Discussion of Numerical Methods used in Positive Displacement Comprehensive Mechanistic Models: Case Study using the Z-Compressor

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Abstract.
Comprehensive mechanistic models have been widely used for simulating positive displacement (PD) compressors or expanders. Such models are based on a thermodynamic analysis of generic control volumes that describe the working chambers. The thermodynamic analysis results in a set of non-linear ordinary differential equations (ODEs) that describe conservation of mass and energy. The derived ODEs are used to predict the evolution of the thermodynamic properties of the working fluid with respect to crank angle or time. The solution scheme of a mechanistic model involves different layers of solvers that handle the step-by-step integration, the cycle-to-cycle continuity as well as the overall energy balance. Since most of the PD machines feature multiple control volumes that merge or split (e.g. scroll-type) or wrap-around a rotor (e.g. screw-type) the integration scheme faces challenges due to the stiffness of the equations or discontinuities in the control volume definition.

In this paper, a discussion of different integration schemes and numerical considerations are proposed that are applied to a novel compressor called the z-compressor which presents a high-degree of intrinsic stiffness. A simplified comprehensive model is developed which is validated against experimental mass flow rate data for a prototype compressor with an average model-predicted error of less than 2\%. This model is used to explore the differences in two ODE solvers from the ODE suite in MATLAB, \textit{(ODE15s, and ODE113)}. These results are further compared against an existing, simplified, Z-compressor model developed in PDSim which uses an explicit, lower order, solver the Adaptive Runge-Kutta (RKF). The results suggest that the semi-implicit solver (\textit{ODE15s}) provides an efficient means for stepping through the compression process ODEs compared to the explicit solvers.

1 Introduction
Comprehensive (also known as chamber or mechanistic) models of compressors are one of best types of models for positive displacement compressor development activities. However, to maximize effectiveness, it is critical that these models function with minimum operational time. These models partially discretize, using control volumes and flow paths, the mass and energy flows through a compressor to account for the most critical phenomenon within the
machine. This can include mass flow paths such as port, valve, and leakage flows plus friction and heat transfer from a plurality of sources or interconnected control volume(s).

The physics of the interconnected control volumes are predicted using a quasi-dynamic, differential form of the mass and energy balance equations, referred to as the compression process equations. One form of these equations, written as a function of compressor crank angle, are:

\[
\frac{d\rho}{d\theta} = \frac{1}{V} \left[ -\rho \frac{dV}{d\theta} + \frac{1}{\omega} \left( \sum m_{in} - \sum m_{out} \right) \right]
\]

and,

\[
\frac{dT}{d\theta} = -\rho h \frac{dV}{d\theta} - \left( uV + \rho V \frac{du}{d\theta} \right) \frac{\partial u}{\partial \rho} \frac{\partial \rho}{\partial \theta} + \frac{1}{\omega} \left( \dot{Q} + \sum m_{in} h_{in} - \sum m_{out} h_{out} \right) \rho V \frac{\partial u}{\partial T}.
\]

These equations are non-linear, first-order, ODE’s, which require numerical solutions. The solution method to these equations has been generalized to be applicable to any positive displacement compressor in recent years [5], and most recently encapsulated in a python-based development framework PDSim [3, 19]. This approach has also been used successfully to predict the behavior and accelerate the development cycles of many legacy and novel compressor technologies such as; scroll [1, 2, 10, 9], screw [15], rotary [13], reciprocating [17], linear [4, 8, 7, 18] and spool [6, 14].

The non-linearity of the compression process equations generates unavoidable numerical stiffness. Some compression mechanisms have intrinsically higher levels of numerical stiffness as a result of unique geometric features and/or coupled dynamic elements such as seals and valves. This has made complete generalization of the comprehensive compression process a bit elusive, as numerical stability and performance has been a secondary consideration even with the most mature platforms, such as PDSim. Most of the above studies rely on low-order, explicit ODE solvers, many with fixed step size, which are not well suited to ODE’s with high levels of numerical stiffness.

This study will aim to evaluate some of the most mature high-order, semi-implicit, non-linear ODE solvers that exist in the MATLAB's [16] ODE solver suite applied to the Z-compressor, which has a high-level of intrinsic numerical stiffness as a result of its geometric profile. The results will explore the efficiency of these solver compared against a more traditional adaptive solver implemented within PDSim.

1.1 The Z-compressor

The Z-compressor, shown in a cutaway in Figure 1, is a rotary style compressor, which uses an angled blade affixed to the compressor rotor which spins inside of a cylindrical housing to generate changes in volume. Suction and discharge processes are separated using a single vertical vane, which is adjacent to the blade, and is controlled via contact with the angled blade as it rotates. This forms four simultaneous chambers that occur on opposite sides of the blade and vane which are out of phase by one-half a rotation. As the main shaft rotates, the angled blade compresses gas against the outer walls of the cylinder and one of the vanes. A discharge reed valve controls the discharge flow process. The Z-compressor was first studied in detail by Jovane ([12, 11]), who developed a comprehensive model of the novel compressor and validated it using data collected from a first generation prototype constructed by LG. This work has been continued by Ziviani and Groll [20] who implemented this model into the PDSim framework and used it to explore design improvements for the Z-compressor.

This combination of two simultaneous necessitates suction and discharge ports aligned axially along the fixed housing of the compressor, on adjacent sides of the vane. This unique geometric attribute provides the numerical challenge, which will be explored in this work. Figure 2 shows
Figure 1: Cutaway view (left) and transparent 3D view (right) of the Z-compressor from Ziviani and Groll [20].

the volume as a function of crank angle for the Z-compressor using the geometric dimensions from Jovane [11] and Ziviani and Groll [19]. This figure shows the four simultaneous volumes that exist within the compressor at any instant (two compression ”c”, and two suction ”s”) and highlights the lower versus upper chambers.

Figure 2: Analytically Determined Compressor Volumes of Z-Compressor Prototype.

2 Model Development
A comprehensive model of the Z-compressor was developed in MATLAB with a goal of exploring the numerical behavior only. However, the model is validated using experimentally obtained mass flow rate data from Jovane [11] for an R410A compressor prototype. This will ensure that
the model has justifiable utility, but does not require more complexities, such as heat balances between the various components and dynamic interaction of the valves with the compression process. Both of which could artificially induce changes to the system stability and make the study more challenging to infer appropriate feedback on the influence of the numerical solver.

The analytical form of the Z-compressor geometry is provided by Ziviani and Groll [20] and Jovane [11]. The dimensions used in both studies match the dimension of this prototype compressor and reflect a total chamber volume of roughly 5.5 cm$^3$, which corresponds to a total compressor displacement of roughly 11 cm$^3$. This volume was used as an input to the compression process equations from Section 1.

The mass flows from the suction and discharge process and leakage paths were modeled using an isentropic compressible flow model. The suction and discharge port areas were considered variable and changed as a function of crank angle to reflect the blade passing over the respective ports. While the prototype included discharge reed valves, the valve was modeled as an ideal valve for the purposes of this study as the influence of the valve was not a primary concern. An ideal valve will allow mass flow out when the cylinder pressure exceeds the set discharge pressure with an area equal to the port area and use an area of zero when the cylinder pressure is below the set discharge pressure.

The compressor is additionally modeled as adiabatic and includes modeled leakage from chamber to chamber. Jovane identified nine leakage paths in the Z-compressor, shown in Figure 3. Along with estimates for the leakage gap widths from the prototype manufacturer. The leakage from chamber to chamber as a result of the clearance of the blade was significantly larger than others (30 microns) and therefore, was selected as the sole source of leakage in the model. This is represented by leakage paths 6-9 in Figure 3 which is the only source of leakage accounted for in this model.

The leakage is modeled as an isentropic compressible flow and given by,

$$ m_{isen} = \rho \cdot Ma \cdot \sqrt{\gamma RT} \cdot A \quad (3) $$

where $\rho$ is the upstream gas density, $Ma$ is the Mach number calculated using the isentropic compressible flow relationships, $\gamma$ is the ratio of specific heats for the working fluid, $R$ is the gas constant, $T$ is the upstream gas temperature, and $A$ is the leakage gap area. The PDSim model includes all the leakage paths [19], but the compression process is kept adiabatic for consistency with the MATLAB model.
Figure 4: Z-compressor model flowchart highlighting the addition of an ODE event manager to account for unique compressor geometry.

2.1 Event Handling and Numerical Methods
The physical attribute in the Z-compressor that makes it numerically interesting is the volume crossover point at crank rotation $\pi$, where the lower chamber transitions from a suction to a compression chamber (or vice-versa) at that instant. While this is not unusual in a geometric model of a compressor, it is typically possible to align this transition with a periodic boundary and utilize successive substitution to account for the transition between chamber types. However, Figure 2 shows that the upper chambers are currently aligned with periodic boundaries at $2\pi$ in this manner. Therefore, adjusting the simulation boundary to some other $\pi$ multiple would still produce at least a single crossover event for any $\pi$ multiple.

To remedy this issue, an additional event handling step is required, which will interrupt the integration steps when a specified condition is satisfied and re-initialize and/or change the model physics. In this case, the volume needs to be re-assigned as the model crosses $\pi$ from either direction to account for the discontinuities in the lower chamber volumes. This process is presented in Figure 4, which shows the overall model flowchart and highlights the event handling procedure. In PDSim, a similar procedure is implemented via a step callback function [19].

The process in Figure 4 is solver agnostic and several ODE solvers were selected to explore the influence of solver order and implicit formulation on the stiffness of the model. The first is the adaptive Runge-Kutta-Fehlberg (RKF) method, which is an explicit, Runge-Kutta method that maintains between 4th and 5th order accuracy, this is the solver built-in to PDSim. The numerical coefficients of the RKF solver are provided in [3]. The second and third solvers
will leverage the ODE Suite in MATLAB [16]. The first is called ODE113, which is also an explicit, adaptive, solver of higher order than the adaptive RKF method. Finally, a solver named ODE15s is used, which is a semi-implicit, adaptive, solver of between 1st and 5th order accuracy. A summary of the numerical methods analyzed is presented in Table 1.

Table 1: ODE solvers used in this study with the type presented and step size error range used.

| Solver | Name         | Implicity | Order | Relative Step Error Range |
|--------|--------------|-----------|-------|---------------------------|
| 1      | Adaptive RKF | explicit  | 4-5th | $\epsilon_{\text{allowed}} = 10^{-8}$  
                                    |            |          | Min. step size: $h_{\text{min}} = 10^{-4}$ |
| 2      | ODE113       | explicit  | 1-13th| $\epsilon_{\text{allowed}} = 5 \cdot 10^{-6} - 5 \cdot 10^{-3}$ |
| 3      | ODE15s       | semi-implicit | 1-5th | $\epsilon_{\text{allowed}} = 10^{-10} - 5 \cdot 10^{-7}$ |

3 Model Results

The resulting comprehensive MATLAB model was compared against experimental data obtained from Jovane [11] using R410A. This data was collected using a hot-gas bypass style compressor load stand. The model was only compared against the data for massflow rate. The compiled input conditions (suction temperature, pressure, discharge pressure, and compressor speed) and corresponding mass flow rates are presented in Table 2 for 18 data points.

Table 2: Operating Conditions and measured mass flow from prototype Z-compressor and massflow predictions from the Jovane [11], the current MATLAB model and PDSim model using R410A.

| Test | $\dot{m}_{\text{exp}}$ | $\dot{m}_J$ | $\dot{m}_{\text{MATLAB}}$ | $\dot{m}_{\text{PDSim}}$ | $T_{\text{suc}}$ | $p_{\text{suc}}$ | $p_{\text{dis}}$ | RPM |
|------|-----------------|-------------|-----------------|-----------------|----------------|----------------|----------------|-----|
| #    | [kg/h]      | [kg/h]      | [kg/h]      | [kg/h]      | [°C]          | [kPa]          | [kPa]          |     |
| 1    | 42.0         | 41.2        | 42.4         | 41.6         | 15.5          | 596            | 1510           | 3496 |
| 2    | 40.4         | 40.7        | 41.6         | 40.6         | 15.9          | 601            | 1780           | 3481 |
| 3    | 49.2         | 48.2        | 48.7         | 48.8         | 20.4          | 705            | 1812           | 3481 |
| 4    | 45.8         | 47.1        | 47.3         | 46.3         | 21.2          | 706            | 2107           | 3464 |
| 5    | 44.0         | 45.5        | 45.3         | 44.3         | 21.2          | 696            | 2384           | 3450 |
| 6    | 57.5         | 55.6        | 55.7         | 55.7         | 20.8          | 793            | 1799           | 3485 |
| 7    | 55.9         | 59.6        | 55.0         | 55.5         | 19.9          | 800            | 2070           | 3468 |
| 8    | 52.0         | 53.3        | 52.4         | 52.6         | 26.3          | 807            | 2405           | 3449 |
| 9    | 51.4         | 51.3        | 50.1         | 50.9         | 25.9          | 792            | 2679           | 3436 |
| 10   | 61.3         | 62.1        | 61.1         | 62.0         | 28.4          | 907            | 2098           | 3469 |
| 11   | 58.4         | 60.3        | 58.8         | 59.3         | 29.3          | 902            | 2400           | 3451 |
| 12   | 56.5         | 59.4        | 57.2         | 57.4         | 27.7          | 897            | 2700           | 3435 |
| 13   | 54.7         | 58.3        | 55.6         | 55.3         | 27.1          | 893            | 2982           | 3420 |
| 14   | 71.0         | 69.7        | 68.1         | 70.1         | 31.9          | 1009           | 2099           | 3473 |
| 15   | 67.8         | 68.0        | 65.8         | 66.9         | 32.3          | 1005           | 2396           | 3454 |
| 16   | 62.7         | 65.6        | 62.9         | 62.6         | 34.2          | 998            | 2712           | 3435 |
| 17   | 61.7         | 65.9        | 62.2         | 60.9         | 32.0          | 1006           | 3047           | 3417 |
| 18   | 58.1         | 61.0        | 57.3         | 58.3         | 36.0          | 975            | 3360           | 3401 |

In the MATLAB model, the leakage flow rates were corrected using a linear parameter estimation technique of the following form,
where \( \dot{m}_{\text{leak}} \) is the mass flow used in the compression process equations and, \( c_f \), is a dimensionless correction factor that is fit using a linear regression analysis based on expected correction assuming linear behavior. First, the estimated correction factor was estimated by using the difference of errors between the model without leakage and with a correction factor of one. The results of this analysis were used in a parameter estimation analysis to explore trends in the suitable correction factor with input variables and found that the most suitable correction factor had the form,

\[
\dot{m}_{\text{leak}} = c_f \cdot \dot{m}_{\text{isen}},
\]

\( c_f = 0.0117 \cdot T_{\text{cond}} - 2.860, \) (5)

where \( T_{\text{cond}} \) is the condensing temperature in K. The model predicted mass flow rate vs. experimental results are compared in Figure 5. The experimental uncertainty of the mass flow measurements reported by Jovane is 0.1 kg/hr.

The Mean Absolute Percentage Errors (MAPE) for the current MATLAB model, the PDSim model, and the Jovane model are 1.8%, 0.98%, and 2.9%, respectively. The results suggest an adequate agreement between model predicted and experimental results. Therefore, the final MATLAB model formulation used to generate these results was utilized to compare the various ODE solvers and the numerical solver built-in into PDSim.

**4 Numerical Results**

Using Test #1 conditions presented in Table 2, the Z-compressor model was exercised using the various ODE solvers presented in Table 1. The first analysis explores the influence of the solver on the step size by fixing the error tolerance for each solver and comparing the results. Figure
6(a) presents this for all three solvers. Since all the solvers considered are using mechanisms to adapt the step size using feedback from the equations the step size can be a surrogate for the stiffness of the ODE system of equations being solved with the step size being inversely related to the equations stiffness. As expected, all the solvers find the highest level of stiffness near $\pi$ with step sizes being reduced, sometimes by several orders of magnitude to account for the difficulty in this transition. The minimum step size prior to the discontinuity at $\pi$ should be as small as possible to minimize the errors associated with the event handling functions. There are also other areas of high stiffness observed which are likely correlated to the start and end of suction and discharge mass flows.

The ODE15s solver takes a very wide range of step sizes, ranging 6 orders of magnitude, but only for small angular displacements. This solver also represents a relatively low number of steps (1,320) with subjectively low amount of noise (continuous significant changes in step size with small angular displacements). The ODE113 solver presents a much smaller range of step sizes with significantly more noise in the step size response and a substantial increase in the number of steps required (21,516) to maintain a significantly lower amount of accuracy. The highest level of stiffness is still observed surrounding a crank angle of $\pi$ but significantly higher stiffness in the areas adjacent to $\pi$. Lastly, the RKF45 solver implemented in PDSim shows fairly constant step size (set by default equal to $10^{-4}$) during the integration with the exception of areas where mass flow rate calculations due to multiple leakage paths and suction/discharge processes occurs. It is interesting to note that ODE113 and RKF45 have similar behavior before and after $\pi$. Due to the fact that the maximum relative step error allowed by the RKF45 solver is significantly lower than that of the other solvers (see Table 1), the total number of steps increases to 41,653 resulting in a very smooth integration at the cost of computational time.

![Graph](image-url)

(a) Step size taken by ODE15s, ODE113, and RKF45 as a function of $\theta$-compressor crank angle with an error tolerance of $5e^{-7}$, $5e^{-3}$ and $1e^{-8}$, respectively.

(b) Required number of steps for $\theta$-compressor model for both ODE15s and ODE113 solvers as a function of input relative error limits.

Figure 6: Numerical results for Z-compressor study

The Figure 6(b) presents the required number of steps for a given input step error tolerance. The lower the step error tolerance the algorithm will attempt to reduce the step size sufficiently
to ensure the accuracy is maintained. This figure shows that the explicit solvers require orders of magnitude more steps in general to achieve a solution. They also tend to have an exponential increase in the required number steps for a given error tolerance. In contrast, the step sizes for the semi-implicit solver tends to increase in number of steps linearly with significantly less steps required for a higher accuracy solution.

The Z-compressor analysis has confirmed that this compressor presents a significantly stiff problem to solve. The semi-implicit solver has shown that it can handle the stiffness effectively while maintaining a relatively lower number of required steps and being significantly less sensitive to the user-selected step error.

5 Conclusions
The Z-compressor is a novel rotary compressor that has been investigated during the last 15 years. The geometry of this mechanism creates a discontinuity, which introduces numerical stiffness into a comprehensive model of the compressor. This stiffness was leveraged to explore the utility of higher-order and semi-implicit, adaptive, ODE solvers than have traditionally been used for these types of compressor models.

A model was developed as a case study and compared against existing experimental data with good predictive capability of the mass flow rate. This model was used a basis to explore three adaptive step-size, ODE solver, algorithms (adaptive RKF, ODE113, ODE15s). Two algorithms were explicit (Adaptive RKF, ODE113) and one was semi-implicit (ODE15s). The numerical analysis suggested that the ODE15s solver provided a solution with significantly higher levels of accuracy and orders of magnitude less steps than the explicit methods as a result of large stiffness in the modeled system. This suggests that for many compressor modeling scenarios a semi-implicit solver would be a good choice in solver to minimize computational effort across a wide range of compressor technologies.

Nomenclature

\begin{align*}
h & \quad \text{Gas enthalpy} \\
h_{\text{next}} & \quad \text{Next solver step size} \\
m & \quad \text{Mass flow rate} \\
m_{\text{in}} & \quad \text{Mass flow rate in} \\
m_{\text{out}} & \quad \text{Mass flow rate out} \\
\dot{Q} & \quad \text{Heat transfer} \\
T & \quad \text{Gas temperature} \\
u & \quad \text{Gas internal energy} \\
V & \quad \text{Compressor volume} \\
V_s & \quad \text{Compressor suction volume} \\
V_c & \quad \text{Compressor compression volume} \\
V_{s,\text{low}} & \quad \text{Lower compressor suction volume} \\
V_{c,\text{low}} & \quad \text{Lower compressor compression volume} \\
\epsilon & \quad \text{Error} \\
\rho & \quad \text{Density} \\
\theta & \quad \text{Crank angle} \\
\omega & \quad \text{Compressor rotational speed}
\end{align*}

Greek

\begin{align*}
\epsilon & \quad \text{Error} \\
\rho & \quad \text{Density} \\
\theta & \quad \text{Crank angle} \\
\omega & \quad \text{Compressor rotational speed}
\end{align*}
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