi_{10,2} & \cdots & \xi_{10,N_c} & -\rho_l^{-1}(\cdot) & -\rho_v^{-1}(\cdot) & 0 & 0 & 0 & \alpha_{40} & \alpha_{41} \\ 0 & \cdots & & 0 & 0 & 0 & -\frac{\partial\psi^L}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial\psi^L}{\partial z_{(3N_c+7)}} \\ 0 & \cdots & & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial\psi^V}{\partial z_{(3N_c+7)}} \\ \xi_{7,1} & \xi_{7,2} & \cdots & \xi_{7,N_c} & 0 & 0 & 0 & 0 & 0 & \alpha_3 & \alpha_4 \end{bmatrix} \in \mathbb{R}^{N_c+6\times 7}$$

which is structurally full row rank if, and only if, $\alpha_3$ and $\alpha_4$ are not both simultaneously zero. If they are, then the first row could be used to eliminate $\xi_7$ and knock out the final row. Assuming that they are non-zero, rank $\left[Z_2^T \mathcal{F}_1|_z\right] = 2N_c + 6 = a$, and Condition 2 is fulfilled.

To test Condition 3, that is:

$$Z_2^T \mathcal{F}_1|_z T_2 = 0$$

the procedure will be as follows. As a simplified form of the matrix $Z_2^T \mathcal{F}_1|_z$ was already calculated above (using only row and column operations), this will be used to determine a nullspace, and then the operations from the right will be inverted to return to the nullspace of $Z_2^T \mathcal{F}_1|_z$. In particular:

$$B := M_1 Z_2^T \mathcal{F}_1|_z M_2 = \begin{bmatrix} I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & I_{N_c} & 0 \\ 0 & J^*_{4,2} & 0 & J^*_{4,4} \end{bmatrix}$$

Where $M_1$ and $M_2$ are the left and right transformation matrices respectively. As the right nullspace is the only required component, only $M_2$ is required. Propose the following $\tilde{T}_2$:

$$\tilde{T}_2 = \begin{array}{cc} \begin{bmatrix} 0 & 0 \\ X & 0 \\ 0 & 0 \\ Y & v \end{bmatrix} & \begin{array}{c} N_c \\ N_c \\ N_c \\ 7 \end{array} \end{array} \in \mathbb{R}^{3N_c+7\times N_c+1}$$

Where $X = [x_1 \ldots x_{N_c}] \in \mathbb{R}^{N_c \times N_c}$ and $Y = \begin{bmatrix} y_1 \\ \vdots \\ y_7 \end{bmatrix} \in \mathbb{R}^{7\times N_c}$ are matrices yet to be determined, partitioned into columns and rows respectively, such that $\tilde{T}_2$ has pointwise maximal rank. $v$ is a vector that will also be determined. These are notational convenience and do not relate to the physical quantities $x$ and $y$. It should hold that:

$$B\tilde{T}_2 = \begin{bmatrix} I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & I_{N_c} & 0 \\ 0 & J^*_{4,2} & 0 & J^*_{4,4} \end{bmatrix} \begin{bmatrix} 0 & 0 \\ X & 0 \\ 0 & 0 \\ Y & v \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{2Nc+6\times N_c+1}$$

This induces the following system of equations:

$$\xi_{13} X - y_1 - y_2 + y_3 + \alpha_{38} y_6 + \alpha_{39} y_7 = 0$$

$$
\begin{aligned}
-y_1 - y_2 + y_3 &= 0 \\
-\rho_l^{-1} y_1 - \rho_v^{-1} y_2 + \xi_{10} X + \alpha_{40} y_6 + \alpha_{41} y_7 &= 0 \\
-\frac{\partial \psi^L}{\partial z_{(3*N_c+3)}} y_3 + y_4 - \frac{\partial \psi^L}{\partial z_{(3*N_c+7)}} y_7 &= 0 \\
y_5 - \frac{\partial \psi^V}{\partial z_{(3*N_c+7)}} y_7 &= 0 \\
\alpha_3 y_6 + \alpha_4 y_7 + \xi_7 X &= 0
\end{aligned}
$$

For an arbitrary column of $Y$, this is equivalent to the following linear system, where $x_i$ is the $i^{th}$ column of $X$:

$$
\begin{bmatrix}
-1 & -1 & 1 & 0 & 0 & \alpha_{38} & \alpha_{39} \\
-1 & -1 & 1 & 0 & 0 & 0 & 0 \\
-\rho_l^{-1}(\cdot) & -\rho_v^{-1}(\cdot) & 0 & 0 & 0 & \alpha_{40} & \alpha_{41} \\
0 & 0 & -\frac{\partial \psi^L}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial \psi^L}{\partial z_{(3N_c+7)}} \\
0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial \psi^V}{\partial z_{(3N_c+7)}} \\
0 & 0 & 0 & 0 & 0 & \alpha_3 & \alpha_4
\end{bmatrix}
\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \end{bmatrix}
=
\begin{bmatrix} -\xi_{13} x_i \\ 0 \\ -\xi_{10} x_i \\ 0 \\ 0 \\ -\xi_7 x_i \end{bmatrix}
$$

Since $\alpha_{38} = -z_{(3N_c+2)}\alpha_3$ and $\alpha_{39} = -z_{(3N_c+2)}\alpha_4$, the final equation is not independent of the first and second equations and hence imposes a consistency condition on the matrix $X$. For any column $x_i$ of $X$, with elements $x_{i,j}$, it must hold that:

$$
-\xi_{13} X = z_{(3N_c+2)} \xi_7 X \implies -\sum_{j=1}^{N_c} \xi_{13,j} x_{i,j} = z_{(3N_c+2)} \sum_{j=1}^{N_c} \xi_{7,j} x_{i,j}
$$

From the expressions for $\xi_{13}$and $\xi_7$, it follows that:

$$
\sum_{j=1}^{N_c} \left( \frac{z_{(3N_c+1)}}{z_{(3N_c+2)}} + K_j \right) x_{i,j} = \sum_{j=1}^{N_c} \left( K_j(\cdot) - 1 \right) x_{i,j} \iff \sum_{j=1}^{N_c} x_{i,j} = 0
$$

Hence, the columns of $X$ should sum to zero. Since $X$ is of size $N_c \times N_c$, it can meet this condition and have rank of at most $N_c - 1$. A trivial basis for this space is obtained by setting pairwise elements opposite and equal and all other elements to zero, for example if $N_c = 3$:

$$
X_{N_c=3} = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ -1 & 0 & 1 \end{bmatrix}
$$

It is noted that the column of zeros above $v$ in the proposed form of $\tilde{T}_2$ also satisfies this condition. Now that $X$ is fixed, it is required to find a feasible $Y$ such that the first block column of $\tilde{T}_2$ is full rank. There are 5 independent equations, and so one possible solution scheme sets $y_1 = 1$ and $y_3 = 0$. This allows the remaining expressions for the other elements to be closed:

$$
\begin{aligned}
y_2 &= -1 \\
y_7 &= \left( \alpha_{41} - \frac{\alpha_{40}\alpha_4}{\alpha_3} \right)^{-1} \left( -\xi_{10} x_i - \left( \rho_v^{-1} - \rho_l^{-1} \right) + \frac{\alpha_{40}}{\alpha_3} \xi_7 x_i \right)
\end{aligned}
$$

$$y_6 = (-\xi_7 x_i - \alpha_4 y_7)\left(\frac{1}{\alpha_3}\right)$$
$$y_4 = \frac{\partial \psi^L}{\partial z_{(3*N_c+7)}} y_7$$
$$y_5 = \frac{\partial \psi^V}{\partial z_{(3*N_c+7)}} y_7$$

The same scheme is used to determine $v$, replacing $x_i$ with zeros. However, this will not provide sufficiently many independent ranks due to the rank deficiency of $X$, and so in the final column of $Y$ a different choice must be made. For this column, set $y_1 = 0$ and $y_3 = 1$, which gives a solution set as follows:

$$y_7 = \left(\alpha_{41} - \frac{\alpha_{40}\alpha_4}{\alpha_3}\right)^{-1}\left(-\xi_{10} x_{N_c} + \rho_v^{-1} + \frac{\alpha_{40}}{\alpha_3}\xi_{15} x_{N_c}\right)$$
$$y_6 = (-\xi_{15} x_{N_c} - \alpha_4 y_7)\left(\frac{1}{\alpha_3}\right)$$
$$y_2 = 1$$
$$y_4 = \frac{\partial \psi^L}{\partial z_{(3*N_c+7)}} y_7 + \frac{\partial \psi^L}{\partial z_{(3*N_c+3)}}$$
$$y_5 = \frac{\partial \psi^V}{\partial z_{(3*N_c+7)}} y_7$$

This gives the following structure for $Y$:

$$\left[\ Y\ \right] = \begin{bmatrix} y_{1,1} & \cdots & y_{1,Nc-1} & y_{1,Nc} \\ y_{2,1} & \cdots & y_{2,Nc-1} & y_{2,Nc} \\ y_{3,1} & \cdots & y_{3,Nc-1} & y_{3,Nc} \\ y_{4,1} & \cdots & y_{4,Nc-1} & y_{4,Nc} \\ y_{5,1} & \cdots & y_{5,Nc-1} & y_{5,Nc} \\ y_{6,1} & \cdots & y_{6,Nc-1} & y_{6,Nc} \\ y_{7,1} & \cdots & y_{7,Nc-1} & y_{7,Nc} \end{bmatrix} = \begin{bmatrix} 1 & \cdots & 1 & 0 \\ -1 & \cdots & -1 & 1 \\ 0 & \cdots & 0 & 1 \\ \xi_{18,1} & & & \xi_{18,N_c} \\ \xi_{17,1} & & & \xi_{17,N_c} \\ \xi_{16,1} & & & \xi_{16,N_c} \\ \xi_{15,1} & & & \xi_{15,N_c} \end{bmatrix}$$

Where the following special definitions apply, given $X = [x_1 \ldots x_{N_c}]$ defined in columns as above, for $i = \{1, 2, ...N_c\}$:

$$\xi_{15,i} = \begin{cases} \left(\alpha_{41} - \frac{\alpha_4\alpha_{40}}{\alpha_3}\right)^{-1}\left(-\xi_{10} x_i - \left(\rho_v^{-1} - \rho_l^{-1}\right) + \frac{\alpha_{40}}{\alpha_3}\xi_7 x_i\right) & i \neq N_c \\ \left(\alpha_{41} - \frac{\alpha_4\alpha_{40}}{\alpha_3}\right)^{-1}\left(-\xi_{10} x_i + \rho_v^{-1} + \frac{\alpha_{40}}{\alpha_3}\xi_7 x_i\right) & i = N_c \end{cases}$$
$$\xi_{16,i} = (-\xi_7 x_i - \alpha_4 \xi_{15,i})\left(\frac{1}{\alpha_3}\right)$$
$$\xi_{17,i} = \frac{\partial \psi^V}{\partial z_{(3N_c+7)}} \xi_{15,i}$$
$$\xi_{18,i} = \begin{cases} \frac{\partial \psi^L}{\partial z_{(3N_c+7)}} \xi_{15,i} & i \neq N_c \\ \frac{\partial \psi^L}{\partial z_{(3N_c+7)}} \xi_{15,i} + \frac{\partial \psi^L}{\partial z_{(3N_c+3)}} & i = N_c \end{cases}$$

And for $v$:

$$v = \begin{bmatrix} 1 \\ -1 \\ 0 \\ \left(\alpha_{41} - \frac{\alpha_4\alpha_{40}}{\alpha_3}\right)^{-1} \left(-\left(\rho_v^{-1} - \rho_l^{-1}\right)\right) \frac{\partial \psi^L}{\partial z_{(3N_c+7)}} \\ \left(\alpha_{41} - \frac{\alpha_4\alpha_{40}}{\alpha_3}\right)^{-1} \left(-\left(\rho_v^{-1} - \rho_l^{-1}\right)\right) \frac{\partial \psi^V}{\partial z_{(3N_c+7)}} \\ \frac{\alpha_4}{\alpha_3\alpha_{41} - \alpha_4\alpha_{40}} \left(\rho_v^{-1} - \rho_l^{-1}\right) \\ \left(\alpha_{41} - \frac{\alpha_4\alpha_{40}}{\alpha_3}\right)^{-1} \left(-\left(\rho_v^{-1} - \rho_l^{-1}\right)\right) \end{bmatrix}$$

Now it remains to determine $T_2 = M_2\tilde{T}_2$, with:

$$M_2 = \begin{bmatrix} I_{N_c} & -\left(J_{2,2} - J_{2,3}J_{3,2}\right) & 0 & -\left(J_{2,4} - J_{2,3}J_{3,4}\right) \\ 0 & I_{N_c} & 0 & 0 \\ 0 & -J_{32} & I_{N_c} & -J_{34} \\ 0 & 0 & 0 & I_7 \end{bmatrix} \in \mathbb{R}^{3N_c+7\times 3N_c+7}$$

This gives:

$$T_2 = M_2\tilde{T}_2 = \begin{bmatrix} I_{N_c} & -\left(J_{2,2} - J_{2,3}J_{3,2}\right) & 0 & -\left(J_{2,4} - J_{2,3}J_{3,4}\right) \\ 0 & I_{N_c} & 0 & 0 \\ 0 & -J_{32} & I_{N_c} & -J_{34} \\ 0 & 0 & 0 & I_7 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ X & 0 \\ 0 & 0 \\ Y & v \end{bmatrix}$$
$$= \begin{bmatrix} X_1 & v_1 \\ X & 0 \\ X_2 & v_2 \\ Y & v \end{bmatrix} \begin{matrix} (N_c) \\ (N_c) \\ (N_c) \\ (7) \end{matrix} \in \mathbb{R}^{3N_c+7\times N_c+1}$$

with the following expressions:

$$\begin{aligned} X_1 &= -\left(J_{2,2} - J_{2,3}J_{3,2}\right)X - \left(J_{2,4} - J_{2,3}J_{3,4}\right)Y \\ X_2 &= -J_{32}X - J_{34}Y \\ v_1 &= -\left(J_{2,4} - J_{2,3}J_{3,4}\right)v \\ v_2 &= -J_{3,4}v \end{aligned}$$

$$-\left(J_{2,4} - J_{2,3}J_{3,4}\right) = \begin{bmatrix} z_{(N_c+1)} & z_{(2N_c+1)} & 0 & 0 & 0 & -z_{(3N_c+2)}\theta_{1,1} & -z_{(3N_c+2)}\theta_{1,2} \\ z_{(N_c+2)} & z_{(2N_c+2)} & \vdots & \vdots & \vdots & -z_{(3N_c+2)}\theta_{2,1} & -z_{(3N_c+2)}\theta_{2,2} \\ \vdots & \vdots & & & & \vdots & \vdots \\ z_{(2N_c)} & z_{(3N_c)} & 0 & 0 & 0 & -z_{(3N_c+2)}\theta_{N_c,1} & -z_{(3N_c+2)}\theta_{N_c,2} \end{bmatrix} \in \mathbb{R}^{N_c\times 7}$$

Then:

$$X_1 = -\left(J_{2,2} - J_{2,3}J_{3,2}\right)X - \left(J_{2,4} - J_{2,3}J_{3,4}\right)Y \in \mathbb{R}^{N_c\times N_c}$$

which has elements:

$$X_1, i, j = \begin{cases} z_{(N_c+i)} - z_{(2N_c+i)} - z_{(3N_c+2)}\left(\theta_{1,i}\xi_{16,j} + \theta_{2,i}\xi_{15,j}\right) - \xi_{13,j}X_{i,j} & j \neq N_c \\ z_{(2N_c+i)} - z_{(3N_c+2)}\left(\theta_{1,i}\xi_{16,j} + \theta_{2,i}\xi_{15,j}\right) - \xi_{13,j}X_{i,j} & j = N_c \end{cases}$$

For the determination of $v_1$:

$$v_1 = \theta_{9,i} = z_{(N_c+i)} - z_{(2N_c+i)} + z_{(3N_c+2)}\left(\rho_v^{-1} - \rho_l^{-1}\right)\left[\theta_{i,2}\frac{\alpha_3}{\alpha_3\alpha_{41} - \alpha_4\alpha_{40}} - \theta_{i,1}\frac{\alpha_4}{\alpha_3\alpha_{41} - \alpha_4\alpha_{40}}\right]$$

It is now left to determine $F_{\dot{z}}T_2$. Recall:

$$F_{\dot{z}} = \begin{array}{c} \begin{bmatrix} I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{array} \begin{array}{c} (N_c) \\ (N_c) \\ (N_c) \\ (6) \end{array} \in \mathbb{R}^{3N_c+6\times 3N_c+7}$$

$$F_{\dot{z}}T_2 = \begin{bmatrix} I_{N_c} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} X_1 & v_1 \\ X & 0 \\ X_2 & v_2 \\ Y & v \end{bmatrix}$$

$$= \begin{bmatrix} X_1 & v_1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{3N_c+6\times N_c+1}$$

And let

$$Z_1 = \begin{bmatrix} I_{N_c} \\ 0 \\ 0 \end{bmatrix} \in \mathbb{R}^{3N_c+6\times N_c}$$

such that:

$$Z_1^T F_{\dot{z}} T_2 = \begin{bmatrix} X_1 & v_1 \end{bmatrix} \in \mathbb{R}^{N_c\times N_c+1}$$

### A.5.2 Case $\mu = 1$

Recall the structure of the Jacobian (with respect to $\dot{z}$ and $\ddot{z}$ only) established in Appendix A.3:

$$\mathcal{F}_1|_{\dot{z},\ddot{z}} = \begin{bmatrix} I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & J_{5,6} & J_{5,7} & J_{5,8} & I_{N_c} & 0 & 0 & 0 \\ I_{N_c} & J_{6,6} & J_{6,7} & J_{6,8} & 0 & 0 & 0 & 0 \\ 0 & J_{7,6} & I_{N_C} & J_{7,8} & 0 & 0 & 0 & 0 \\ J_{8,5} & J_{8,6} & J_{8,7} & J_{8,8} & 0 & 0 & 0 & 0 \end{bmatrix} \begin{array}{c} (N_c) \\ (N_c) \\ (N_c) \\ (6) \\ (N_c) \\ (N_c) \\ (N_c) \\ (6) \end{array} \in \mathbb{R}^{6N_c+12\times 6Nc+14}$$

As per Hypothesis 1, the left nullspace of this matrix is required. A candidate for the Matrix $Z_2$ is as follows:

$$
Z_2 = \left[\begin{array}{ccc}
0 & 0 & 0 \\
I_{N_c} & 0 & 0 \\
0 & I_{N_c} & 0 \\
0 & 0 & I_6 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{array}\right]
\begin{array}{c}
(N_c) \\ (N_c) \\ (N_c) \\ (6) \\ (N_c) \\ (N_c) \\ (N_c) \\ (6)
\end{array}
\in \mathbb{R}^{6N_c+12 \times 2Nc+6} \tag{A.15}
$$

This satisfies Condition 1:

$$
Z_2^T \mathcal{F}_1|_{\dot{z},\ddot{z}} = \left[\begin{array}{cccccccc}
0 & I_{Nc} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & I_{N_c} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & I_6 & 0 & 0 & 0 & 0
\end{array}\right]
\left[\begin{array}{cccccccc}
I_{N_c} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & J_{5,6} & J_{5,7} & J_{5,8} & I_{N_c} & 0 & 0 & 0 \\
I_{N_c} & J_{6,6} & J_{6,7} & J_{6,8} & 0 & 0 & 0 & 0 \\
0 & J_{7,6} & I_{N_C} & J_{7,8} & 0 & 0 & 0 & 0 \\
J_{8,5} & J_{8,6} & J_{8,7} & J_{8,8} & 0 & 0 & 0 & 0
\end{array}\right]
\begin{array}{c}
(N_c) \\ (N_c) \\ (N_c) \\ (6) \\ (N_c) \\ (N_c) \\ (N_c) \\ (6)
\end{array}
$$

$$
= \left[\begin{array}{cccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right] \in \mathbb{R}^{2Nc+6 \times 6N_c+14}
$$

And Condition 2:

$$
Z_2^T \mathcal{F}_1|_{z} = \left[\begin{array}{cccccccc}
0 & I_{Nc} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & I_{N_c} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & I_6 & 0 & 0 & 0 & 0
\end{array}\right]
\left[\begin{array}{cccc}
0 & J_{1,2} & J_{1,3} & J_{1,4} \\
I_{N_c} & J_{2,2} & J_{2,3} & J_{2,4} \\
0 & J_{3,2} & I_{N_c} & J_{3,4} \\
J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4} \\
0 & J_{5,2} & J_{5,3} & J_{5,4} \\
0 & J_{6,2} & J_{6,3} & J_{6,4} \\
0 & J_{7,2} & 0 & J_{7,4} \\
J_{8,1} & J_{8,2} & J_{8,3} & J_{8,4}
\end{array}\right]
\begin{array}{c}
(N_c) \\ (N_c) \\ (N_c) \\ (6) \\ (N_c) \\ (N_c) \\ (N_c) \\ (6)
\end{array}
$$

$$
= \left[\begin{array}{cccc}
I_{N_c} & J_{2,2} & J_{2,3} & J_{2,4} \\
0 & J_{3,2} & I_{N_c} & J_{3,4} \\
J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4}
\end{array}\right] \in \mathbb{R}^{2Nc+6 \times 3N_c+7}
$$

This is the same matrix that results in the $\mu = 0$ case and hence the relevant rank conditions follow from the results in the previous section. The matrices $T_2$ and $Z_1$ are therefore the same as those determined in the case where $\mu = 0$.

## A.6 Quasi-linear DAE Analysis

It is required to investigate the conditions described in Theorem 2.3, as applied to System 1. First, note that, with $E, h$ defined in (3.15 - 3.17), the partial derivative of $h$, given in terms of the matrices in Appendix A.3, is as follows:

$$h_z(t,z) = \begin{bmatrix} I_{N_C} & J_{2,2} & J_{2,3} & J_{2,4} \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} \\ J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4} \end{bmatrix} \in \mathbb{R}^{2N_c+6\times 3N_c+7}$$

A condition for a system to be d-index $1$ is that matrix $\begin{bmatrix} E \\ h_z \end{bmatrix}$ has full rank:

$$\begin{aligned} \text{rank} \begin{bmatrix} E \\ h_z \end{bmatrix} &= \text{rank} \begin{bmatrix} -I_{N_c} & 0 & 0 & 0 \\ I_{N_C} & J_{2,2} & J_{2,3} & J_{2,4} \\ 0 & J_{3,2} & I_{N_c} & J_{3,4} \\ J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4} \end{bmatrix} \\ &= N_c + \text{rank} \begin{bmatrix} J_{2,2} & J_{2,3} & J_{2,4} \\ J_{3,2} & I_{N_c} & J_{3,4} \\ J_{4,2} & J_{4,3} & J_{4,4} \end{bmatrix} \end{aligned}$$

To investigate further, define the following groupings for convenience:

$$\begin{aligned} J^*_{2,2} &= J_{2,2} - J_{2,3}J_{3,2} \\ J^*_{2,4} &= J_{2,4} - J_{2,3}J_{3,4} \\ J^*_{4,2} &= J_{4,2} - J_{4,3}J_{3,2} \\ J^*_{4,4} &= J_{4,4} - J_{4,3}J_{3,4} \\ J^{**}_{4,4} &= J^*_{4,4} - J^*_{4,2}\left(J^*_{2,2}\right)^{-1} J^*_{2,4} \end{aligned}$$

Then:

$$\begin{aligned} \text{rank} \begin{bmatrix} J_{2,2} & J_{2,3} & J_{2,4} \\ J_{3,2} & I_{N_c} & J_{3,4} \\ J_{4,2} & J_{4,3} & J_{4,4} \end{bmatrix} &= \text{rank} \begin{bmatrix} (J_{2,2} - J_{2,3}J_{3,2}) & 0 & (J_{2,4} - J_{2,3}J_{3,4}) \\ J_{3,2} & I_{N_c} & J_{3,4} \\ (J_{4,2} - J_{4,3}J_{3,2}) & 0 & (J_{4,4} - J_{4,3}J_{3,4}) \end{bmatrix} \begin{array}{l} R_1 - J_{2,3}R_2 \\ \\ R_3 - J_{4,3}R_2 \end{array} \\ &= \text{rank} \begin{bmatrix} J^*_{2,2} & 0 & J^*_{2,4} \\ J_{3,2} & I_{N_c} & J_{3,4} \\ J^*_{4,2} & 0 & J^*_{4,4} \end{bmatrix} = \text{rank} \begin{bmatrix} J^*_{2,2} & 0 & J^*_{2,4} \\ 0 & I_{N_c} & 0 \\ J^*_{4,2} & 0 & J^*_{4,4} \end{bmatrix} \text{ eliminate} \\ &= I_{N_c} + \text{rank} \begin{bmatrix} J^*_{2,2} & J^*_{2,4} \\ J^*_{4,2} & J^*_{4,4} \end{bmatrix} \end{aligned}$$

Note the form of $J^*_{2,2}$, given below:

$$J^*_{2,2} = \left[\begin{array}{ccccc} \xi_{13,1} & 0 & \cdots & & 0 \\ 0 & \xi_{13,2} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & \xi_{13,N_C} \end{array}\right] \in \mathbb{R}^{N_c \times N_c}$$

along with the System 1 assumptions, guarantees that the matrix is non-singular and hence:

$$\begin{aligned}
\text{rank}\left[\begin{array}{cc} J^*_{2,2} & J^*_{2,4} \\ J^*_{4,2} & J^*_{4,4} \end{array}\right] &= \text{rank}\left[\begin{array}{cc} I_{N_c} & \left(J^*_{2,2}\right)^{-1} J^*_{2,4} \\ J^*_{4,2} & J^*_{4,4} \end{array}\right] \\
&= \text{rank}\left[\begin{array}{cc} I_{N_c} & \left(J^*_{2,2}\right)^{-1} J^*_{2,4} \\ 0 & \left(J^*_{4,4} - J^*_{4,2}\left(J^*_{2,2}\right)^{-1} J^*_{2,4}\right) \end{array}\right] \quad R_2 - J^*_{4,2} R_1 \\
&= \text{rank}\left[\begin{array}{cc} I_{N_c} & \left(J^*_{2,2}\right)^{-1} J^*_{2,4} \\ 0 & J^{**}_{4,4} \end{array}\right] \\
&= \text{rank}\left[\begin{array}{cc} I_{N_c} & 0 \\ 0 & J^{**}_{4,4} \end{array}\right] \quad \text{eliminate} \\
&= I_{N_c} + \text{rank}\left[J^{**}_{4,4}\right]
\end{aligned}$$

Obviously, $J^{**}_{4,4}$ must be determined. First:

$$J_{2,3}J_{3,4} = \left[\begin{array}{ccccccc} 0 & 0 & 0 & 0 & 0 & -z_{(3N_c+2)}\theta_{1,1} & -z_{(3N_c+2)}\theta_{1,2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & -z_{(3N_c+2)}\theta_{2,1} & -z_{(3N_c+2)}\theta_{2,2} \\ & & & & & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & -z_{(3N_c+2)}\theta_{N_c,1} & -z_{(3N_c+2)}\theta_{N_c,2} \end{array}\right] \in \mathbb{R}^{N_c \times 7}$$

$$J^*_{2,4} = \left[\begin{array}{ccccccc} -z_{(N_c+1)} & -z_{(2N_c+1)} & 0 & 0 & 0 & z_{(3N_c+2)}\theta_{1,1} & z_{(3N_c+2)}\theta_{1,2} \\ -z_{(N_c+2)} & -z_{(2N_c+2)} & \vdots & \vdots & \vdots & z_{(3N_c+2)}\theta_{2,1} & z_{(3N_c+2)}\theta_{2,2} \\ \vdots & \vdots & & & & \vdots & \vdots \\ -z_{(2N_c)} & -z_{(3N_c)} & 0 & 0 & 0 & z_{(3N_c+2)}\theta_{N_c,1} & z_{(3N_c+2)}\theta_{N_c,2} \end{array}\right] \in \mathbb{R}^{N_c \times 7}$$

$$J^*_{4,2} = \left[\begin{array}{cccc} 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{10,1} & \xi_{10,2} & & \xi_{10,N_c} \\ 0 & \cdots & & 0 \\ 0 & \cdots & & 0 \\ \xi_{7,1} & \xi_{7,2} & \cdots & \xi_{7,N_c} \end{array}\right] \in \mathbb{R}^{6 \times N_c}$$

$$J_{4,3}J_{3,4} = \left[\begin{array}{ccccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \bar{\alpha}_{24} & \bar{\alpha}_{25} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right] \in \mathbb{R}^{6,7}$$

$$J_{4,4}^{*} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ -\rho_l^{-1}(\cdot) & -\rho_v^{-1}(\cdot) & 0 & 0 & 0 & \alpha_1 - \bar{\alpha}_{24} & \alpha_2 - \bar{\alpha}_{25} \\ 0 & 0 & -\frac{\partial \psi^L}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial \psi^L}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial \psi^V}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 0 & \alpha_3 & \alpha_4 \end{bmatrix} \in \mathbb{R}^{6,7}$$

$$J_{4,2}^{*} \left(J_{2,2}^{*}\right)^{-1} J_{2,4}^{*} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\alpha_{22} + \rho_l^{-1}(\cdot) & -\alpha_{23} + \rho_v^{-1}(\cdot) & 0 & 0 & 0 & -\alpha_{24} + \alpha_1 & -\alpha_{25} + \alpha_2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\alpha_{26} & -\alpha_{27} & 0 & 0 & 0 & -\alpha_{28} + \alpha_3 & -\alpha_{29} + \alpha_4 \end{bmatrix}$$

Finally, this gives $J_{4,4}^{**}$:

$$J_{4,4}^{**} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ \alpha_{22} & \alpha_{23} & 0 & 0 & 0 & \alpha_{24} & \alpha_{25} \\ 0 & 0 & -\frac{\partial \psi^L}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial \psi^L}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial \psi^V}{\partial z_{(3N_c+7)}} \\ \alpha_{26} & \alpha_{27} & 0 & 0 & 0 & \alpha_{28} & \alpha_{29} \end{bmatrix} \in \mathbb{R}^{6,7}$$

Now the rank of this matrix will be investigated in detail:

$$\text{rank} \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ \alpha_{22} & \alpha_{23} & 0 & 0 & 0 & \alpha_{24} & \alpha_{25} \\ 0 & 0 & -\frac{\partial \psi^L}{\partial z_{(3N_c+3)}} & 1 & 0 & 0 & -\frac{\partial \psi^L}{\partial z_{(3N_c+7)}} \\ 0 & 0 & 0 & 0 & 1 & 0 & -\frac{\partial \psi^V}{\partial z_{(3N_c+7)}} \\ \alpha_{26} & \alpha_{27} & 0 & 0 & 0 & \alpha_{28} & \alpha_{29} \end{bmatrix} = \text{rank} \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ \alpha_{22} & \alpha_{23} & 0 & 0 & 0 & \alpha_{24} & \alpha_{25} \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \alpha_{26} & \alpha_{27} & 0 & 0 & 0 & \alpha_{28} & \alpha_{29} \end{bmatrix} \begin{matrix} \\ R_2 - R_1 \\ \\ \\ \text{eliminate} \\ \\ \end{matrix}$$

$$\begin{aligned} \text{rank} \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ \alpha_{22} & \alpha_{23} & 0 & 0 & 0 & \alpha_{24} & \alpha_{25} \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \alpha_{26} & \alpha_{27} & 0 & 0 & 0 & \alpha_{28} & \alpha_{29} \end{bmatrix} &= 3 + \text{rank} \begin{bmatrix} -1 & -1 & 0 & 0 \\ \alpha_{22} & \alpha_{23} & \alpha_{24} & \alpha_{25} \\ \alpha_{26} & \alpha_{27} & \alpha_{28} & \alpha_{29} \end{bmatrix} \\ &= 3 + \text{rank} \begin{bmatrix} -1 & -1 & 0 & 0 \\ \alpha_{22} & \alpha_{23} & \alpha_{24} & \alpha_{25} \\ \alpha_{26} & \alpha_{27} & \alpha_{28} & \alpha_{29} \end{bmatrix} \\ &= 3 + \text{rank} \begin{bmatrix} -1 & -1 & 0 & 0 \\ 0 & (\alpha_{23} - \alpha_{22}) & \alpha_{24} & \alpha_{25} \\ 0 & (\alpha_{27} - \alpha_{26}) & \alpha_{28} & \alpha_{29} \end{bmatrix} \begin{matrix} \\ R_2 + \alpha_{22} R_1 \\ R_3 + \alpha_{26} R_1 \end{matrix} \\ &= 4 + \text{rank} \begin{bmatrix} (\alpha_{23} - \alpha_{22}) & \alpha_{24} & \alpha_{25} \\ (\alpha_{27} - \alpha_{26}) & \alpha_{28} & \alpha_{29} \end{bmatrix} \end{aligned}$$

Therefore, an equivalent condition to the system in question having s-index $0$ is that the block

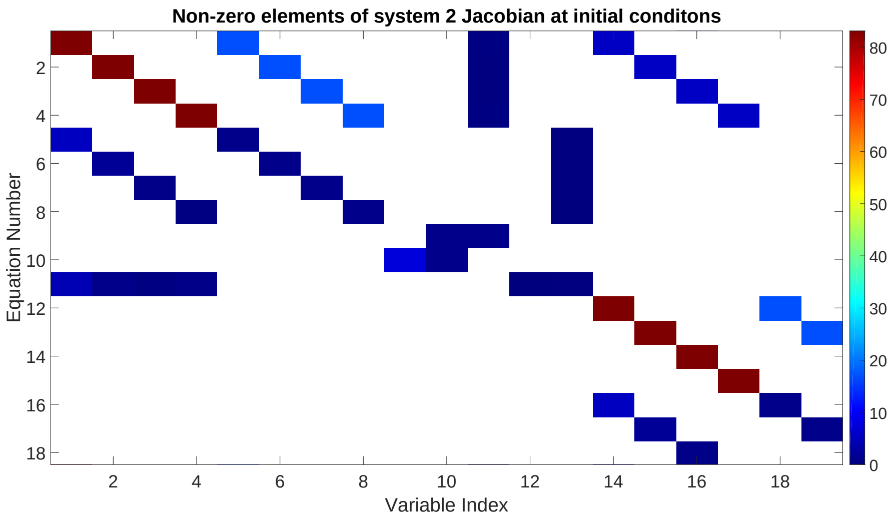
$$\begin{bmatrix} (\alpha_{23}-\alpha_{22}) & \alpha_{24} & \alpha_{25} \\ (\alpha_{27}-\alpha_{26}) & \alpha_{28} & \alpha_{29} \end{bmatrix} \tag{A.16}$$

has full row rank for all admissible states.

# B System 2 Jacobian

In this section, the Jacobians needed for testing Hypothesis 1 for the second system of equations are derived and analysed. The Jacobians are given for both $\mu = 0$ and $\mu = 1$.

The structure of the Jacobians can be visualised for the base case steady-state conditions derived in Section 5.5. While this does not give a fully general picture as the time-derivatives are all zero, and only simple closure models are applied, it allows the scaling and general structure of the initial matrix to be observed. The variable indices can be interpreted using Table 3 in Section 4.1. Whitespace means the value is zero.



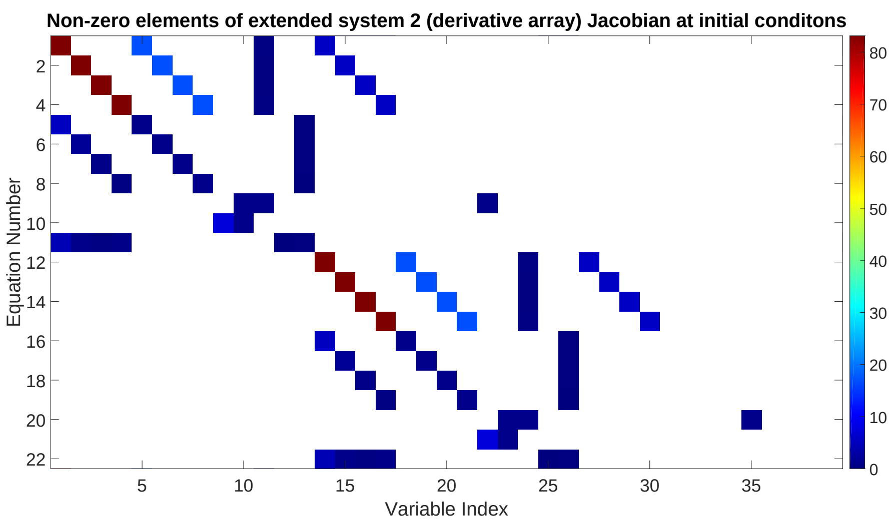




Figure 32: Jacobian of derivative array for system 2, $\mu = 0$ (top) and $\mu = 1$ (bottom) for sample problem at steady-state initial conditions.

## B.1 Time Derivative of System 2

In order to form the derivative array, the derivatives of the nonlinear DAE system given in (4.1-4.5) are needed. These are given as follows:

$$\begin{aligned} 0 = {} & \dot{z}_{(2N_c+1)}\dot{z}_i + z_{(2N_c+1)}\ddot{z}_i - \dot{\phi}_{(N_c+1)}\left(\phi_i - z_i\right) \\ & - \phi_{(N_c+1)}\left(\dot{\phi}_i - \dot{z}_i\right) + \dot{z}_{(2N_c+3)}\left(z_{(N_c+i)} - z_i\right) + z_{(2N_c+3)}\left(\dot{z}_{(N_c+i)} - \dot{z}_i\right) \end{aligned} \tag{B.1}$$

$$0 = \dot{z}_{(N_c+i)} - \left[\frac{\partial K_i\left(\cdot\right)}{\partial z_{(2N_c+4)}}\dot{z}_{(2N_c+4)}z_i + \frac{\partial K_i\left(\cdot\right)}{\partial z_{(2N_c+5)}}\dot{z}_{(2N_c+5)}z_i + K_i\left(\cdot\right)\dot{z}_i\right] \tag{B.2}$$

$$0 = \ddot{z}_{(2N_c+1)} - \dot{\phi}_{(N_c+1)} + \dot{z}_{(2N_c+2)} + \dot{z}_{(2N_c+3)} \tag{B.3}$$

$$0 = \dot{z}_{(2N_c+2)} - \left[\frac{\partial \psi_L\left(\cdot\right)}{\partial z_{(2N_c+1)}}\dot{z}_{(2N_c+1)} + \frac{\partial \psi_L\left(\cdot\right)}{\partial z_{(2N_c+5)}}\dot{z}_{(2N_c+5)}\right] \tag{B.4}$$

$$0 = \sum_{i=1}^{N_c}\left[\left(\frac{\partial K_i\left(\cdot\right)}{\partial z_{(2N_c+4)}}\dot{z}_{(2N_c+4)} + \frac{\partial K_i\left(\cdot\right)}{\partial z_{(2N_c+5)}}\dot{z}_{(2N_c+5)}\right)z_i + \left(K_i\left(\cdot\right) - 1\right)\dot{z}_i\right] \tag{B.5}$$

## B.2 Parameter Groups

For notational convenience, frequently used or complex expressions are grouped here, into a few broad categories. Most of the listed groups are used in forming the system Jacobian, and in expressing the matrices that are needed to determine the rank of various blocks.

The parameters are loosely grouped as follows. $\theta$ and $\xi$ are used to denote shorthand for columns and rows respectively, where a single generating expression is given for the entire vector. $\alpha$ denotes scalar groups that appear as elements in the final matrices.

The column vectors $\theta$ are given as:

$$
\begin{aligned}
\theta_{i,1} &= z_{(Nc+i)} - z_i \\
\theta_{i,2} &= \left[ -z_i \frac{\partial K_i\left(\cdot\right)}{\partial z_{(2N_c+4)}} \right] \\
\theta_{i,3} &= \left[ -z_i \frac{\partial K_i\left(\cdot\right)}{\partial z_{(2N_c+5)}} \right] \\
\theta_{i,4} &= \dot{z}_{(N_c+i)} - \dot{z}_i \\
\theta_{i,5} &= -\left[ \frac{\partial K_i\left(\cdot\right)}{\partial z_{(3N_c+4)}} \dot{z}_{(3N_c+4)} + \frac{\partial K_i\left(\cdot\right)}{\partial z_{(3N_c+5)}} \dot{z}_{(3N_c+5)} \right] \\
\theta_{i,6} &= \left( -\left[ \frac{\partial^2 K_i\left(\cdot\right)}{\partial z^2_{(2N_c+4)}} \dot{z}_{(3N_c+4)} + \frac{\partial^2 K_i\left(\cdot\right)}{\partial z_{(2N_c+4)} \partial z_{(2N_c+5)}} \dot{z}_{(2N_c+5)} \right] z_i - \frac{\partial K_i\left(\cdot\right)}{\partial z_{(2N_c+4)}} \dot{z}_i \right) \\
\theta_{i,7} &= \left( -\left[ \frac{\partial^2 K_i\left(\cdot\right)}{\partial z_{(2N_c+5)} \partial z_{(2N_c+4)}} \dot{z}_{(2N_c+4)} + \frac{\partial^2 K_i\left(\cdot\right)}{\partial z^2_{(2N_c+5)}} \dot{z}_{(2N_c+5)} \right] z_i - \frac{\partial K_i\left(\cdot\right)}{\partial z_{(3N_c+5)}} \dot{z}_i \right)
\end{aligned}
$$

The row vectors $\xi$ are given as:

$$
\begin{aligned}
\xi_{1,i} &= K_i\left(\cdot\right) - 1 \\
\xi_{2,i} &= \left( \frac{\partial K_i(\cdot)}{\partial z_{(2N_c+4)}} \dot{z}_{(2N_c+4)} + \frac{\partial K_i(\cdot)}{\partial z_{(2N_c+5)}} \dot{z}_{(2N_c+5)} \right)
\end{aligned}
$$

Finally, the parameters $\alpha$ are given as:

$$
\begin{aligned}
\alpha_1 &= \phi_{(N_c+1)} - z_{(2N_c+3)} \\
\alpha_2 &= \sum_{i=1}^{N_c} \left( \frac{\partial K_i\left(\cdot\right)}{\partial z_{(2N_{c+4})}} z_i \right) \\
\alpha_3 &= \sum_{i=1}^{N_c} \left( \frac{\partial K_i\left(\cdot\right)}{\partial z_{(3N_{c+5})}} z_i \right) \\
\alpha_4 &= \dot{\phi}_{(N_c+1)} - \dot{z}_{(2N_c+3)} \\
\alpha_5 &= \dot{z}_{(2N_c+1)} + \phi_{(N_c+1)} - z_{(2N_c+3)} \\
\alpha_6 &= -\left[ \frac{\partial^2 \psi_L\left(\cdot\right)}{\partial z_{(2N_c+1)} \partial z_{(2N_c+5)}} \dot{z}_{(2N_c+5)} + \frac{\partial^2 \psi_L\left(\cdot\right)}{\partial z^2_{(2N_c+1)}} \dot{z}_{(2N_c+1)} \right]
\end{aligned}
$$

$$\alpha_7 = -\left[\frac{\partial^2 \psi_L(\cdot)}{\partial z^2_{(2N_c+5)}}\dot{z}_{(2N_c+5)} + \frac{\partial^2 \psi_L(\cdot)}{\partial z_{(2N_c+5)}\partial z_{(2N_c+1)}}\dot{z}_{(2N_c+1)}\right]$$

$$\alpha_8 = \sum_{i=1}^{Nc}\left[\frac{\partial K_i(\cdot)}{\partial z_{(2N_c+4)}}\dot{z}_i + \left(\frac{\partial^2 K_i(\cdot)}{\partial z^2_{(2N_c+4)}}\dot{z}_{(2N_c+4)} + \frac{\partial^2 K_i(\cdot)}{\partial z_{(2N_c+4)}\partial z_{(2N_c+5)}}\dot{z}_{(2N_c+5)}\right) z_i\right]$$

$$\alpha_9 = \sum_{i=1}^{Nc}\left[\frac{\partial K_i(\cdot)}{\partial z_{(2N_c+5)}}\dot{z}_i + \left(\frac{\partial^2 K_i(\cdot)}{\partial z_{(2N_c+5)}\partial z_{(2N_c+4)}}\dot{z}_{(2N_c+4)} + \frac{\partial^2 K_i(\cdot)}{\partial z^2_{(2N_c+5)}}\dot{z}_{(2N_c+5)}\right) z_i\right]$$

$$\alpha_{10} = \frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+1)}} + \frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+5)}}$$

$$\alpha_{11} = -\frac{\alpha_3}{\alpha_4}$$

$$\alpha_{12} = \left(\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+1)}}\right)^{-1}\left(1 + \frac{\alpha_2}{\alpha_3}\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+5)}}\right)$$

$$\alpha_{13} = -\frac{\alpha_2}{\alpha_3}$$

## B.3 Jacobian of the Derivative Array for System 2

The Jacobian of the derivative array is constructed in the following way:

$$\mathcal{F}_1|_{z,\dot{z},\ddot{z}} = \begin{bmatrix} F|_z & F|_{\dot{z}} & F|_{\ddot{z}} \\ \dot{F}|_z & \dot{F}|_{\dot{z}} & \dot{F}|_{\ddot{z}} \end{bmatrix}$$

$$F|_z = \frac{\partial}{\partial z_i} F\left(t, z, \dot{z}\right) = \begin{bmatrix} J_{1,1} & J_{1,2} & J_{1,3} \\ J_{2,1} & J_{2,2} & J_{2,3} \\ J_{3,1} & J_{3,2} & J_{3,3} \end{bmatrix} \in \mathbb{R}^{2N_c+3 \times 2N_c+5}$$

$$F|_{\dot{z}} = \frac{\partial}{\partial \dot{z}_i} F\left(t, z, \dot{z}\right) = \begin{bmatrix} J_{1,4} & J_{1,5} & J_{1,6} \\ J_{2,4} & J_{2,5} & J_{2,6} \\ J_{3,4} & J_{3,5} & J_{3,6} \end{bmatrix} \in \mathbb{R}^{2N_c+3 \times 2N_c+5}$$

$$F|_{\ddot{z}} = \frac{\partial}{\partial \ddot{z}_i} F\left(t, z, \dot{z}\right) = \begin{bmatrix} J_{1,7} & J_{1,8} & J_{1,9} \\ J_{2,7} & J_{2,8} & J_{2,9} \\ J_{3,7} & J_{3,8} & J_{3,9} \end{bmatrix} \in \mathbb{R}^{2N_c+3 \times 2N_c+5}$$

$$\dot{F}|_z = \frac{\partial}{\partial z_i} \frac{dF}{dt}\left(t, z, \dot{z}, \ddot{z}\right) = \begin{bmatrix} J_{4,1} & J_{4,2} & J_{4,3} \\ J_{5,1} & J_{5,2} & J_{5,3} \\ J_{6,1} & J_{6,2} & J_{6,3} \end{bmatrix} \in \mathbb{R}^{2N_c+3 \times 2N_c+5}$$

$$\dot{F}|_{\dot{z}} = \frac{\partial}{\partial \dot{z}_i} \frac{dF}{dt}\left(t, z, \dot{z}, \ddot{z}\right) = \begin{bmatrix} J_{4,4} & J_{4,5} & J_{4,6} \\ J_{5,4} & J_{5,5} & J_{5,6} \\ J_{6,4} & J_{6,5} & J_{6,6} \end{bmatrix} \in \mathbb{R}^{2N_c+3 \times 2N_c+5}$$

$$\dot{F}|_{\ddot{z}} = \frac{\partial}{\partial \ddot{z}_i} \frac{dF}{dt}\left(t, z, \dot{z}, \ddot{z}\right) = \begin{bmatrix} J_{4,7} & J_{4,8} & J_{4,9} \\ J_{5,7} & J_{5,8} & J_{5,8} \\ J_{6,7} & J_{6,8} & J_{6,9} \end{bmatrix} \in \mathbb{R}^{2N_c+3 \times 2N_c+5}$$

$$J_{1,1} = \begin{bmatrix} \alpha_1 & 0 & \cdots & & 0 \\ 0 & \alpha_1 & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & \alpha_1 \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{1,2} = \begin{bmatrix} z_{(2N_c+3)} & 0 & \cdots & & 0 \\ 0 & z_{(2N_c+3)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & z_{(2N_c+3)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{1,3} = \begin{bmatrix} \dot{z}_1 & 0 & \theta_{1,1} \\ \vdots & & \\ & & \\ \dot{z}_{N_c} & 0 & \theta_{N_c,1} \end{bmatrix} \in \mathbb{R}^{N_c \times 5}$$

$$J_{1,4} = \begin{bmatrix} z_{(2N_c+1)} & 0 & \cdots & & 0 \\ 0 & z_{(2N_c+1)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & z_{(2N_c+1)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{1,5} = 0 \in \mathbb{R}^{N_c \times N_c}$$
$$J_{1,6} = 0 \in \mathbb{R}^{N_c \times 5}$$
$$J_{1,7} = 0 \in \mathbb{R}^{N_c \times N_c}$$
$$J_{1,8} = 0 \in \mathbb{R}^{N_c \times N_c}$$
$$J_{1,9} = 0 \in \mathbb{R}^{N_c \times 5}$$

$$J_{2,1} = \begin{bmatrix} -K_1(\cdot) & 0 & \cdots & & 0 \\ 0 & -K_2(\cdot) & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & -K_{N_c}(\cdot) \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{2,2} = I_{N_c} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{2,3} = \begin{bmatrix} 0 & 0 & 0 & \theta_{1,2} & \theta_{1,3} \\ \vdots & \vdots & \vdots & \theta_{2,2} & \theta_{2,3} \\ & & & \vdots & \vdots \\ & & & & \\ 0 & 0 & 0 & \theta_{N_c,2} & \theta_{N_c,3} \end{bmatrix} \in \mathbb{R}^{N_c \times 5}$$

$$J_{2,4} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{2,5} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{2,6} = 0 \in \mathbb{R}^{N_c \times 5}$$

$$J_{2,7} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{2,8} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{2,9} = 0 \in \mathbb{R}^{N_c \times 5}$$

$$J_{3,1} = \begin{bmatrix} 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ \xi_{1,1} & \cdots & \xi_{1,2} \end{bmatrix} \in \mathbb{R}^{3\times N_c}$$

$$J_{3,2} = 0 \in \mathbb{R}^{5\times N_c}$$

$$J_{3,3} = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ -\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+1)}} & 1 & 0 & 0 & -\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+5)}} \\ 0 & 0 & 0 & \alpha_2 & \alpha_3 \end{bmatrix} \in \mathbb{R}^{3\times 5}$$

$$J_{3,4} = 0 \in \mathbb{R}^{3\times N_c}$$

$$J_{3,5} = 0 \in \mathbb{R}^{3\times N_c}$$

$$J_{3,6} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \in\in \mathbb{R}^{3\times 5}$$

$$J_{3,7} = 0 \in \mathbb{R}^{3\times N_c}$$

$$J_{3,8} = 0 \in \mathbb{R}^{3\times N_c}$$

$$J_{3,9} = 0 \in \mathbb{R}^{3\times 5}$$

$$J_{4,1} = \begin{bmatrix} \alpha_4 & 0 & \cdots & & 0 \\ 0 & \alpha_4 & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & \alpha_4 \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{4,2} = \begin{bmatrix} \dot{z}_{(2N_c+3)} & 0 & \cdots & & 0 \\ 0 & \dot{z}_{(2N_c+3)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & \dot{z}_{(2N_c+3)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{4,3} = \begin{bmatrix} \ddot{z}_1 & 0 & \theta_{1,4} & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \ddot{z}_{N_c} & 0 & \theta_{N_c,4} & 0 & 0 \end{bmatrix} \in \mathbb{R}^{N_c \times 5}$$

$$J_{4,4} = \begin{bmatrix} \alpha_5 & 0 & \cdots & & 0 \\ 0 & \alpha_5 & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & \alpha_5 \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{4,5} = \begin{bmatrix} z_{(2N_c+3)} & 0 & \cdots & & 0 \\ 0 & z_{(2N_c+3)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & z_{(2N_c+3)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{4,6} = \begin{bmatrix} \dot{z}_1 & 0 & \theta_{1,5} & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \dot{z}_{N_c} & 0 & \theta_{N_c,5} & 0 & 0\vdots \end{bmatrix} \in \mathbb{R}^{N_c \times 5}$$

$$J_{4,7} = \begin{bmatrix} z_{(2N_c+1)} & 0 & \cdots & & 0 \\ 0 & z_{(2N_c+1)} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & z_{(2N_c+1)} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{4,8} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{4,9} = 0 \in \mathbb{R}^{N_c \times 5}$$

$$J_{5,1} = \begin{bmatrix} \theta_{1,6} & 0 & \cdots & & 0 \\ 0 & \theta_{2,6} & & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & \theta_{N_c,6} \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,2} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,3} = \begin{bmatrix} 0 & 0 & 0 & \theta_{1,4} & \theta_{1,5} \\ \vdots & \vdots & \vdots & \theta_{2,6} & \theta_{2,7} \\ & & & \vdots & \vdots \\ 0 & 0 & 0 & \theta_{N_c,4} & \theta_{N_c,5} \end{bmatrix} \in \mathbb{R}^{N_c \times 5}$$

$$J_{5,4} = \begin{bmatrix} -K_1(\cdot) & 0 & \cdots & & 0 \\ 0 & -K_2(\cdot) & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & & \\ & \vdots & & \ddots & \\ 0 & & & \cdots & -K_{N_c}(\cdot) \end{bmatrix} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,5} = I_{N_C} \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,6} = \begin{bmatrix} 0 & 0 & 0 & \theta_{1,2} & \theta_{1,3} \\ \vdots & \vdots & \vdots & \theta_{2,2} & \theta_{2,3} \\ & & & \vdots & \vdots \\ 0 & 0 & 0 & \theta_{N_c,2} & \theta_{N_c,3} \end{bmatrix} \in \mathbb{R}^{N_c \times 5}$$

$$J_{5,7} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,8} = 0 \in \mathbb{R}^{N_c \times N_c}$$

$$J_{5,9} = 0 \in \mathbb{R}^{N_c \times 5}$$

$$
J_{6,1} = \begin{bmatrix} 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ \xi_{2,1} & \cdots & \xi_{2,N_c} \end{bmatrix} \in \mathbb{R}^{3\times N_c}
$$

$$
J_{6,2} = 0 \in \mathbb{R}^{5\times N_c}
$$

$$
J_{6,3} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ \alpha_6 & 0 & 0 & 0 & \alpha_7 \\ 0 & 0 & 0 & \alpha_8 & \alpha_9 \end{bmatrix} \in \mathbb{R}^{3\times 5}
$$

$$
J_{6,4} = \begin{bmatrix} 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ \xi_{1,1} & \cdots & \xi_{1,N_c} \end{bmatrix} \in \mathbb{R}^{3\times N_c}
$$

$$
J_{6,5} = \begin{bmatrix} 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \end{bmatrix} \in \mathbb{R}^{3\times N_c}
$$

$$
J_{6,6} = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ -\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+1)}} & 1 & 0 & 0 & -\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+5)}} \\ 0 & 0 & 0 & \alpha_2 & \alpha_3 \end{bmatrix} \in \mathbb{R}^{3\times 5}
$$

$$
J_{6,7} = 0 \in \mathbb{R}^{3\times N_c}
$$

$$
J_{6,8} = 0 \in \mathbb{R}^{3\times N_c}
$$

$$
J_{6,9} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{3\times 5}
$$

The total Jacobian is given as:

$$
\mathcal{F}_1|_{z,\dot{z},\ddot{z}} = \begin{bmatrix} J_{1,1} & J_{1,2} & J_{1,3} & J_{1,4} & 0 & 0 & 0 & 0 & 0 \\ J_{2,1} & I_{N_c} & J_{2,3} & 0 & 0 & 0 & 0 & 0 & 0 \\ J_{3,1} & 0 & J_{3,3} & 0 & 0 & J_{3,6} & 0 & 0 & 0 \\ J_{4,1} & J_{4,2} & J_{4,3} & J_{4,4} & J_{4,5} & J_{4,6} & J_{4,7} & 0 & 0 \\ J_{5,1} & 0 & J_{5,3} & J_{5,4} & I_{N_c} & J_{5,6} & 0 & 0 & 0 \\ J_{6,1} & J_{6,2} & J_{6,3} & J_{6,4} & 0 & J_{6,6} & 0 & 0 & J_{6,9} \end{bmatrix} \in \mathbb{R}^{4N_c+6\times 6N_c+15} \tag{B.6}
$$

## B.4 Ranks of System 2 Jacobian Elements

In order to test Hypothesis 1, the ranks of the matrices $\mathcal{F}_0|_{z,\dot{z}} = F|_{z,\dot{z}}$ and $\mathcal{F}_0|_{\dot{z}}$ must be determined. Recalling:

$$\mathcal{F}_0|_{z,\dot{z}} = F|_{z,\dot{z}} = \begin{bmatrix} J_{1,1} & J_{1,2} & J_{1,3} & J_{1,4} & 0 & 0 \\ J_{2,1} & I_{N_c} & J_{2,3} & 0 & 0 & 0 \\ J_{3,1} & 0 & J_{3,3} & 0 & 0 & J_{3,6} \end{bmatrix} \begin{matrix} (N_c) \\ (N_c) \\ (3) \end{matrix} \in \mathbb{R}^{2N_c+3\times 4N_c+10}$$

note that, under Assumptions 4.1, $z_{(2N_c+1)} \neq 0$ and hence $J_{1,4}$ is invertible as it is a diagonal matrix with non-zero elements. This gives:

$$\begin{aligned}
\text{rank}\begin{bmatrix} J_{1,1} & J_{1,2} & J_{1,3} & J_{1,4} & 0 \\ J_{2,1} & I_{N_c} & J_{2,3} & 0 & 0 \\ J_{3,1} & 0 & J_{3,3} & 0 & J_{3,6} \end{bmatrix} &= \text{rank}\begin{bmatrix} J_{1,4}^{-1}J_{1,4}^{-1}J_{1,1} & J_{1,4}^{-1}J_{1,2} & J_{1,4}^{-1}J_{1,3} & I_{N_c} & 0 \\ J_{2,1} & I_{N_c} & J_{2,3} & 0 & 0 \\ J_{3,1} & 0 & J_{3,3} & 0 & J_{3,6} \end{bmatrix} \quad \text{multiply by } J_{1,4}^{-1} \\
&= \text{rank}\begin{bmatrix} 0 & 0 & 0 & I_{N_c} & 0 \\ J_{2,1} & I_{N_c} & J_{2,3} & 0 & 0 \\ J_{3,1} & 0 & J_{3,3} & 0 & J_{3,6} \end{bmatrix} \quad \text{eliminate} \\
&= \text{rank}\begin{bmatrix} 0 & 0 & 0 & I_{N_c} & 0 \\ 0 & I_{N_c} & 0 & 0 & 0 \\ J_{3,1} & 0 & J_{3,3} & 0 & J_{3,6} \end{bmatrix} \quad \text{eliminate} \\
&= 2N_c + \text{rank}\begin{bmatrix} J_{3,1} & J_{3,3} & J_{3,6} \end{bmatrix}
\end{aligned}$$

Where:

$$\begin{aligned}
\text{rank}\begin{bmatrix} J_{3,1} & J_{3,3} & J_{3,6} \end{bmatrix} &= \text{rank}\begin{bmatrix} 0 & \cdots & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & \cdots & 0 & -\frac{\partial\psi^L(\cdot)}{\partial z_{(2N_c+1)}} & 1 & 0 & 0 & -\frac{\partial\psi^L(\cdot)}{\partial z_{(2N_c+5)}} & 0 & 0 & 0 & 0 & 0 \\ \xi_{1,1} & \cdots & \xi_{1,2} & 0 & 0 & 0 & \alpha_2 & \alpha_3 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \\
&= 3
\end{aligned}$$

so long as $\alpha_2$, $\alpha_3$ and $\xi_{1,i}$, $\forall i$ are not simultaneously zero. Therefore,

$$\text{rank}\left[\mathcal{F}_0|_{z,\dot{z}}\right] = 2N_c + 3$$

It is also required to determine the rank of the Jacobian with respect to $\dot{z}$ only, which is given by:

$$\text{rank}\left[F|_{\dot{z}}\right] = \text{rank}\begin{bmatrix} J_{1,4} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & J_{3,6} \end{bmatrix}$$

As mentioned previously, $J_{1,4}$ is non-zero diagonal and hence full rank, while $J_{3,6}$ has a single non-zero element, which gives that:

$$\text{rank}\left[F|_{\dot{z}}\right] = \text{rank}\begin{bmatrix} J_{1,4} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & J_{3,6} \end{bmatrix} = N_c + 1$$

## B.5 System 2 Reduced Order Projection Matrices

Recall that:

$$\mathcal{F}_0|_{\dot{z}} = F|_{\dot{z}} = \begin{array}{cc} \begin{bmatrix} J_{1,4} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & J_{3,6} \end{bmatrix} & \begin{array}{c} (N_c) \\ (N_c) \\ (3) \end{array} \end{array} \in \mathbb{R}^{2N_c+3 \times 2N_c+5}$$

A candidate for the Matrix $Z_2$ is as follows:

$$Z_2 = \begin{array}{cc} \begin{bmatrix} 0 & 0 \\ I_{N_c} & 0 \\ 0 & 0 \\ 0 & I_2 \end{bmatrix} & \begin{array}{c} (N_c) \\ (N_c) \\ (1) \\ (2) \end{array} \end{array} \in \mathbb{R}^{2N_c+3 \times Nc+2}$$

This satisfies Condition 1:

$$Z_2^T \mathcal{F}_0|_{\dot{z}} = \begin{bmatrix} 0 & I_{N_c} & 0 & 0 \\ 0 & 0 & 0 & I_2 \end{bmatrix} \begin{array}{cc} \begin{bmatrix} J_{1,4} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & J_{3,6} \end{bmatrix} & \begin{array}{c} (N_c) \\ (N_c) \\ (3) \end{array} \end{array} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{Nc+2 \times 2N_c+5}$$

And Condition 2:

$$Z_2^T \mathcal{F}_0|_{z} = \begin{bmatrix} 0 & I_{N_c} & 0 & 0 \\ 0 & 0 & 0 & I_2 \end{bmatrix} \begin{array}{cc} \begin{bmatrix} J_{1,1} & J_{1,2} & J_{1,3} \\ J_{2,1} & I_{N_c} & J_{2,3} \\ J_{3,1} & 0 & J_{3,3} \end{bmatrix} & \begin{array}{c} (N_c) \\ (N_c) \\ (3) \end{array} \end{array} = \begin{bmatrix} J_{2,1} & I_{N_c} & J_{2,3} \\ \tilde{J}_{3,1} & 0 & \tilde{J}_{3,3} \end{bmatrix} \in \mathbb{R}^{Nc+2 \times 2N_c+5}$$

with

$$\tilde{J}_{3,1} = \begin{bmatrix} 0 & \cdots & 0 \\ \xi_{1,1} & \cdots & \xi_{1,2} \end{bmatrix} \in \mathbb{R}^{2 \times N_c}$$

$$\tilde{J}_{3,3} = \begin{bmatrix} -\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+1)}} & 1 & 0 & 0 & -\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+5)}} \\ 0 & 0 & 0 & \alpha_2 & \alpha_3 \end{bmatrix} \in \mathbb{R}^{2 \times 5}$$

This matrix clearly has full row rank if $\alpha_2$ and $\alpha_3$ are not simultaneously zero, but it can be transformed into an easier form from which the nullspace can be determined:

$$\begin{bmatrix} J_{2,1} & I_{N_c} & J_{2,3} \\ \tilde{J}_{3,1} & 0 & \tilde{J}_{3,3} \end{bmatrix} \sim \begin{bmatrix} 0 & I_{N_c} & 0 \\ \tilde{J}_{3,1} & 0 & \tilde{J}_{3,3} \end{bmatrix}^{\text{eliminate}} =: B$$

As in the system 1 case, this involves multiplying from the left by a permutation matrix $M_2$ such that $Z_2^T \mathcal{F}_0|_z M_2 = B$. Now the kernel of $B$, $\tilde{T}_2$ can be determined. Propose:

$$\tilde{T}_2 = \begin{array}{cc} \begin{bmatrix} I_{N_c} & 0 \\ 0 & 0 \\ Y_1 & Y_2 \end{bmatrix} & \begin{array}{c} (N_c) \\ (N_c) \\ (5) \end{array} \end{array} \in \mathbb{R}^{2N_c+5 \times Nc+3}$$

such that:

$$\begin{bmatrix} 0 & I_{N_c} & 0 \\ \tilde{J}_{3,1} & 0 & \tilde{J}_{3,3} \end{bmatrix} \begin{bmatrix} I_{N_c} & 0 \\ 0 & 0 \\ Y_1 & Y_2 \end{bmatrix} \begin{matrix} (N_c) \\ (N_c) \\ (5) \end{matrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{matrix} (N_c) \\ (1) \\ (1) \end{matrix} \in \mathbb{R}^{N_c+2\times N_c+3}$$

This induces the following equations for the $i^{th}$ column of $Y_1$:

$$-\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+1)}} y_1 + y_2 - \frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+5)}} y_5 = 0$$
$$\xi_1 x_1 + \alpha_2 y_4 + \alpha_3 y_5 = -\xi_{1,i}$$

This leaves 5 unknowns in 2 equations; hence set $y_1 = y_5 = y_3 = 0 \implies y_2 = 0$ and:

$$y_4 = -\frac{\xi_{1,i}}{\alpha_2}$$

Which gives

$$Y_1 = \begin{bmatrix} 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ -\frac{\xi_{1,1}}{\alpha_2} & \cdots & -\frac{\xi_{1,N_c}}{\alpha_2} \\ 0 & \cdots & 0 \end{bmatrix}$$

For the matrix $Y_2$, the following homogeneous equations are induced:

$$-\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+1)}} y_1 + y_2 - \frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+5)}} y_5 = 0$$
$$\alpha_2 y_4 + \alpha_3 y_5 = 0$$

It is necessary to have 3 independent solutions in order for $\tilde{T}_2$ to have full rank. For the first column, trivially set $y_3 = 1$ and all other elements to zero. For the second column, set $y_1 = y_5 = 1$ and $y_3 = 0$, leading to:

$$y_2 = \frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+1)}} + \frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+5)}}$$
$$y_4 = -\frac{\alpha_3}{\alpha_2}$$

Alternately, set $y_4 = y_2 = 1$ and $y_3 = 0$, which gives:

$$y_1 = \left(\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+1)}}\right)^{-1} \left(1 + \frac{\alpha_2}{\alpha_3} \frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+5)}}\right)$$
$$y_5 = -\frac{\alpha_2}{\alpha_3}$$

This allows $Y_2$ to be fully defined:

$$Y_2 = \begin{bmatrix} 0 & 1 & \alpha_{12} \\ 0 & \alpha_{10} & 1 \\ 1 & 0 & 0 \\ 0 & \alpha_{11} & 1 \\ 0 & 1 & \alpha_{13} \end{bmatrix}$$

It is required to find a $T_2$ s.t. $T_2 = M_2\tilde{T}_2$, with:

$$M_2 = \begin{bmatrix} I_{N_c} & 0 & 0 \\ -J_{2,1} & I_{N_c} & -J_{2,3} \\ 0 & 0 & I_5 \end{bmatrix}$$

Now this $T_2$can be specified:

$$T_2 = \begin{bmatrix} I_{N_c} & 0 & 0 \\ -J_{2,1} & I_{N_c} & -J_{2,3} \\ 0 & 0 & I_5 \end{bmatrix} \begin{bmatrix} I_{N_c} & 0 \\ 0 & 0 \\ Y_1 & Y_2 \end{bmatrix} = \begin{array}{c} \begin{bmatrix} I_{N_c} & 0 \\ \tilde{Y}_1 & \tilde{Y}_2 \\ Y_1 & Y_2 \end{bmatrix} \end{array} \begin{array}{c} (N_c) \\ (N_c) \\ (5) \end{array} \in \mathbb{R}^{2N_c+5\times Nc+3}$$

with:

$$\begin{aligned} \tilde{Y}_1 &= -J_{2,1} - J_{2,3}Y_1 \\ \tilde{Y}_2 &= -J_{2,3}Y_2 \end{aligned}$$

Now, the final requirement is that $F_{\dot{z}}T_2$ has rank $d$, where:

$$F_{\dot{z}}T_2 = \begin{bmatrix} J_{1,4} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & J_{3,6} \end{bmatrix} \begin{bmatrix} I_{N_c} & 0 \\ \tilde{Y}_1 & \tilde{Y}_2 \\ Y_1 & Y_2 \end{bmatrix} = \begin{bmatrix} J_{1,4} & 0 \\ 0 & 0 \\ 0 & J_{3,6}Y_2 \end{bmatrix} \in \mathbb{R}^{2N_c+3\times N_c+3}$$

and:

$$J_{3,6}Y_2 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & \alpha_{12} \\ 0 & \alpha_{10} & 1 \\ 1 & 0 & 0 \\ 0 & \alpha_{11} & 1 \\ 0 & 1 & \alpha_{13} \end{bmatrix} = \begin{bmatrix} 0 & 1 & \alpha_{12} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

As mentioned previously, $J_{1,4}$ has full rank $N_c$ by assumption, and hence:

$$\text{rank}\,[F_{\dot{z}}T_2] = N_c + 1$$

Finally, a smooth matrix-valued function $Z_1$, such that $Z_1F_{\dot{z}}T_2$ has full rank $d = N_c + 1$, is given as:

$$Z_1 = \begin{bmatrix} I_{Nc} & 0 \\ 0 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{array}{c} (N_c) \\ (N_c) \\ (1) \\ (1) \\ (1) \end{array} \in \mathbb{R}^{2N_c+3\times N_c+1}$$

It follows that:

$$Z_1 F_{\dot{z}} T_2 = \begin{bmatrix} I_{Nc} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} J_{1,4} & 0 \\ 0 & 0 \\ 0 & J_{3,6} Y_2 \end{bmatrix} = \begin{array}{c} \begin{bmatrix} J_{1,4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & \alpha_{12} \end{bmatrix} \end{array} \begin{array}{c} (N_c) \\ (1) \end{array} \in \mathbb{R}^{N_c+1 \times N_c+3}$$

and has rank $d = N_c + 1$.

## B.6 Quasi-linear DAE Analysis

It is required to investigate the conditions described in Theorem 2.3, as applied to System 2. First, note that, with $E, h$ defined in (4.7-4.9), the partial derivative of $h$, given in terms of the matrices in Appendix B.3, is as follows:

$$h_z(t,z) = \begin{bmatrix} J_{2,1} & I_{N_c} & J_{2,3} \\ \tilde{J}_{3,1} & 0 & \tilde{J}_{3,3} \end{bmatrix} \in \mathbb{R}^{N_c+2 \times 2N_c+5}$$

where, just as above:

$$\tilde{J}_{3,1} = \begin{bmatrix} 0 & \cdots & 0 \\ \xi_{1,1} & \cdots & \xi_{1,2} \end{bmatrix} \in \mathbb{R}^{2 \times N_c}$$

$$\tilde{J}_{3,3} = \begin{bmatrix} -\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+1)}} & 1 & 0 & 0 & -\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+5)}} \\ 0 & 0 & 0 & \alpha_2 & \alpha_3 \end{bmatrix} \in \mathbb{R}^{2\times 5}$$

A condition for a system to be d-index 1 is that matrix $\begin{bmatrix} E \\ h_z \end{bmatrix}$ has full rank:

$$\text{rank} \begin{bmatrix} E \\ h_z \end{bmatrix} = \text{rank} \begin{bmatrix} \tilde{E}_1 & 0 & \hat{E}_1 \\ J_{2,1} & I_{N_c} & J_{2,3} \\ \tilde{J}_{3,1} & 0 & \tilde{J}_{3,3} \end{bmatrix} = N_c + \text{rank} \begin{bmatrix} \tilde{E}_1 & \hat{E}_1 \\ \tilde{J}_{3,1} & \tilde{J}_{3,3} \end{bmatrix}$$

Where:

$$\begin{aligned} \text{rank} \begin{bmatrix} \tilde{E}_1 & \hat{E}_1 \\ \tilde{J}_{3,1} & \tilde{J}_{3,3} \end{bmatrix} &= \text{rank} \begin{bmatrix} -z_{(2N_c+1)} I_{N_c} & 0 \\ 0 & \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \end{bmatrix} \\ \tilde{J}_{3,1} & \tilde{J}_{3,3} \end{bmatrix} \\ &= N_c + \text{rank} \begin{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \end{bmatrix} \\ \tilde{J}_{3,3} \end{bmatrix} \\ &= N_c + \text{rank} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+1)}} & 1 & 0 & 0 & -\frac{\partial \psi^L(\cdot)}{\partial z_{(2N_c+5)}} \\ 0 & 0 & 0 & \alpha_2 & \alpha_3 \end{bmatrix} \\ &= N_c + 2 + \text{rank} \begin{bmatrix} \alpha_2 & \alpha_3 \end{bmatrix} \end{aligned}$$

and the matrix has full row rank if and only if $\alpha_2$ and $\alpha_3$ are not both simultaneously zero.

# C Code and Implementation

Code to solve the problems described in Section 5.6 was developed and implemented in Matlab® 2014b. In developing code for the solution of the two systems of flash equations considered in this work, a modular approach was taken. The codes are available from `https://github.com/jpjanet/Dynamic_flash_codes/`. The overall structure of the program written is depicted below:

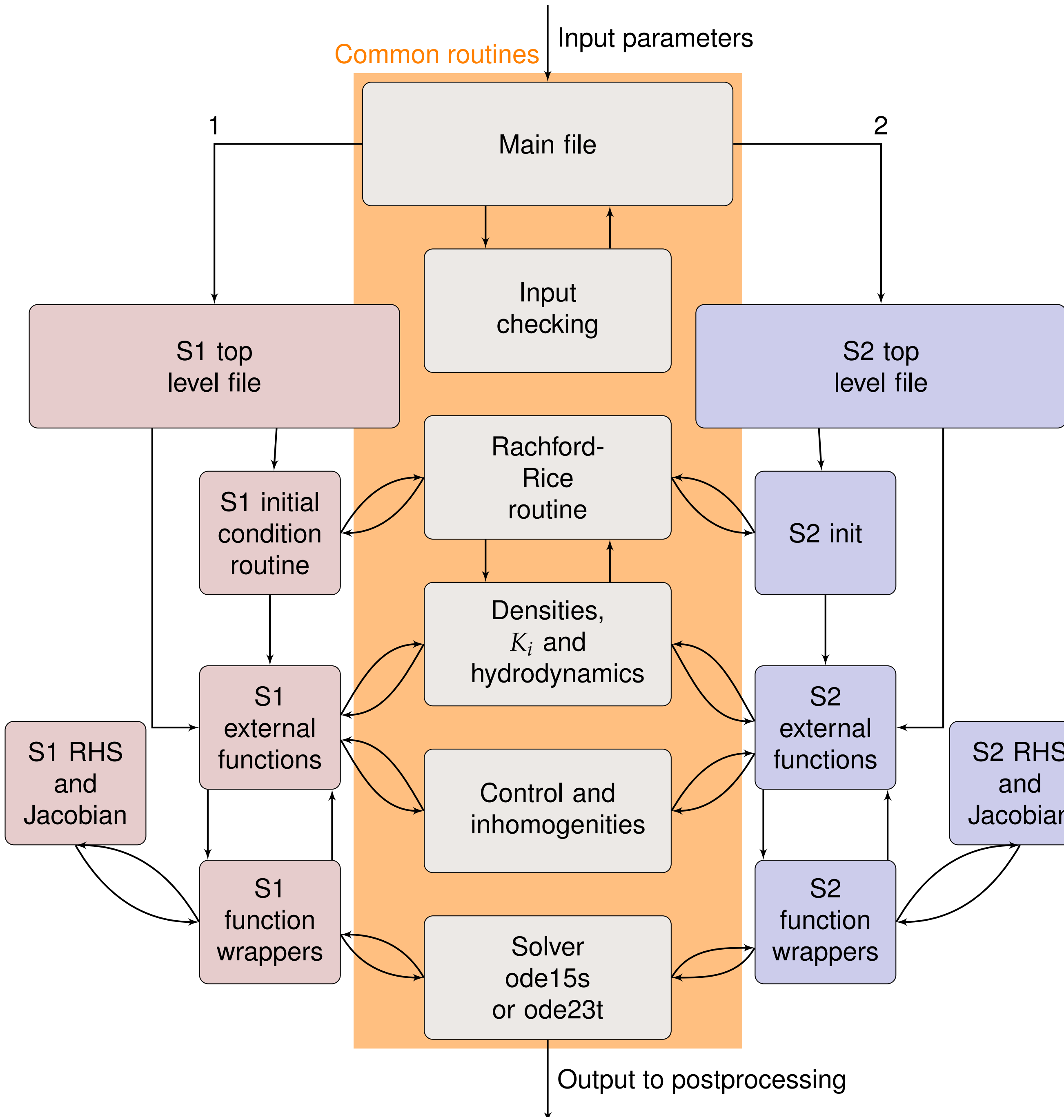



Figure 33: Schematic depiction of code logic

There are a number of routines, for example the equilibrium function $K_i$ (Equation (5.3) in Section 5.1), the phase densities and the tank hydrodynamics that are common to both systems. Hence, these functions are grouped together into a series of common m-files that could easily be switched out. This allows for different equilibrium/tank models to be inserted with minimal changes.

The code begins with a top-level file, *dynamic_flash_mainfile.m*, in which the test case, tolerance and other high-level parameters are entered. This code then invokes separate scripts for the two systems, with the same data, in order to provide an easy comparison. The top-level file invokes the System 1 solver first and the System 2 solver afterwards, but these could run in parallel in theory. Each system's main script (*s1_explicit_function.m* or *s2_explicit_function.m*) begins by invoking a routine to calculate consistent initial conditions by the Rachford-Rice method, as described in Section 5.5. The Rachford-Rice function is set up to be used by both systems - the system initial condition file simply assigns the output of the routine (which is in physical variables) to the correct indices in the state variable vector for each system.

Next, the system script creates wrappers to the common function handles as required for the current test case, for example selecting the time-varying temperature function for Test Case 1 or the control for Test Case 3. Because each system function can select which state variables it passes to the external functions, the same common function can be specified in physical variables for both systems. The script also creates function handles for the system right hand side (RHS), left hand side (mass matrix) and Jacobians. The equations are solved in the form given in Equations (3.15-3.17) and (4.7-4.9).

The system functions then pass the wrapped function handles to the ODE code, using the solver specified in the top-level file. The results of the solver are then returned to the top-level script environment so that they are in the workspace after the code is complete. Depending on the options specified, the results can be passed to automatic post-processing, where the figures like those given in Section 6 are plotted.

## C.1 Instructions

This section provides a short guide for using the codes provided to simulate the test cases given in Section 5.6. All of the code files are commented sufficiently to explain the functioning of the files, so only usage instructions are given here. These codes were written and tested in Matlab® 2014b, and compatibility with other versions has not been established.

The codes are provided in a package that contains three sub-directories: *common*, *system1* and *system2*. The only file that needs to be edited and invoked is *dynamic_flash_mainfile.m*, which lives in the top level directory. The code supports two methods of operation. Firstly, the code can be provided with a single tolerance and test case, in which case the code executes as per Figure 33 above - first System 1, and then System 2, are solved for the given parameters. This method of operation is called **Default Mode**.

Alternatively, if **both** *tol* is a vector and *clock* is set on, the code will detect this and switch into an alternate behaviour. If these two conditions are fulfilled, the code will instead sweep through the procedure depicted in Figure 33 **for each tolerance, both solvers and each test case**. As Test Case 3 takes longer to complete, the third test case can be excluded by setting the parameter *include3* to $0$. Effectively, this mode compares the solution time across all combinations of test case, solver and system for the vector of tolerances specified. Hence, this operation is called **Comparison Mode**.

In order to protect against lockout resulting from long run times, Test Case 3 will not simulate for tolerances tighter than $5 \times 10^{-7}$ in this mode. Instead, it will run for all tolerances larger than this value (the other two test cases will proceed normally). If it is desired to use strict tolerances for Test Case 3, consider running the test individually using **Default Mode**, where no such restrictions are enforced.

The inputs that are intended to be edited by the user in *dynamic_flash_mainfile.m* are given in Table 12 below:

Table 12: Input parameters to *dynamic_flash_mainfile.m*

| Parameter | Values | Default Mode | Comparison Mode |
|---|---|---|---|
| *testcase* | $1,2,3$ | Choice of test case for current run. | No effect (all test cases will be timed) |
| *integrator* | *ode15s*,*ode23t* | Select which solver to use | No effect, both solvers are automatically compared |
| *stats* | *on*, *off* | Enable display of all available solver output (number of runs, successful timesteps etc) | |
| *gain* | $\geq 0$ | Control gain for Test Case 3 (if *testcase*$= 3$) | Test Case 3 control gain |
| *tspan* | $[a, b]$ | Time span for integration (from $a$ to $b$) with $0 \leq a < b$ | |
| *tol* | $> 0$ | Integration error tolerance (absolute), should be scalar | Integration error tolerance (absolute), should be a vector of different tolerances |
| *clock* | $0, 1$ | Times the current run if set to $1$, averaged over *clock_reps* runs | Must be set to $1$ to enable Comparison Mode. Averaged over *clock_reps* runs |
| *clock_reps* | $\in \mathbb{N}$ | Natural number, the number of times to repeat the solver and average the results. No effect if *clock*$= 0$ | |
| *include3* | $0, 1$ | No effect | Enables $(= 1)$ Test Case 3 in the comparison. This may increase run time |
| *jtest* | $0, 1$ | Enable $(= 1)$ to check the Jacobians numerically. Enabling this option will print the result of the test to the workspace | |
| *plotting* | $0, 1$ | Enables automatic plotting of figures as in Section 6 | No effect, time-comparison plots are generated by default |

The variables returned to the workspace depend on the mode of operation. For the **Default Mode**, the variables returned to the workspace are as in Table 13 below. The variables are all returned in physical units corresponding to those given in Section 5.5. For matrices with components as columns, the order is from light to heavy, such that the first column corresponds to propane.

Table 13: Returned values in Default Mode

| Varaible name | Description |
|---|---|
| *tt1*,*tt2* | Vector of discrete times (integrator timesteps), for Systems 1 and 2 respectively. |
| *x1*,*x2* | Matrix of species liquid composition (as columns) at the times specified in *tt1* and *tt2* for Systems 1 and 2 respectively. |
| *y1*,*y2* | Matrix of species vapour composition (as columns) at the times specified in *tt1* and *tt2* for Systems 1 and 2 respectively. |
| *M1*,*M2* | Vector with total molar hold-up in the vessel at the times specified in *tt1* and *tt2* for Systems 1 and 2 respectively. |
| *L1*,*L2* | Vector with molar liquid discharge rate at the times specified in *tt1* and *tt2* for Systems 1 and 2 respectively. |
| *V1*,*V2* | Vector with molar vapour discharge rate at the times specified in *tt1* and *tt2* for Systems 1 and 2 respectively. |
| *P1*,*P2* | Vector with internal total pressure at the times specified in *tt1* and *tt2* for Systems 1 and 2 respectively. |
| *T1*,*T2* | Vector with temperature (control) at the times specified in *tt1* and *tt2* for Systems 1 and 2 respectively. |
| *Mi* | Matrix of species molar outflow (as columns) at the times specified in *tt1* and *tt2* for System 1 only. |
| *Ml* | Vector with molar liquid hold-up in the vessel at the times specified in *tt1* and *tt2* for System 1 only. |
| *Mv* | Vector with molar vapour hold-up in the vessel at the times specified in *tt1* and *tt2* for System 1 only. |

The return types for operation in **Comparison Mode** are given in Table 14 below. As opposed to the results from **Default Mode**, the state variables are not returned to the workspace. Instead, the code returns matrices containing the solution time and number of timesteps taken for the various combinations of test case, system and solver.

Table 14: Returned values in Comparsion Mode

| Varaible name | Description |
|---|---|
| *TIME_INFO_15s_1* | Matrix, comprising of the solution times for Test Case 1 using *ode15s*. The number of rows correspond to the elements in the vector *tol*. The first column contains the solution time for System 1, and the second column contains the number of timesteps taken by the integrator. The third and fourth columns contain the solution time and number of timesteps for System 2, respectively. |
| *TIME_INFO_15s_2* | Matrix, as above, but for Test Case 2. |
| *TIME_INFO_15s_3* | Matrix, as above, but for Test Case 3. Only returned if *include3*$= 1$ in *dynamic_flash_mainfile.m*. Note that the code will not attempt Test Case 3 for tolerances tighter than $5 \times 10^{-7}$, in order to ensure fast solution time. To time Test Case 3 at tighter tolerances, use **Default Mode** with *clock*$= 1$. |
| *TIME_INFO_23t_1* | Matrix, the same as *TIME_INFO_15s_1*, but using *ode23t* as the solver. |
| *TIME_INFO_23t_2* | Matrix, the same as *TIME_INFO_15s_2*, but using *ode23t* as the solver. |
| *TIME_INFO_23t_3* | Matrix, the same as *TIME_INFO_15s_3*, but using *ode23t* as the solver. |