Numerical investigation of injector geometry effects on fuel stratification in a GCI engine

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Abstract

Injectors play an important role in direct injection (DI) gasoline compression ignition (GCI) engines by affecting the in-cylinder mixture formation and stratification, which in turn impacts combustion and emissions. In this work, the effects of two different injector geometries, a 7-hole solid-cone injector and an outwardly opening hollow-cone injector, on fuel mixture stratification in a GCI engine were investigated by computational simulations. Three fuels with similar autoignition kinetics, but with different physical properties, were studied to isolate the effect of the combustion chemistry on combustion phasing. In addition, start of injection (SOI) sweeps relevant to low-load engine operating conditions were performed. The results show that physical properties of the fuel do not have significant influence when using a hollow-cone injector. Richer mixtures were observed at all the studied SOI (-40 to -14 CAD aTDC) cases, which can be attributed to the nature of the hollow cone spray. At later SOIs (-18 and -14 CAD aTDC), the richer mixtures are accompanied by lower mean in-cylinder temperature due to the charge cooling effect, which surpasses the equivalence ratio effect. The effect of fuel physical properties on combustion phasing was evident in multi-hole injection cases, which can be attributed to the differences in mixture stratification and equivalence ratio distribution at the time of ignition.

Key words

Light naphtha; multi-hole spray; hollow-cone spray; stratification

1- Introduction

Growing environmental concerns demand modern combustion engine research towards reduced emissions and higher efficiencies more than ever before. In the light duty application, gasoline compression ignition (GCI) engines have been considered a promising technology to enable

throttle-less operation at diesel-like efficiencies. Recent studies explored fuels in the octane number range of 60-85 [1-5] as optimal candidates for GCI operation. Compared to diesel, the longer ignition delay times of these fuels result in enough time for mixing and consequent leaner burning. Hence, soot and NO_x emissions are reduced, while maintaining a high efficiency. The level of in-cylinder fuel mixing or stratification can be controlled by varying the start of injection (SOI) timings, which has been extensively investigated [2-6]. Other factors which affect GCI engine operations are fuel type [1-5, 7-10], level of exhaust gas recirculation (EGR) [11, 12] and supercharging [13].

High fidelity computational fluid dynamic simulations with detailed chemical kinetics enable the optimization of engine performance and exploration of fuel properties effects on pollutant formation and engine efficiency [14]. However, real fuels (e.g. gasoline, diesel and jet fuels) consist of a wide range of components which pose a real challenge to chemical kinetics modelers. Surrogate fuels present an efficient and prevalent methodology to model complex real fuels [15]. Surrogate fuels are mixtures of a smaller number of hydrocarbons to mimic the chemical and physical properties of real fuels with affordable computational costs [2, 3, 7, 16]. The most commonly used surrogates are primary reference fuels (PRF), which are blends of iso-octane and n-heptane matching the octane numbers (ON) of the real fuel. In addition, ternary mixtures of PRF and toluene were also proposed as potential fuel surrogates [17, 18]. However, Pitz et al. [19] discussed the importance of matching more properties between gasoline and its surrogate; these targets include the chemical composition, H/C ratio, density and evaporation characteristics. The importance of formulating surrogates that match both chemical and physical properties for diesel fuels to replicate the mixing-controlled and kinetically-controlled phenomena occurring in real engines was discussed by Farrell et al. [20]. Moreover, developing

chemical/physical surrogates for jet fuels was investigated by Colket et al. [21, 22], these resulted in several methodologies for formulating multicomponent surrogates [14, 23]. The surrogate becomes more complicated when more target properties are included in the formulation process. Hence, careful considerations need to be made when selecting appropriate surrogate components and target properties.

The performance of fully blended fuels and their surrogates in GCI engines was studied recently. Badra et al. [2] conducted GCI experiments in single cylinder 4 valve engine with an outwardly-opening piezo-electric hollow-cone gasoline direct injection (GDI) injector using three fuels; primary reference fuel (PRF) 62 (62% by volume *iso*-octane and 38% *n*-heptane), Saudi Aramco light naphtha (SALN) and Haltermann straight run naphtha (HSRN). They performed a start of injection sweep from -60 to -11 CAD aTDC to study the fuel effect on the engine combustion as well as emissions. The measured research octane numbers (RON) for SALN and HSRN are 62 and 60, respectively, and their motored octane number (MON) are 60 and 58.3, respectively. From chemical kinetics perspective, the three fuels have similar ignition characteristics. This was confirmed by showing that the three fuels have similar combustion phasing and emissions at SOI earlier than -30 CAD aTDC, despite the apparent differences in the physical properties.

A similar work was performed by Naser et al. [24] in a single cylinder compression ignition engine (AVL 5404) equipped with a Bosch 7 hole injector for light naphtha (LN) with a measured RON of 65 and PRF65 across SOI sweep from -40 to -19 CAD aTDC. PRF65 was chosen as the kinetic surrogate of LN as recommended by Javed et al. [25]. However, the engine results showed significant differences in the combustion phasing of the two fuels at GCI relevant injection timings (-19 to -40 CAD aTDC). The work concluded that primary reference fuels are suitable surrogates only for HCCI tests where combustion processes are driven primarily by

chemical kinetics. In PPCI modes, however, combustion processes are also controlled by the physical properties of the fuels, leading to observed differences.

The aforementioned contradicting results from two studies with nearly similar operating conditions may be conjectured to be the effect of different injectors employed in the two engines. Both hollow-cone and multi-hole injectors are commonly used in GCI engines [4, 5, 9, 24, 26] or spray-guided gasoline spark ignition engines [27]. To corroborate the hypothesis, a comparison study of the two injectors in an identical engine configuration is necessary. To our knowledge, comparing the performance of both types of injectors in the same engine has not been investigated before.

In this work, numerical simulations using the CONVERGETM software package [28] were conducted to provide a clear understanding of the different findings from the above two experimental studies [2, 24]. Three fuels with similar chemical kinetics are tested; PRF62, light naphtha (LN) and Haltermann straight run naphtha (HSRN) for SOI sweep from -40 to -14 CAD aTDC at part load-conditions. Inert simulations (reactions turned off) were also conducted to examine further details of in-cylinder stratification for different injectors. Both the inert and reactive simulations with the three fuels were conducted using hollow-cone and solid-cone multi-hole injectors with the same engine geometry. Detailed analysis of the results was performed and discussions about the similarities and differences between the two injectors and the three fuels were provided.

2- Numerical Setup

Full cycle 3D engine simulations in CONVERGETM were conducted using the Reynolds-averaged Navier-Stokes (RANS) with the renormalization group (RNG k- ϵ) model, and the

multi-zone SAGE combustion sub-model [29] with the bin sizes of temperature and equivalence ratio of 5 K and 0.05, respectively.

For the modeling of spray dynamics, the Lagrangian discrete parcel method was used. As for the spray break-up models, Sim et al. [30] modified the Kelvin-Helmholtz-Rayleigh-Taylor (KH-RT) model [30][30] for the Lagrangian spray parcels produced from the outwardly-opening hollow-cone spray. The model was validated against constant volume spray [30] and engine data [3], and yielded good prediction in 3D engine simulations [3]. Moreover, the 3D engine simulations with the hollow-cone spray using the same three fuels studied here were successfully validated in our recent work [2]. Therefore, the models, parameters and approach that were utilized in [2] are implemented here without any modifications for the GCI engine simulations with the hollow-cone injector.

For the multi-hole Bosch injector, the standard spray models implemented in CONVERGE were optimized and validated against the Engine combustion network (ECN4) spray G data [31], which is close to the injection parameters considered in this study in terms of the spray angle (80°), injection pressure (200 bar) and the utilized fuel (iso-octane). A Lagrangian discrete parcel method was used for spray modeling by introducing parcels (groups of droplets) of liquid into the gas phase computational domain with Rosin-Rammler distributions. As a breakup algorithm of liquid spray, the modified Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) model is mainly used without an ad hoc breakup length [32].

The injection size distribution model was based on the nozzle exit diameter for better accuracy. Furthermore, the dynamic drag model was implemented by determining the droplet drag coefficient as part of the simulation, accounting for variations in the drop shape through a drop

distortion parameter. The effect of the turbulent flow on spray drops was modeled using the turbulent dispersion model by accounting fluctuating velocities [33]. For collision model, the traditional O'Rourke collision scheme [33] and no-time-counter (NTC) method [34] were extended with Post and Abraham's inclusion of collision regimes [35]. For spray evaporation, Frossling's [36] evaporation model was implemented. More details about the spray and turbulent models and validation can be found in [37].

Grid independence was obtained with base grid 4 mm coupled with fixed embedding scale of 4 for the injector spray and scale of 2 for the whole cylinder, in addition to temperature and velocity adaptive mesh refinement (AMR) for 1 m/s and 2.5 K difference, respectively with a scale of 4 [2]. A variable time step algorithm is used with maximum and minimum values of 10^{-4} and 10^{-8} respectively. The order of accuracy of the temporal and spatial schemes is first and second respectively.

The fuels used in the study were the straight-run light naphtha (LN), Haltermann straight-run naphtha (HSRN) and PRF62. These fuels have been chosen to have close cetane and octane numbers and different physical characteristics as shown in Table 1. The temperature ranges of the boiling characteristics for these fuels are shown in Fig. 1. LN is highly paraffinic (>90%) and have low sensitivity ($S = \text{RON} - \text{MON}$) of about 2. On the other hand, HSRN has more than 20% aromatics and naphthenes, which are reflected as a lower sensitivity of 1.7. The boiling range of HSRN is wider than LN, while PRF62 has a very narrow boiling range as expected from the similar boiling temperatures of n-heptane (98.4°C) and iso-octane (99°C).

Table 1. Properties of the tested fuels.

Fuel	LN	HSRN	PRF62
DCN from IQT	34.7	34.2	34.2
RON	62	60	62
MON	60	58.3	62
Sensitivity	2	1.7	0
Density (kg/m ³) at 15°	661	705	695
Lower heating value (LHV) (MJ/kg)	45.1	44.6	44.4
Hydrogen to carbon (H/C) ratio	2.175	2.146	2.262
Normal-paraffins vol.%	53.3	36	38
Iso-paraffins vol.%	38.7	40.8	62
Aromatics vol.%	1.14	8.94	0
Naphthenes vol.%	6.87	14.24	0
Sulfur (ppm)	<1	14	0
Final boiling point (FBP (°C))	90.7	138	99

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151 To eliminate the effect of chemistry in the simulations, PRF62 (59% and 41% by mole *iso*-
152 octane and *n*-heptane, respectively) was used for all three fuels with a skeletal reaction
153 mechanism [38]. However; the liquid physical properties of each fuel (e.g. density, viscosity,
154 surface tension, specific heat capacity) were enforced on the chemical PRF surrogate, so that any
155 differences in the results are attributed to their physical properties. The liquid physical properties
156 were calculated from the properties of the three components surrogate developed by Ahmed et
157 al. [39] for LN and Badra et al. [2] for HSRN using mass basis additivity. The formulation of
158 these surrogates aimed to match the evaporation of a single real fuel droplet.

Figure 1. Distillation curves of the tested fuels using American Society for Testing and Materials (ASTM) D86 method.

The simulations for both injectors are conducted in the GDI engine geometry used in the study of Badra et al. [2, 3]. The GDI engine is a 4-valve single cylinder engine with 499 cm³ displacement, 84 mm bore and 90 mm stroke. The geometrical compression ratio of the engine was 14:1, but was adjusted to 13.85:1 in the simulations to match the motored pressure traces from experiments in order to compensate for non-idealities of the real engine such as blow-by [2]. The intake air pressure and temperature were 1.2 bar and 304 K, respectively. The temperature of the liner and head were set to 403 K, while the piston temperature was at 423 K. For all SOI, the same amount of fuel at 10 mg was injected. The injection parameters are listed in Table 2. The trapezoidal injection rate shape with a ramp up and down presented in [2, 3] was used for all the hollow-cone and multi-hole simulations. More details about the simulated engine and its operating conditions can be found in [2, 3].

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Table 2. Injection parameters

Injector	Hollow-cone	Multi-hole
Injection pressure (bar)	130	300
Injected Mass (mg/cycle)	≈ 10	≈ 10
Injection duration (CAD)	≈ 4	≈ 4
SOI (CAD aTDC)	-40 to -14	-40 to -14
Spray angle ($^{\circ}$)	100	72
Number of holes	single hole	7 holes
Hole diameter (mm)	0.62	0.18

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175 **3- Results and discussion**

176 Figure 2 shows the simulated crank angle corresponding to 50% of total heat release (CA50) for
177 all the cases using the multi-hole and hollow-cone injectors. For the multi-hole injector, different
178 combustion phasings are observed for the tested fuels at all SOIs, which is in agreement with the
179 findings of the AVL experiments [24]. On the other hand, the cases with the hollow-cone
180 injector do not show significant differences in the combustion phasings of the three fuels at all
181 SOIs. This again agrees with the findings of Badra et al. [2]. Comparing the simulation results of
182 the two injectors showed that the hollow-cone injector resulted in earlier combustion phasing for
183 SOIs -40 and -30 aTDC, while the opposite trend is seen for SOIs -18 and -14 CAD aTDC. The
184 results were found to be consistent for the three fuels. The comparison of combustion phasing for

PRF 62 using both multi-hole and hollow-cone injectors can be found in supplementary material.

Figure 2. Simulated CA50 for the three fuels using multi-hole injector (left) and hollow-cone injector (right)

Figure 2 shows that the present simulations successfully reproduced the different experimental trends observed in [2, 24], such that the data were further analyzed to examine the main effects of the two different injectors. Note that any observed differences are attributed to the physical properties of the fuel exclusively because the simulations of three fuels utilize the same combustion kinetics of PRF62.

Therefore, to isolate the mixing behavior, inert non-reacting runs were conducted for all the fuels and SOIs. Figures 3 and 4 present the in-cylinder total liquid and vapor mass histories from the non-reacting cases. These quantities affect the spray penetration and subsequent fuel/air mixing characteristics of evaporating sprays. Figure 3 shows that the hollow-cone injector produces a much larger amount of in-cylinder liquid for all SOIs. As a related outcome, Fig. 4 shows that the total vapor mass is significantly lower for the hollow-cone injector case. This is attributed to the nature of the two injectors; the hollow-cone spray allows liquid parcels to cluster at the

nozzle exit and results in slower evaporation. In addition, the spray exit area of the hollow-cone injector is larger due to the nature of the outwardly opening injections. The total injection area of the hollow-cone and multi-hole (all 7 holes counted) injectors are 0.302 mm^2 and 0.178 mm^2 , respectively. The smaller injection cross-sectional area of the multi-hole injector leads to higher injection velocities, as shown in Fig. 5. This higher injection velocity increases the instability of the droplet due to the higher shear stress on the surface, which results in easier break-up and evaporation [40].

Regarding the differences between the three fuels, it is evident from Figs. 3 and 4 that the liquid mass of the LN is lower than those of the PRF62 and HSRN for the same SOI and injector type. This is mainly due to the lower boiling point of the LN compared to PRF62 and HSRN as seen in Fig.1.

Figure 3. Liquid spray mass at different SOIs using hollow-cone (red lines) and solid-cone injectors (black lines) for PRF, LN and HSRN

Figure 4. Fuel vapor in-cylinder mass at different SOIs using hollow-cone injector (red lines) and solid-cone injector (black lines) for LN, PRF 62 and HSRN

Figure 5. Spray exit velocity using hollow-cone injector (red lines) and solid-cone injector (black lines) for LN (dashed line), PRF 62 (solid line) and HSRN (dotted lines) at SOI -40°(a), -30°(b), -18°(c) and -14°(d)

Figure 6 shows the temperature-equivalence ratio maps colored by fuel mass fraction in addition to the mass average temperature and equivalence ratio at TDC for LN. The mass average temperature and equivalence ratio are calculated using the following equations;

$$\Phi_{\text{mean}} = \frac{\sum \Phi_i m_i}{\text{Total injected fuel mass}} \quad (1)$$

$$T_{\text{mean}} = \frac{\sum T_i m_i}{\text{Total injected fuel mass}} \quad (2)$$

where T_i , m_i and Φ_i denote the temperature, fuel mass and equivalence ratio of i -th cell in the computational domain. It is noted here that only the fuel containing cells are accounted for when calculating Φ_{mean} and T_{mean} because of the m_i term which by definition is zero for cells with no fuel. Similar T - Φ maps for PRF 62 and HSRN can be found in the supplementary material.

The figure also shows that, for both injectors, a later SOI increases equivalence ratio due to less time available for mixing. The mass-averaged in-cylinder temperatures are also lower for later SOI because richer fuel pockets are formed and the evaporative cooling of the fuel reduces the temperature of the fuel containing cells. Please note that, if all the cells in the cylinder domain are considered for calculation in Eq. (1) and (2), the in-cylinder T_{mean} will be the same for fuels with similar latent heat of vaporization regardless of the SOI. In addition, at the same SOI, the hollow-cone injector always produces richer mixtures and a lower mass average temperatures compared to the solid-cone injector.

The mass-average temperatures and equivalence ratios for all cases are summarized in Fig.7. For all three fuels, the distinct trends resulting from the two injectors are evident.

The nature of both sprays is further investigated here. The percentage of the unused air is calculated at TDC for all SOI cases as:

$$\% \text{ unused air} = \frac{\text{mass of air in fuel free bins}}{\text{total mass of incylinder air}} \times 100 \quad (3)$$

Figure 8 clearly shows that the percentage of unused air is always higher in the hollow-cone injector because fuel parcels are clustered and the equivalence ratios are higher. The multi-hole solid-cone injector penetrates further into the chamber and vaporizes more rapidly, resulting in leaner and hotter mixtures.

-40 **-30** **-18**

-14

Figure 6. T- Φ maps colored by fuel mass fraction at TDC for LN at different SOIs; using solid-cone and hollow-cone injector.

Figure 7. Calculated mass-average temperature (left) and mass-average equivalence ratio (right) for different fuels using hollow-cone (hollow squares) and solid-cone (solid circles) injections. Lines are for eye guidance.

Figure 8. Percentage of unused air for different fuels at different SOIs using solid-cone injector (solid symbols) and hollow-cone injector (hollow symbols). Lines are for eye guidance.

Both equivalence ratio and temperature distributions affect ignition. To assess the relative significance between the two factors, constant volume ignition delay time (IDT) calculations were carried out at the different T_{mean} and Φ_{mean} values reported in Fig.7 and a representative pressure of 40 bar. Simulations were performed in CHEMKIN-PRO [41] using the same reaction mechanism by Liu et al. [38]. The results are shown in Fig.9. The IDT are also presented in CADs.

At the earlier injection cases (SOI -40 and -30 CAD), the difference between the in-cylinder mass-average temperatures of the two injector cases is small, as previously seen in Fig.7. Consequently, the equivalence ratio differences dominate and the richer hollow-cone injection cases ignite faster as evident from the combustion phasings presented in Fig.2. On the other hand, the difference in the mass-average temperature becomes large at later injection cases (SOI -18 and -14 shown in Fig.7) and overrides the effects of the equivalence ratio differences. Accordingly, the hotter solid-cone injection cases ignite faster as also shown earlier in the

combustion phasings (CA50). In summary, the combustion phasing trends in Fig.2 can be explained by the distinct spray characteristics of the two different nozzles; the subsequent ignition can be properly captured by the homogeneous ignition model as the ignition locations are locally well mixed.

Figure 9. Simulated IDT for the three fuels conducted at 40 bar and the calculated T_{mean} and Φ_{mean} for different SOIs using solid-cone injector (solid symbols) and hollow-cone injector (hollow symbols). IDT are shown in ms and CAD. Lines are for eye guidance.

However, the simplified homogeneous IDT analysis is not sufficient to explain the differences observed between the combustion phasings of the fuels in the multi-hole injection engine experiments [24]. Figure 9 shows that the calculated ignition delay times are identical for the three fuels at each SOI. Note that ignition favors a locally richer and hotter spot. Therefore, the probability density functions (PDF) for the in-cylinder equivalence ratio and temperature at TDC are investigated in Figs. 10 and 11. To generate PDFs, all computational cells were classified into bins according to their equivalence ratio or temperature ranges and the total volume of each

bin was determined. Figure 10 shows the Φ range favored by combustion (close to stoichiometry). The total equivalence ratio PDF can be found in supplementary material (Fig. S4). It is clear that the PDF for the three fuels are similar at all SOIs for the hollow-cone injection, which explains the similar combustion phasings presented in Fig.2. Some differences between the three fuels are observed in the highly rich regions where lower temperatures prevent autoignition. However, differences are observed in the multi-hole injector. For all cases considered, PRF62 and HSRN have similar PDF distributions in the multi-hole injection case. The similar densities and surface tensions of the two fuels (Fig.12) contribute to the similarities in the PDF distributions because the droplet breakup is directly affected by these two physical properties. In addition, the distillation curves of PRF62 and HSRN (Fig.1) are not very different and hence the evaporation of the two fuels is expected to be similar when injected into the relatively hotter in-cylinder region. However, the differences in the distillation curves of PRF62 and HSRN yield some minor differences in the PDF distributions, as can be seen in Fig.10 especially at later SOIs. However, the narrower boiling point range of LN results in leaner mixtures compared to PRF62 and HSRN. Specifically, at the earlier injection cases (-40 and -30 CAD), PRF and HSRN show richer mixtures compared to LN resulting in their earlier CA50 presented in Fig.2. In later injection cases of -18 and -14 CAD, LN shows richer mixtures than PRF 62 and HSRN which explains its earlier CA50 in Fig.2. LN parcels break up and evaporate easier due to its physical properties. Figure 5 shows that LN cases always have a higher injection velocity for all SOIs because of its lower density, as shown in Fig.12. This, in addition to its lower surface tension clearly seen in Fig.12, facilitates the breakup of LN compared to PRF 62 and HSRN. Furthermore, according to the evaporation curves in Fig.1, LN is more volatile than

307 PRF and HSRN and hence easier to evaporate. This agrees with the liquid mass profiles shown
308 in Fig.3, where lower in-cylinder liquid mass is observed for LN.

309 Figure 11 shows the temperature PDF for all the investigated cases across a narrow temperature
310 range. The total temperature PDF can be found as supplementary material (Fig.S5). The
311 temperature PDF for the three fuels is identical in case of multi-hole injection, attributing the
312 difference in their combustion phasing to their equivalence ratio distribution, as discussed earlier.
313 However, the hollow-cone cases show some slight discrepancies in the temperature PDF of the
314 three fuels, which didn't affect the ignition characteristics of the mixtures as interpreted by their
315 similar CA50. With early injection, the LN cases are very lean compared to PRF and HSRN
316 cases resulting in later CA50. For late injection cases, the time available for mixing is not
317 enough, so PRF62 and HSRN mixtures are leaner compared to LN mixtures, which impedes
318 ignition.

Figure 10. Equivalence ratio PDF at TDC for the three fuels LN, HSRN and PRF 62 using hollow-cone injector and solid-cone injector

Figure 11. Temperature PDF at TDC for the three fuels LN (dashed line), HSRN (dotted lines) and PRF 62 (straight lines) using hollow-cone injector (red lines) and solid-cone injector (black lines).

Figure 12. Computed surface tension and density for the three fuels; PRF 62 (red dotted line), LN (straight line) and HSRN (dashed line).

4- Conclusions

The effects of injector geometry on gasoline compression ignition engine (GCI) were numerically investigated by sweeping SOI from -40 to -14 CAD aTDC and using three fuels with different physical properties (i.e., PRF 62, LN, HSRN). It was found that a hollow-cone injector creates richer mixtures which are accompanied by lower in-cylinder temperatures. At early injection cases, the hollow-cone injector cases showed earlier combustion phasing than the multi-hole injector. However, at later injection cases, the in-cylinder temperature for the multi-hole injection cases was higher than that of hollow-cone injection, overriding the equivalence ratio effect and resulted in earlier ignition.

The effects of the physical properties of different fuels were also studied. The equivalence ratio PDF across the ignitable range varies for fuels injected via the multi-hole injector, resulting in combustion phasing differences. However, the hollow-cone injection cases showed similar

equivalence ratio distributions for all fuels. It was concluded that though primary reference fuels were able to replicate the ignition delay time of real fuels with the same octane number in shock tube and rapid compression machines [25, 42], their actual performance in engines can be markedly different. The present study demonstrates the importance of formulating surrogates that match the physical properties of the real fuels in addition to the octane number [14, 19, 39] .

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