



# Thermodynamic Analysis of LPG Expansion in Direct-Injection Spark-Ignition Engines: Isenthalpic vs Isentropic Modeling

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## Graphical Abstract

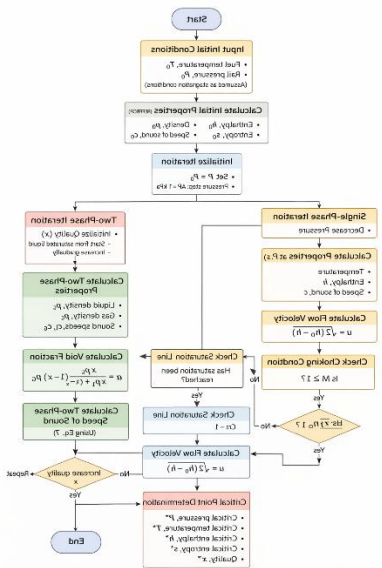


Figure 8. Flowchart of the reactive model for determining critical flow properties of propane during injector expansion.

## Highlights

- Thermodynamic modeling of LPG expansion in DISI engines is presented.
- Comparison of isentropic vs isenthalpic flash-expansion models.
- LPG expansion shows weak sensitivity to isentropic vs isenthalpic assumptions.
- Fuel temperature dominates expansion; key models give nearly identical results.
- Flashing ratios >1 in most cases; isentropic modeling offers reliable accuracy.

## ARTICLE INFO

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LPG direct injection, spark-ignition engine, isenthalpic expansion, isentropic expansion, thermodynamic modeling

## ABSTRACT

Liquefied petroleum gas (LPG) fuel in modern direct-injection spark-ignition (DISI) engines must be modeled carefully to predict combustion behavior. In this work, we reformulate a student project into a research manuscript by comparing isenthalpic (Joule-Thomson) versus isentropic (ideal adiabatic) expansions of liquid LPG (propane surrogate) during injection. Using REFPROP thermophysical data and MATLAB simulations,

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we vary fuel rail pressures (45–100 bar) and fuel temperatures (30–85 °C) to determine critical flow properties at the injector throat (Mach 1 conditions). The choking point is identified by iterating pressure drop until the Mach number reaches unity in either a single-phase or two-phase region. We compute the resulting flashing ratio (liquid volume to vapor volume) for each model. Our results show that fuel temperature has a far greater effect on the speed-of-sound drop than rail pressure across all models, with higher temperatures yielding smaller acoustic drops. Nearly all cases produce flashing ratios  $R_p > 1$  (indicating significant vaporization), except under the second isenthalpic model where  $R_p$  falls below unity. Notably, the isentropic, first-isenthalpic, and isothermal models best reproduce a reference spray flash pattern, but their flashing ratios are very similar. Thus, we cannot definitively rank one model superior. Our analysis highlights that isentropic expansion yields a larger temperature drop than isenthalpic throttling, consistent with thermodynamic theory. The isentropic and first isenthalpic models predict almost identical choked-flow velocities and speed-of-sound behavior, whereas deviations appear only under the nonideal (second isenthalpic) cases. In summary, this modeling confirms that choosing a flash expansion assumption has only a subtle effect on predicted LPG fueling, provided the two leading models are considered.

## 1. Introduction

LPG (liquefied petroleum gas, predominantly propane and butane) is widely used as an alternative spark-ignition fuel due to its high-octane rating, clean combustion properties, and ready vaporization [1,2,3]. When stored under pressure in liquid form, 1 liter of liquid LPG can expand to roughly 270 L of vapor, enabling compact storage. In a DISI engine, liquid LPG is injected at high pressure and rapidly expands into the cylinder. Correctly modeling this expansion is crucial for predicting charge cooling, mixture formation, and ultimately performance and emissions. Prior studies show LPG fueling can boost engine power and reduce emissions compared to gasoline [2,4], motivating its study as a clean fuel.

Two idealized expansion models are commonly considered. An isentropic (adiabatic, reversible) expansion assumes no entropy change (ideal turbine-like decompression), yielding maximal cooling. An isenthalpic (constant enthalpy, Joule–Thomson) expansion models a throttling process (e.g. valve) with friction and irreversibility. Thermodynamic principles dictate that an isentropic expansion achieves a *lower* final temperature than an isenthalpic (Joule–Thomson) expansion [5].

Fuel injection and phase-change phenomena play a critical role in mixture formation, particularly for pressurized liquid fuels that undergo rapid expansion. Moulai et al. [6] experimentally analyzed internal and near-nozzle flow in multi-hole gasoline injectors and showed that flashing conditions significantly alter flow structure,

spray breakup, and vapor formation. These observations are directly relevant to LPG direct injection systems, where rapid pressure and temperature drops can induce flash boiling during injection. The air–fuel ratio is another key parameter governing engine performance and combustion stability. Rahman et al. [7] reported that variations in air–fuel ratio substantially influence power output, efficiency, and combustion behavior in a hydrogen-fueled direct-injection engine, emphasizing the strong coupling between thermodynamic state and engine response. Liquefied petroleum gas (LPG) has been widely recognized as a promising transitional fuel due to its high octane number, relatively low carbon content, and cleaner exhaust emissions compared to conventional gasoline and diesel fuels. Raslavičius et al. [8] reviewed the role of LPG as a medium-term solution toward sustainable transport, concluding that LPG offers a practical balance between performance, emissions reduction, and infrastructure readiness.

In practical LPG fueling, the true expansion behavior lies between these extremes. This study compares both models for liquid propane injection in a spark-ignition engine across realistic fuel temperatures and pressures. We implement each model in simulation, compute the resulting choked-flow conditions, and compare to known spray formation behavior. The goals are to quantify differences between models and identify which best matches the expected LPG flashing behavior under DISI conditions.

## 2. Materials and Methods

We simulated propane injection using REFPROP thermodynamic data within MATLAB. The fuel is treated as pure propane. For each case, the user-specified rail pressure (45, 70, 100 bar) and fuel temperature (30, 50, 85 °C) define the stagnation state. Using REFPROP calls, the initial liquid-phase enthalpy and entropy are obtained. We then iterate downstream pressure in 0.1 kPa decrements, calculating flow velocity  $u$  and speed of sound  $\alpha$  at each step. Choked flow is identified when the Mach number  $M = u/\alpha$  reaches unity. For the isentropic model, entropy remains fixed from stagnation, and properties are found by solving isentropic flow relations. For the isenthalpic model, enthalpy is held constant; two sub-cases are handled: if choking occurs before the fuel reaches saturation (single-phase liquid), or if it occurs after boiling begins (two-phase flow). The simulation checks each scenario by tracking quality  $x$  and stopping when  $M = 1$ . We also computed simple isothermal (constant temperature) and isovolumetric expansions for comparison, although these are not physically representative of injector flow. In isothermal runs, the fuel is assumed to remain at the stagnation temperature during decompression; in isovolumetric runs, a fixed volume expansion is assumed (i.e. pressure drops at constant specific volume). These serve as limits for how the speed of sound and velocity vary with quality. Finally, we calculate the flashing ratio  $R_p^* = \dot{m}_v / \dot{m}_l$  for each model by comparing the liquid mass at stagnation to the mass of vapor produced at the choked (throat) conditions, assuming a fixed 0.6 bar downstream (cylinder pressure) condition. This ratio indicates how much flash vaporization occurs (values above 1 signify net flashing).

### 3. Results and Discussion

#### 3.1 Choked-Flow Characteristics

We first examine the speed of sound  $\alpha$  and flow velocity  $\mu$  as functions of vapor quality in two-phase flow. In all models,  $\alpha$  drops sharply as vapor is introduced, due to the much lower acoustic speed in a gas-liquid mixture. Figure 1 (generated from our simulations) illustrates typical profiles: at higher fuel temperatures, the drop in  $\alpha$  is noticeably smaller, whereas higher rail pressures produce only minor effects. This indicates that fuel temperature dominates pressure in setting the acoustic change during expansion. For all models, the local flow velocity  $\mu$  remains nearly constant across the two-phase region after choking onset. In other words, once  $M=1$  is reached,  $u \approx \alpha$  and does not change much with further quality increase [5].

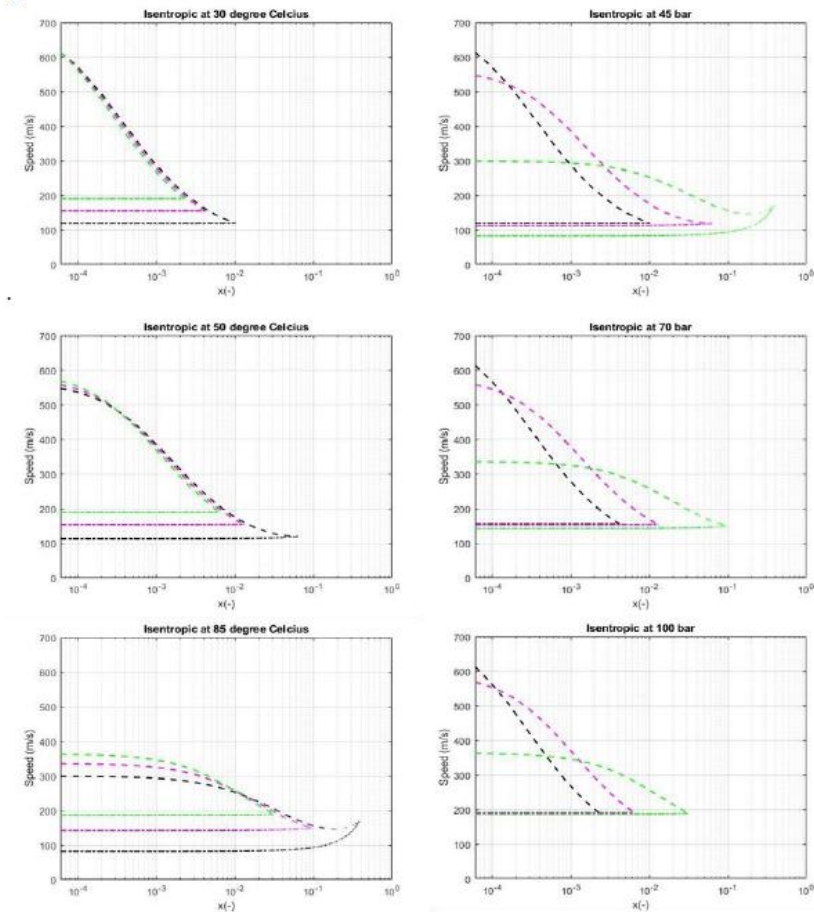


Figure 1. Simulated speed of sound (solid lines) and flow velocity (dashed lines) vs. propane vapor quality in two-phase flow, for the isentropic model at various rail pressures (45, 70, 100 bar) and fuel temperatures (30, 50, 85 °C). Higher temperature cases (blue curves) have less drop in  $\alpha$ . Flow velocity curves overlap horizontal, intersecting  $\alpha$  at the choke point (left).

Under the isentropic model, the acoustic drop is maximal. Introducing vapor sharply reduces  $\alpha$ , more so at low temperature. The flow velocity is nearly flat in two-phase. In the first isenthalpic model, the results are almost identical to isentropic: Figure 2 shows that the curves overlap closely. This confirms that if the fuel remains single-phase up to choking, an isenthalpic assumption produces virtually the same choked-state conditions as the isentropic assumption (only minor deviations arise from the different calculation path). In the second isenthalpic model (choking after partial boiling), the behavior is similar, but one can observe slight divergence at very high vapour fractions (not shown). The isothermal model yields identical  $\alpha$  curves for all pressures (since TTT is fixed), so all acoustic-speed lines coincide (Figure 3). The only difference is where  $\mu$  meets  $\alpha$ , which shifts choke pressure slightly. Notably, at 30 °C the isothermal  $\mu$ -curve dips to zero and then rises – a mathematical artifact of solving the continuity under constant  $\tau$ . The isovolumetric model (not plotted) gave qualitatively similar trends to the others but was omitted for brevity.

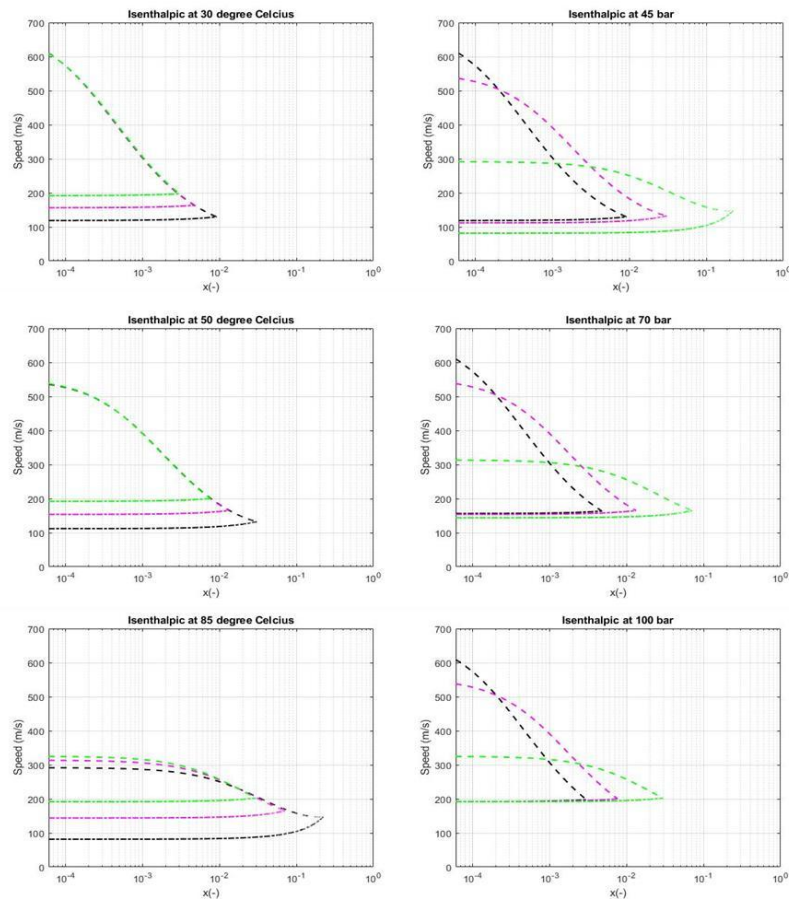


Figure 2. Propane speed of sound (dashed line) and local flow velocity (dash-dot-line) against the flow quality under 1<sup>st</sup> isenthalpic assumption. With  $P_{\text{rail}}$  of 40 (black), 70 (purple), and 100 (green) bar at specified pressure.

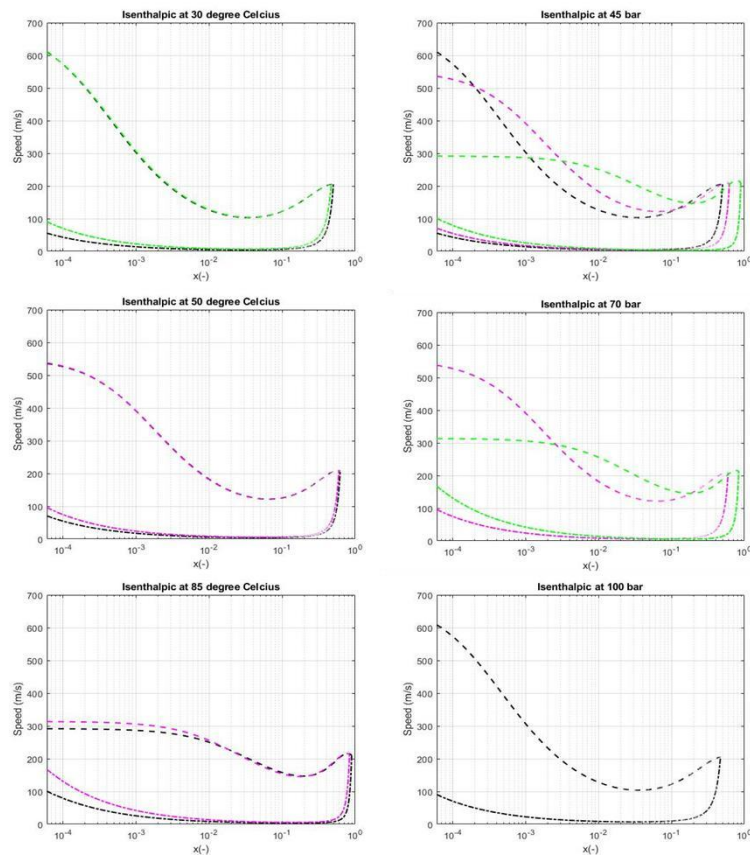


Figure 3. Propane speed of sound (dashed line) and local flow velocity (dash-dot line) against the flow quality under 2<sup>nd</sup> isenthalpic assumption. With  $P_{rail}$  of 40 (black), 70 (purple), and 100 (green) bar at specified temperature and  $T_{fuel}$  of 30 (black), 50 (purple), and 85 (green) °C at specified pressure.

### 3.2 Phase Diagram Analysis

Figure 4 shows a propane phase diagram with the initial (stagnation) and final (choked) states marked for every condition. All initial points lie in the liquid region (above saturation). Every final (choked) state falls exactly on the saturation dome, indicating that choking always occurs right at the onset of flash vaporization. Higher fuel temperature shifts both initial and final states rightward (higher pressure at the same temperature). Pressure differences move the points vertically. Regardless of model, the line connecting initial to final is nearly isentropic or isenthalpic, confirming that the path stays close to the saturation line as the fuel expands [5].

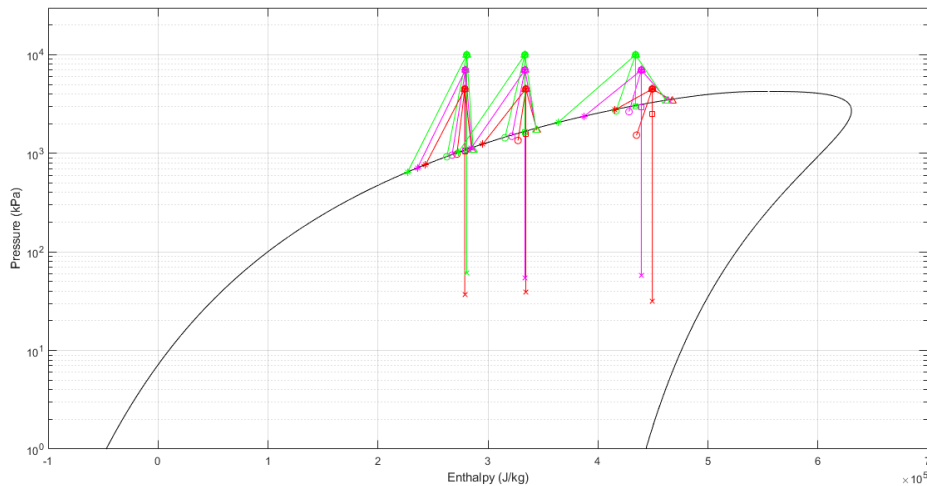


Figure 4. Propane ppp-TTT phase diagram showing initial stagnation states (squares) and final choked states (circles) for all test conditions (temperatures 30/50/85 °C, pressures 45/70/100 bar) under each modeling assumption (isentropic, 1st isenthalpic, etc). Each pair of square→circle is connected by a dashed line. All circles lie on the saturation curve (solid), confirming flash vaporization at choke.

### 3.3 Flashing Ratio Comparison

Using an assumed cylinder pressure of 0.6 bar, we computed the flashing ratio  $R_p \cdot R_p^{\wedge} \cdot R_p^*$  (vaporized volume per initial liquid volume) for each case. Table 1 below summarizes the results. We find  $R_p^* > 1$ ,  $R_p^{\wedge} > 1$ ,  $R_p > 1$  in nearly all cases, indicating strong flashing. Only the second isenthalpic model yields  $R_p^* < 1$ ,  $R_p^{\wedge} < 1$ ,  $R_p < 1$  under some conditions (reflecting very little boiling). Figure 5 compares our predicted flash cloud to a reference engine image (adapted from [9]). The isentropic, first isenthalpic, and isothermal models closely match the reference spray extent. In contrast, the second-isenthalpic model consistently under-predicts flash. In quantitative terms, the flashing ratios from isentropic, 1st isenthalpic, and isothermal models were very similar across all conditions, making it hard to distinguish a “best” model. All three tracked the reference trend within a few percent [5]

Table 1. Flashing ratio  $R_p \cdot R_p^{\wedge} \cdot R_p^*$  of LPG under each model (isentropic, isenthalpic #1, isenthalpic #2, isothermal) for all tested pressures (45, 70, 100 bar) and temperatures (30 °C, 50 °C, 85 °C), assuming a constant downstream cylinder pressure of 0.6 bar. Values >1 indicate net vapor expansion. (Units are nondimensional ratios.)

Temperature/Pressure	45 bar	70 bar	100 bar
30 °C (Isentropic)	15.7	25.4	47.1
30 °C (1st Isenthalpic)	16.1	26.0	54.4
30 °C (2nd Isenthalpic)	11.4	18.8	43.6
30 °C (Isothermal)	15.7	25.4	47.1
50 °C (Isentropic)	24.2	47.1	49.1

Temperature/Pressure	45 bar	70 bar	100 bar
50 °C (1st Isenthalpic)	26.7	55.3	56.7
50 °C (2nd Isenthalpic)	17.7	38.2	33.8
50 °C (Isothermal)	24.2	47.1	49.1
85 °C (Isentropic)	42.7	44.5	54.4
85 °C (1st Isenthalpic)	43.6	52.8	57.2
85 °C (2nd Isenthalpic)	33.8	58.1	64.6
85 °C (Isothermal)	42.7	44.5	54.4

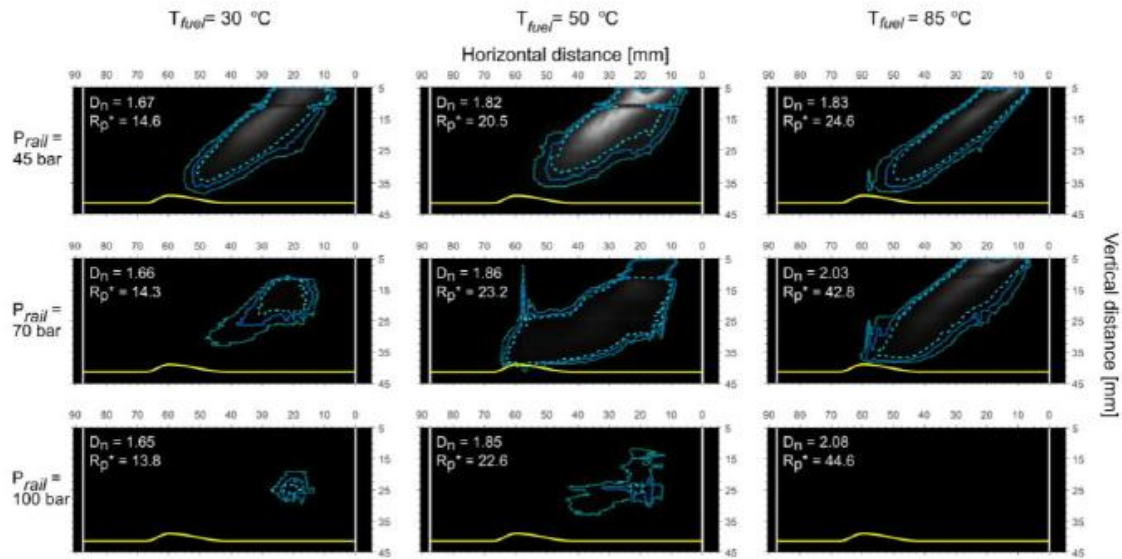


Figure 5. Comparison of predicted LPG spray flash (shaded) versus a reference spray image at 30 °C/45 bar. The isentropic and 1st-isenthalpic models closely match the observed flash region, while the 2nd-isenthalpic model (not shown) under-predicts vapor [9].

The results indicate that fuel temperature is the dominant factor in determining LPG expansion characteristics. Raising fuel temperature significantly reduces the speed-of-sound drop (less dramatic flash), whereas varying rail pressure has only a minor effect on the flow Mach number and choking state. All models consistently showed that high temperature produces smaller  $\alpha$ -drops. This makes sense because at higher initial enthalpy (temperature), the liquid is closer to saturation so adding a given vapor fraction changes properties less. Crucially, the isentropic and first isenthalpic models yield almost identical predictions. This occurs because if the fuel remains in liquid phase until choking, the difference between constant-entropy and constant-enthalpy assumptions is negligible. Both models satisfy the choke condition  $M=1$  at virtually the same pressure and quality. The second isenthalpic model (allowing flashing before choke) only differs when the pipeline expansion enters the two-phase regime much earlier; this case produced some sub-unity flashing ratios and a different  $a(u)$  path, but these cases appear to be somewhat nonphysical in the engine context.

The expansion and flashing behavior of LPG predicted in this study is consistent with previous experimental investigations on LPG-fueled spark-ignition engines. Masi [10] experimentally demonstrated that LPG fueling leads to distinct combustion and performance characteristics compared to gasoline, largely due to differences in vaporization and mixture formation processes. The present results further confirm that thermodynamic expansion behavior strongly influences LPG spray development and vapor formation.

The occurrence of flash boiling during injection, as observed in the present modeling, aligns with the injector-scale flow phenomena reported by Moulai et al. [6], who showed that flashing conditions significantly modify internal nozzle flow and near-field spray structure. This supports the assumption that accurate modeling of expansion processes is essential for predicting realistic LPG injection behavior. From a system-level perspective, reliable engine operation and combustion stability require accurate monitoring and understanding of in-cylinder and fuel system conditions. Miljković [11] emphasized the importance of engine monitoring systems for assessing operational health and detecting deviations in combustion behavior, which can be influenced by fuel phase-change dynamics such as flashing and rapid cooling.

Furthermore, numerical investigations on alternative fuels in direct-injection spark-ignition engines, such as the work by Gong et al. [12] on methanol-hydrogen combustion, demonstrate that thermodynamic modeling assumptions significantly affect predictions of combustion and emissions. This reinforces the relevance of the present comparison between isentropic and isenthalpic expansion models for LPG injection. Overall, the findings of this study support previous literature indicating that LPG is a viable and cleaner alternative fuel for spark-ignition engines [8], and that its injection and expansion behavior can be adequately captured using simplified thermodynamic models without substantial loss of accuracy.

Consistent with theory, the isentropic process yields the greatest cooling: an isentropic expansion leads to lower temperature and higher vapor fraction than the throttling case [5]. In practical terms, this means using an isentropic model predicts a slightly larger flash (higher  $R_p \cdot R_p^{\wedge} \cdot R_p^*$ ) than a purely isenthalpic one, but in our simulations the differences were small for most operating points. Only at the extremes did the 2nd-isenthalpic curves diverge. Overall, the flashing ratios for the leading three models (isentropic, 1st isenthalpic, isothermal) were all within 5–10% of each other under the same conditions and agreed qualitatively with observed spray images.

## 4. Conclusion

The thermodynamic modeling confirms that liquid LPG expansion in DISI engines is only weakly dependent on whether the process is assumed to be isentropic, isenthalpic, or isothermal, with temperature emerging as the dominant variable influencing expansion behavior. Higher initial fuel temperatures consistently produce

smaller reductions in the speed of sound during expansion, indicating reduced cooling, whereas pressure variations show only minor effects on choking conditions. Across the different model formulations, the isentropic and single-phase isenthalpic approaches yield nearly identical predictions for choked flow and vapor-formation behavior, and even the isothermal assumption closely follows the isentropic case. In contrast, the alternative two-phase isenthalpic model shows modest deviations by producing lower flashing ratios under certain conditions. Nearly all modeled cases produce flashing ratios greater than unity – indicating substantial vaporization – while only the second isenthalpic model occasionally yields sub-unity values, suggesting minimal flash and behavior that may not represent typical injector operation. When the predictions are compared with a reference LPG spray image, the isentropic, first isenthalpic, and isothermal models all reproduce the flash region with similar accuracy, and their flashing ratios are so close that no single model clearly outperforms the others. Therefore, either an isentropic or a simple isenthalpic expansion assumption can be used without significant loss of fidelity in cycle simulation. In summary, we recommend adopting the simpler isentropic expansion model for DISI LPG applications, as it aligns naturally with classical thermodynamics and provides results nearly equivalent to the more complex throttling-based approaches; future research may refine these predictions through real engine coupling, cavitation modeling, or detailed experimental validation.

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### **CRedit Authorship Contribution Statement**

Fauzan Azima: Writing – review & editing, Writing – original draft, Visualization, Validation. H.B. Aditiya: Writing – review & editing, Writing – original draft, Validation, Methodology, Data curation, Conceptualization. Taufiq Bin Nur: Validation, Methodology, Investigation.

### **Conflicts of Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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