

Numerical simulations of n–heptane spray in high pressure and temperature environments

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Abstract

In this study n-heptane spray in supercritical environments was simulated using commercial CFD (Computational Fluid Dynamic) software AVL Fire. The numerical results were analyzed in terms of global spray parameter, and spray penetration. The results obtained were compared with experimental data available at Sandia National Laboratories. N-heptane spray simulations were performed in the same conditions as in the Sandia experiments. The goal of the study was to assess whether the Lagrangian approach performs well in engine relevant conditions in terms of spray global parameters. Not included in this assessment was the influence of supercritical mixing on liquid-gas interphase. The major element was the potential for practical application of the commercial CFD code in terms of properly representing global spray parameters and thus mixture formation in supercritical conditions, which is one of the core aspects in whole engine process simulation. The key part of the study was mesh optimization. Therefore, the influence of mesh density on both the accuracy of calculations and the calculation time was determined, taking into consideration detailed experimental data as initial conditions for the subsequent calculations. This served as a basis to select the optimal mesh with regard to both accuracy of the results obtained and time duration of the calculations. As a determinant of accuracy, the difference within a range of evaporated fuel stream was used. Using selected mesh the set of numerical calculations were performed and the results were compared with experimental ones taken from the literature. Several spray parameters were compared: spray tip penetration, temperature of the gaseous phase and mixture fraction in the gaseous phase. The numerical results were very consistent in respect of spray tip penetration. The other parameters were influenced by specific features of the Lagrangian approach. Nevertheless the results obtained showed that the Lagrangian approach may be used for engine relevant conditions.

Keywords: CFD, n-heptane, spray, injection, supercritical mixing,

1. Introduction

Injection into environments of pressure and temperature exceeding fuel critical parameters is attracting high interest due to trends for downsizing and turbocharging. Supercritical mixing was studied for many years with respect to rocket propulsion. In terms of reciprocating engines it was first noticed by some researchers [1–4] that this aspect should be taken into account in compression ignition engines. This statement seems to be confirmed in particular by the findings of Rachedi et al. [5] who noticed that for a swirling injector the behavior of a supercritical hydrocarbon jet and a supercritical CO₂ jet was similar in most investigated aspects.

A study made by Dahms et al. [6] showed that the mixing behavior of hydrocarbon fuels changes when the temperature of the surrounding gas exceeds the critical temperature of the injectant, but the influence of the backpressure was not investigated in terms of exceeding the value of critical pressure of injected hydrocarbon fuel. They performed a set of experiments to image the structure of n-dodecane jets in conditions of relevance to diesel engines. They used long-distance microscopy to visualize jets propagating from the injector. They noticed that, for higher temperatures, darker regions signifying light-scatter and extinction by liquid were still apparent in some locations. However, the transition from liquid to gaseous state appeared to be much smoother than in low-temperature conditions.

These findings are important in terms of Computational Fluid Dynamics simulations used in the engine optimization process. Fuel injection models used for predicting the mixing process in internal combustion engine are based on the

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assumption that the fuel jet undergoes disintegration and breakup typical for liquid fuels. According to Pilch and Erdman [7], the breakup of the liquid drop depends on the Weber number, which is a dimensionless number describing the relation between the fluid's inertia force and surface tension force.

When a liquid fuel is injected into a high temperature and pressure environment, the phenomena involved in the mixing process may become different than occurs during mixing in subcritical conditions. This results in all the knowledge concerning liquid fuel injection in subcritical regimes gained during previous investigations having limited application.

Therefore the main objective of this study was to compare experimental results (from Sandia) of a research n-heptane injector with numerical modelling of the same injector. The main goal of this comparison was to check the behavior of Lagrangian spray under supercritical temperature in the combustion chamber as well as to determine differences between numerical and experimental results.

2. Numerical model

Numerical simulations were performed with AVL Fire CFD software based on the Finite Volume approach. The simulations were done using the RANS method (Reynolds Averaged Navier-Stokes). During the injection turbulent conditions of the flow had to be modelled. For this purpose the k - ϵ model was chosen. An eddy-viscosity model based on Durbin's elliptic relaxation concept is proposed, which solves a transport equation for the velocity scales ratio $f^{1/4} t_2 = k$ instead of t_2 , thus making the model more robust and less sensitive to grid nonuniformities [8].

The next model which is very important for proper modelling of injection is the spray model. For liquid phase representation the Discrete Droplet Model (DDM) was used. This approach in stochastic form was originally proposed by Dukowicz [9] and it is a more practical approach than the Continuous Droplet Model (CDM) because of the lower computational requirements. In DDM the spray is represented by finite numbers of parcels, where each parcel contains a group of similar droplets. Spray equations are implemented for only one droplet from each parcel, resulting in lower calculation costs [10]. If DDM is used, appropriate submodels need to be chosen for break-up and vaporization of droplets. A primary breakup model was not included and the injected liquid entered the computational domain as droplets of nozzle diameter size. The WAVE submodel was chosen for secondary break-up of the droplets. the Dukowicz submodel was chosen to model vaporization. The surrounding gas was treated as ideal gas and no real gas effects were included. This was done deliberately in order to focus on the performance of the conventional approach to liquid spray modelling in high temperature and high pressure environments. A previous comparison for similar solver settings [11] was limited to qualitative analysis due to the limited availability of experimental data.

3. Boundary and initial conditions

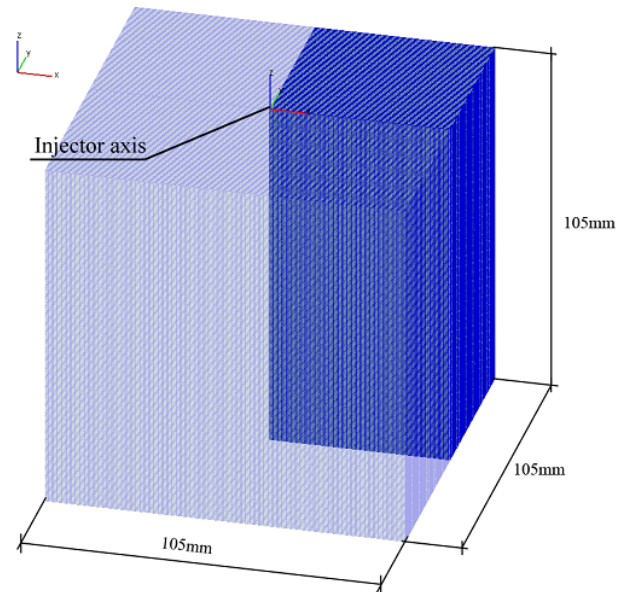


Figure 1: Model used for calculations. Location of the injector

A combustion chamber used in the experiments in Sandia and available in [12] was simplified to a cube model with dimensions $105 \times 105 \times 105$ mm. The model was limited by the walls of the cube and, to speed up the calculations, only one quarter of the model with symmetry conditions was used. The injector nozzle axis was perpendicular to the wall at its central point (Fig. 1). The parameters of the boundary and initial conditions are shown in Table 1. The parameters of n-heptane during injection are presented in Table 2.

The injection rate was set as a table according to "recommended" values from [12]. The injection rate is shown in Fig. 2.

Table 1: Initial and boundary conditions [12]

Parameter	Value
Nominal ambient temperature, K	1,000
Nominal oxygen mole fraction, %	0
Nominal ambient temperature, K	1,000
Nominal ambient density, kg/m^3	14.8

Table 2: Parameters of injection [12]

Description	Value
Temperature, K	373
Nominal injection pressure difference, MPa	150
Injection duration, ms	6.94
Nozzle diameter, mm	0.1

The temperature of the gas in the combustion chamber was higher than 540K, which is the critical temperature of n-heptane. The pressure in the chamber at the start of injection was also higher than the critical pressure of n-heptane, which is 2.74 MPa.

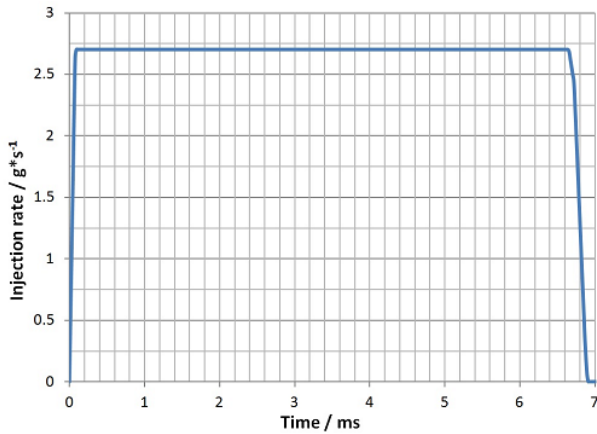


Figure 2: Injection rate (from [12])

4. Computational mesh

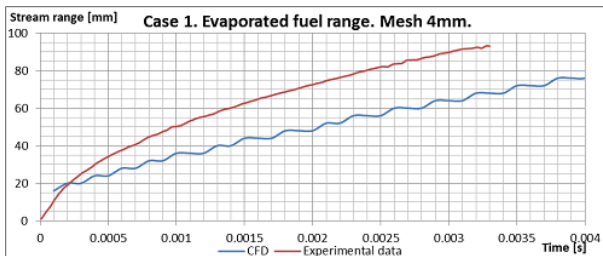


Figure 3: Comparison of range of evaporated fuel stream. Size of single element 4 mm

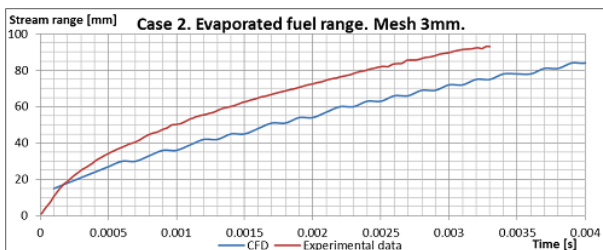


Figure 4: Comparison of range of evaporated fuel stream. Size of single element 3mm.

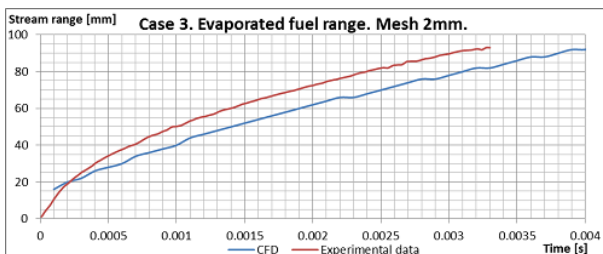


Figure 5: Comparison of range of evaporated fuel stream. Size of single element 2 mm

One quarter of the chamber volume was meshed several times with cells of different size. That was done to select

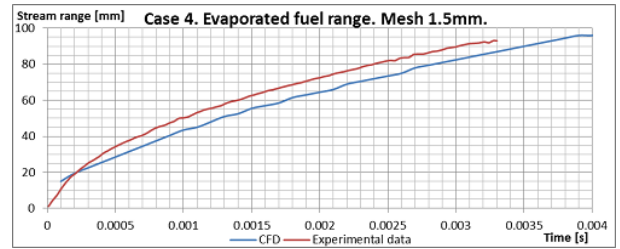


Figure 6: Comparison of range of evaporated fuel stream. Size of single element 1.5 mm

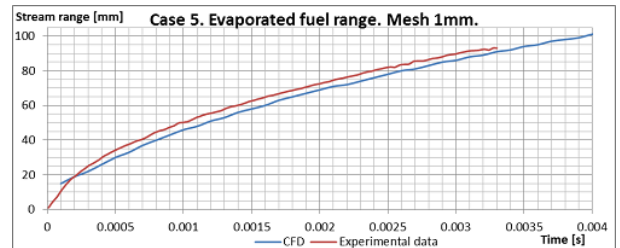


Figure 7: Comparison of range of evaporated fuel stream. Size of single element 1 mm

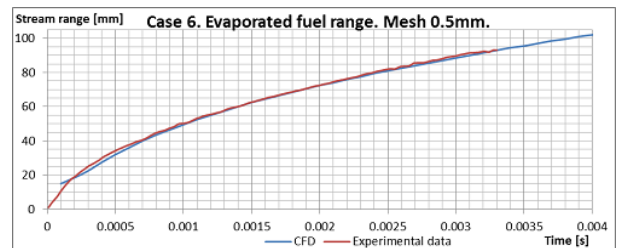


Figure 8: Comparison of range of evaporated fuel stream. Size of single element 0.5 mm.

the most appropriate cell size, thereby providing relatively low computation time while avoiding the negative influence of mesh density on the accuracy of results derived from simulation. As a determinant of accuracy, the difference within a range of evaporated fuel stream was used. The mesh independence study was started for mesh of size 4, 3, 2, 1.5, 1 and 0.5 mm. The comparisons of the range of evaporated fuel stream for each case are shown in Figs. 3–8.

The average differences and standard deviations for the test meshes are provided in Table 3.

Table 3: Collation of average differences and standard deviations

	Element size, mm	Average difference, mm	Standard deviation, mm
Case 1	4	18.9	8.20
Case 2	3	14.6	5.79
Case 3	2	9.37	3.88
Case 4	1.5	6.73	2.65
Case 5	1	3.71	2.65
Case 6	0.5	0.709	1.13

In order to clarify the influence of cell size on spray penetration, the measured average differences and standard deviations were shown in Fig. 9.

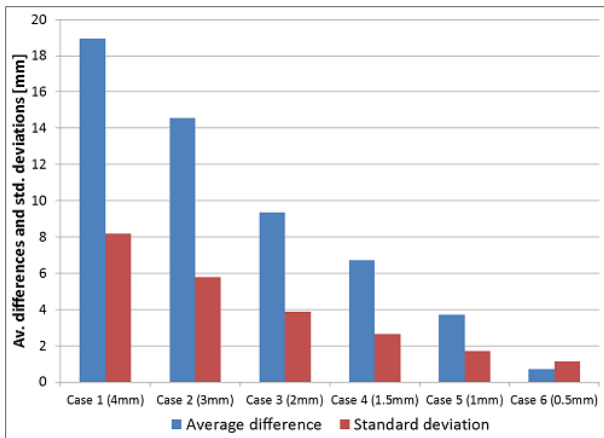


Figure 9: Spray penetration average differences and standard deviations (between experimental and numerical results)

For further simulations, mesh of cell size of 0.5 mm was chosen.

5. Results

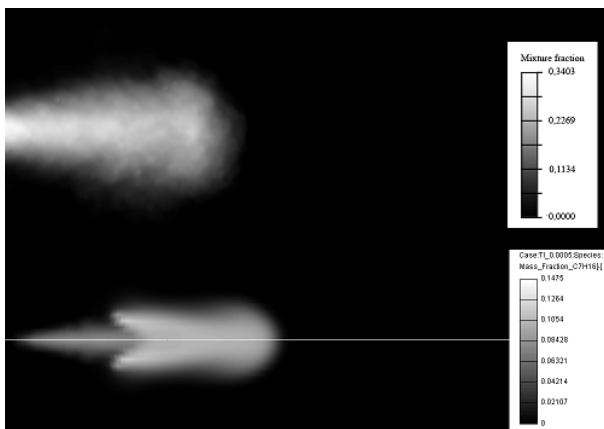


Figure 10: Collation of experimental results [3] and numerical results of mixture fraction in 0.5 ms of injection

The simulation results obtained were collated for the purpose of comparison with the experimental data available at Sandia. In Figs. 10–13 the comparison of mixture fraction is shown.

Similarly, the results are shown for the temperature field in the axial plane downstream of the injector axis. A comparison of the temperature results is shown in Figs. 14–17.

The most striking difference between the sets of results is the clearly visible step change in the distance of the injector exit. This area is located around 12 ÷ 15 mm from the injector nozzle. This may be linked with sudden annihilation of droplets, which is shown in Fig. 18. This effect

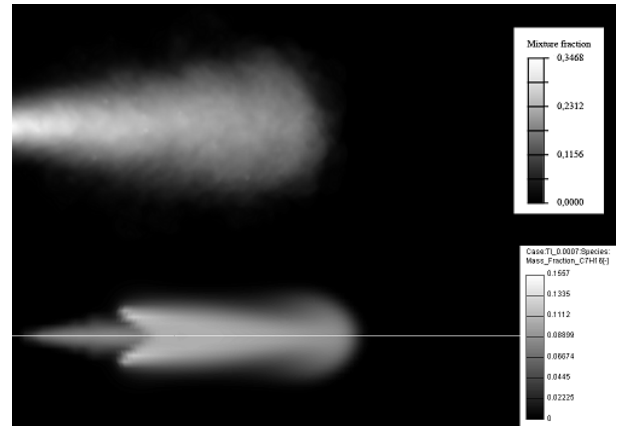


Figure 11: Collation of experimental results [3] and numerical results of mixture fraction in 0.7 ms of injection

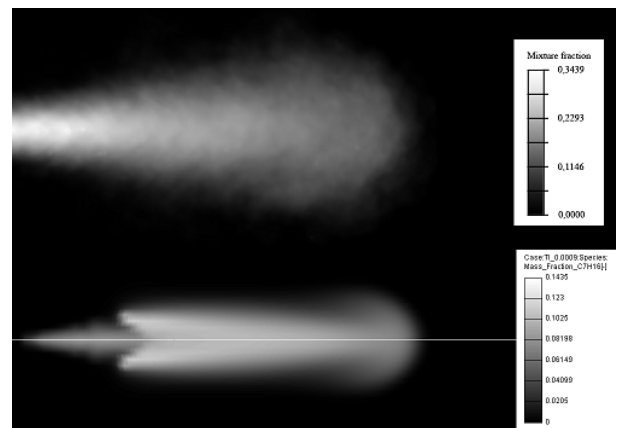


Figure 12: Collation of experimental results [3] and numerical results of mixture fraction in 0.9 ms of injection

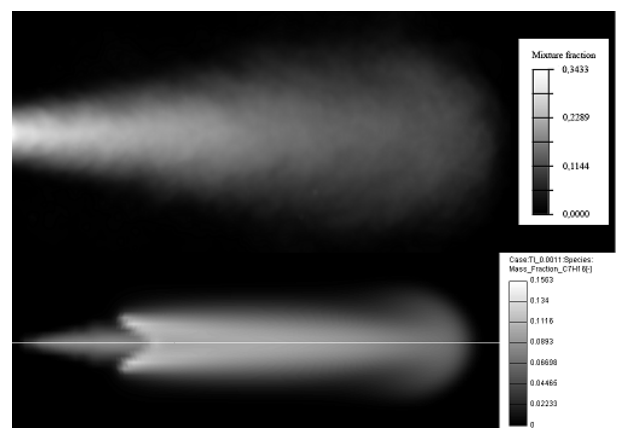


Figure 13: Collation of experimental results [3] and numerical results of mixture fraction in 1.1 ms of injection.

may be regarded as a drawback of omitting real gas effects near the critical point. When droplets reach the critical temperature they become treated as gaseous phase. Therefore in the downstream area after the annihilation of droplets, a high concentration of evaporated fuel is observed



Figure 14: Collation of experimental results [3] and numerical results of temperature in 0.5 ms of injection



Figure 17: Collation of experimental results [3] and numerical results of temperature in 1.1 ms of injection



Figure 15: Collation of experimental results [3] and numerical results of temperature in 0.7 ms of injection

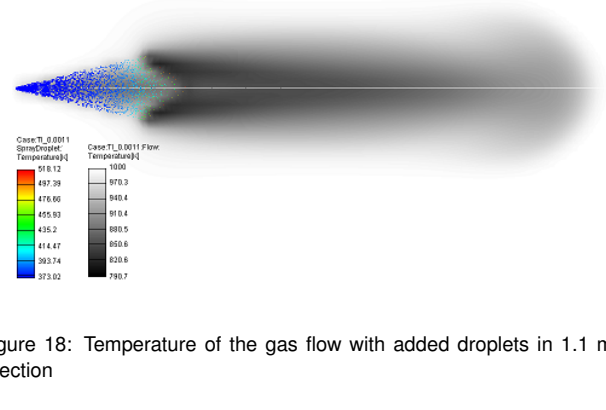


Figure 18: Temperature of the gas flow with added droplets in 1.1 ms of injection

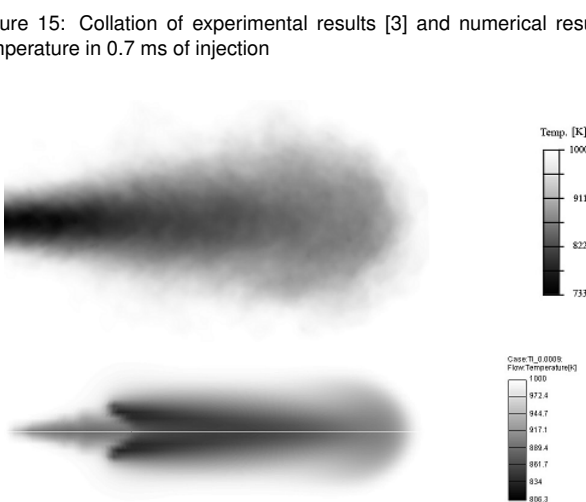


Figure 16: Collation of experimental results [3] and numerical results of temperature in 0.9 ms of injection

(Figs. 10–13). The immediate phase change of relatively cold droplets (compared to surrounding gas) influenced the temperature in the same way (Figs. 14–17).

Fig. 18. The droplet temperature was superimposed on the gaseous surrounding temperature field. One can clearly

see that the droplets annihilate before the critical temperature of n-heptane is reached.

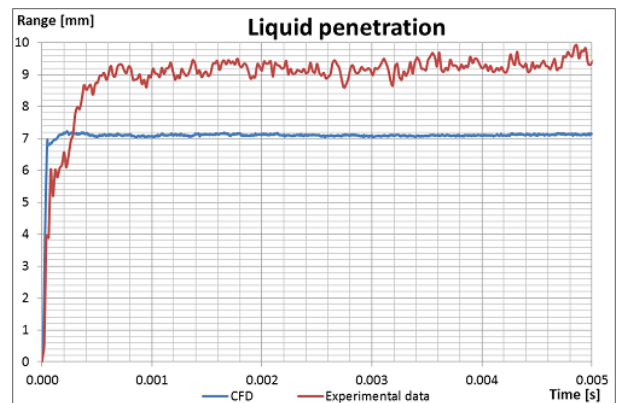


Figure 19: Comparison of liquid penetration during time of injection.

In addition to the mixture fraction and temperature field, the global spray parameter was compared, specifically liquid length. The comparison of liquid length for experiment and numerical simulation is shown in Fig. 19.

The average difference between these results comes to about 1.88 mm. This difference results from the fact that in the Lagrangian approach the liquid core needs to be defined arbitrarily. Moreover, the threshold of the scattering signal

represents the liquid core. However, once these values are defined, the liquid length evolution should be similar. Therefore the initial growth rate is more important than the stable maximum value. This in turn is consistent.

6. Summary and Conclusions

The numerical results were very consistent in terms of spray tip penetration. The other parameters were influenced by specific features of the Lagrangian approach. The specific observations are summarized below:

- The mesh with single element size 0.5 mm is a good approximation of the investigated injector.
- The spray tip penetration obtained in numerical simulation was consistent with experimental results.
- There is a clearly visible step change in fuel vapor mass fraction at a distance of 12–15 mm from the injector nozzle exit. Similar behavior was observed for the temperature field. This may be linked with sudden annihilation of droplets, which is shown in Fig. 17. This effect may be regarded as a drawback of omitting real gas effects near the critical point.
- The maximum temperature of droplets was lower than the critical value for n-heptane.

Even though there are some deficiencies in the proper representation of spray, especially in terms of temperature and fuel vapor concentration, global spray parameters such as tip penetration are represented very accurately. One needs to be aware that both the Lagrangian approach for liquid droplets representation and the ideal gas assumption for continuous phase assure high computational savings, which is crucial in terms of engine simulations. Taking into account all these aspects, one can draw the conclusion that the Lagrangian approach may be used for spray simulation in engine relevant conditions.

Acknowledgments

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