

Statistical Approach on Visualizing Multi-Variable Interactions in a Hybrid Breakup Model under ECN Spray Conditions

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ABSTRACT

The Direct Numerical Simulation (DNS) approach to solving the fundamental transport equations down to the smallest scales of motion is favorable should the requirement be a truly predictive solution of fluid dynamic problems, but the simulation run times are unacceptable for most practical industrial applications. Despite the steadily increasing computational capabilities, Reynolds Averaged Navier-Stokes (RANS) based frameworks remain the most commercially viable option for high volume sectors, like automotive. The sub models within RANS simplify the description of key physical phenomena and include several numerical constants. These so-called “tuning constants” introduce multivariable dependencies that are almost impossible to untangle with local sensitivity studies. This paper addresses the prevailing difficulties in setting up an adequate diesel spray simulation which arise from the mentioned multi-variable interactions of these “tuning constants”, by applying a statistical approach named Design of Experiments (DoE).

Often combined with an optimizer, DoE is commonly used to find an optimum set of engine parameters for set criteria at reduced experimental effort. In this case, the methodology was applied to determine an optimal set of “tuning constants” for the simulations which best matched experimental data at five conditions taken from the Engine Combustion Network (ECN) database. Multi-variable DoE were run for each condition. Stochastic response models (SPM’s) highlighted crucial simulation sensitivities of the turbulent dissipation constant C_2 and liquid/gas-phase momentum transfer at injection pressure swings. Further, a comparison of the breakup models which produced matching simulations exhibited patterns which correspond with physical processes. Lastly, it was shown that while a single set of the constants can give reasonable results in the space explored, there is merit in adjusting key constants to suit the operating condition in the search for accuracy.

CITATION: Nsikane, D., Mustafa, K., Ward, A., Morgan, R. et al., "Statistical Approach on Visualizing Multi-Variable Interactions in a Hybrid Breakup Model under ECN Spray Conditions," *SAE Int. J. Engines* 10(5):2017, doi:10.4271/2017-24-0104.

INTRODUCTION

A combination of tightening emission regulations and shortening product development cycles is challenging wide spread product development practices. Due to the growing complexity of ICEs, prototyping and experimental engine mapping is not only expensive, but also time consuming. The emergence of Computer Aided Engineering (CAE) has brought relief to these pressures. In particular, Computational Fluid Dynamics (CFD) tools have facilitated the research and development of in-cylinder processes like port flow, injection events, combustion and emission production processes. As engine development becomes progressively more virtual, the expectations for accurate simulations will rise.

Engineering flows are predominantly turbulent. The accuracy of the simulation is highly dependent on the approach to model the turbulent motion. The three main approaches are Direct Numerical Simulation (DNS), Large Eddy Simulation (LES) and Reynolds-Averaged Navier-Stokes (RANS). The characteristics of each method are shown in [Table 1](#).

Up to now, due to its favorable simulation durations, the chosen method in most commercial environments is typically RANS. Since RANS applies a statistical approach in which all fluctuating motion is absorbed into turbulence models, information about the detailed flow characteristics is lost. In order to offset the loss of this information semi-empirical sub models can be used to approximate the influence of complicated flows like high speed jets. The disadvantage of sub models is that they introduce a large number of user-defined input

variables. This paper addresses the prevailing difficulties in setting up an adequate diesel spray simulation which arise from multi-variable interactions of tuning constants in sub models in a RANS based approach. It is important to note that since diesel engines are characterized by diffusion combustion, the rate of combustion is directly influenced by the propagation of the fuel and therefore it is critical to model the fuel spray accurately if an engine simulation is to be credible.

Table 1. Characteristics of DNS, LES and RANS [1]

DNS	LES	RANS
• Highly resolved grid • Predicts every detail of turbulent motion to the smallest scale • Highest level of physical accuracy • No tuning required • Very computationally expensive	• Directly computes large eddies like in DNS • Models small eddies like in RANS • Requires fine grids • Good level of physical accuracy • Computationally expensive	• Fluctuating turbulent motion is modelled using a statistical approach (turbulence modelling) • Least level of physical accuracy • Highly dependent on tuning • Computationally efficient

An example of the importance of tuning constants in the context of diesel spray models is given in Figure 1, where two simulations were run under identical boundary conditions and the liquid and vapor spray penetration compared to the results of an experiment. The default model constants were selected based on literature and suggestions from the software manual, likely to have been validated at a select number of scenarios. It is clear that the results are not close to the measurement data. However, the model can be tuned to deliver an accurate match. Being able to pre-define these model constants for a new case is therefore a crucial step in eliminating time consuming tuning iterations and the need to wait for hardware and experimental data, delivering a truly predictive but practical simulation.

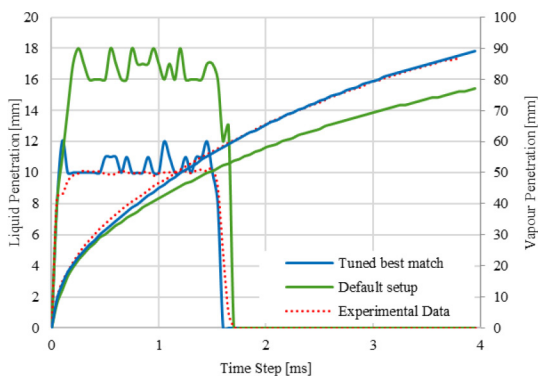


Figure 1. Simulation with default vs tuned model constants compared with measured non-reacting ECN Spray A ($T_{amb}=900K$, $P_{inj}=150MPa$)

Starting from an ‘out-of-the-box’ setup, this paper demonstrates how an extensive parametric study arrived at an acceptable ‘spray match’ using a Design of Experiment (DoE) approach. Additionally, a justification of the selected sub models and analysis of the physical expression is presented. The goal of this is to highlight sensitivities and quantify the ranges the tuning constants should be set within. A thorough investigation into the physical expression of selected parameters explains the rationale behind the change between conditions.

The investigated cases are all taken from existing non-reactive spray bombs gathered by the Engine Combustion Network (ECN) and is openly accessible through their website [2]. The data sets all use n-dodecane, a single component Diesel surrogate, which was injected into a quiescent chamber under varying charge pressures and temperatures over a range of fuel injection pressures.

ECN Conditions

The ECN is a collaboration between the experimental and computational research communities with the focus on in-cylinder processes. The goal of the ECN is to establish an open-source library of experiments under strictly controlled laboratory conditions, with which computational models, and fundamental understanding of in-cylinder processes can be progressed. The ECN further offer suggestions to standardize the post-processing of computational results to ensure comparability amongst participants. The experimental and computational results shape the outcome of regular ECN meetings, which identify further research gaps and thus guiding combustion research in a more structured way. [2, 3, 4]

Despite the rigorous control of the ECN target experimental conditions, results between institutions vary. For example, while variations in vapor penetration between institutes are small, liquid penetration results vary by up to 17%. These variations arise from measurement uncertainties due to different measurement techniques and component tolerances, wear and decay [5]. Nevertheless, the ECN offers one of the most comprehensive data sets that is publicly available.

ECN “Spray A” utilizes an injector with a (single) nominal nozzle diameter of 90µm and rail pressures of 150MPa. This condition represents a light duty DI injection system running at part-load conditions, and with moderate EGR rates. A list of selected specifications and baseline operating conditions is presented in Table 2.

Table 2. ECN Spray A injector specifications and operating conditions [6]

Charge gas temperature	900 K
Charge gas pressure	near 6.0 MPa
Charge gas density	22.8 kg/m ³
Charge gas oxygen (by volume)	15% O ₂ (reacting); 0% O ₂ (non-reacting).
Fuel injector nominal nozzle outlet diameter	0.090 mm
Nozzle K factor	K = 1.5
Discharge coefficient	C _d = 0.86,
Fuel injection pressure	150 MPa prior to start of injection
Fuel	n-dodecane
Fuel temperature at nozzle	363 K (90°C)
Injection duration	1.5 ms
Injection mass	3.5 – 3.7 mg

Influential Diesel Injection Parameters

Some of the most influential parameters driving the fuel/air mixing process in the cylinder are parameters like injection pressure, charge gas temperature and density [7, 8, 9]. In [10] Naber and Siebers found that with increasing chamber air density, spray dispersion and air entrainment were increased. This was confirmed by Huang *et al* in [11], where it was shown that higher charge gas temperatures and subsequently reduced gas density led to enhanced heat transfer between the gas phase and the liquid fuel. The consequence was a decrease of fuel viscosity reducing flow resistance and subsequently increasing further spray propagation. The effects of fuel injection pressure on a diesel spray plume was studied by Agarwal *et al* in [12], where it was shown that vapor penetration significantly increases with rising injection pressure.

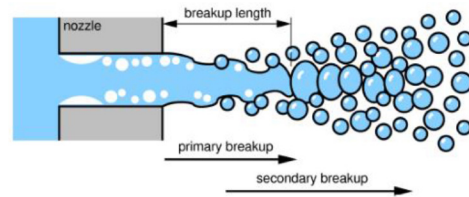
Computational Implementation of Fuel Injection

In contrast to experiments, simulations assume exact boundary conditions but simplify the real physics in favor of computational efficiency. The tradeoff between run time and accuracy is a very important consideration for practical CFD applications. While DNS simulations are entirely inappropriate for commercial purposes due to runtimes of up to 25 million core hours for a combusting bio-diesel case [13], LES has been receiving increasing interest. Nevertheless, a direct comparison between the performance of RANS and LES in [14] by Som *et al* showed that LES had a time penalty of approximately an order of magnitude in both reactive and non-reactive cases but produced better results. If LES is not a feasible choice, researchers and engineers still have the choice between RANS models of varying complexity. Notable attempts to improve physical accuracy and reduce tuning efforts have been undertaken for example by Som *et al* in [15], Abani *et al* [16] and Lee *et al* in [17].

Another possible route to improve simulations is to select more basic models but improve tuning capabilities. That this can work is shown in the work by Wang *et al* in [18], where he concluded that a well-tuned simple model was capable of predicting the combustion characteristics at a higher computational efficiency. To avoid losing the advantage of faster simulations to excessive tuning iterations, predefining tuning constants based on defined boundary conditions using intelligent tuning could be a potential solution. The work by Pei *et al* in [19] and [20] conducted a large parametric study in which a statistical approach called Global Sensitivity Analysis (GSA) was applied to a high number of simulations, and the dependency of simulation constants on ECN boundary condition quantified.

Spray breakup can be divided into two separate processes commonly termed as *primary* and *secondary breakup* (Figure 2) [21]. This describes the disintegration of a coherent liquid jet into a dispersed collection of droplets. Subsequently, the droplets undergo secondary breakup where the liquid droplets become unstable and further breakup into smaller droplets.

Real spray breakup



Existing breakup models

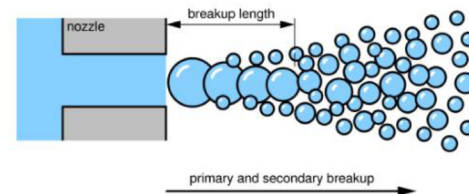


Figure 2. Real spray breakup vs common breakup models [22]

The breakup model used in this work is called the KH-RT hybrid breakup model and is based on the model developed by Beale and Reitz in [23]. It applies Kelvin-Helmholtz (KH) and Rayleigh-Taylor (RT) instability theory on droplet surfaces to approximate breakup. This model is selected because it is available in practically every commercial CFD package running with the RANS method. Due to the detailed investigation into the model constants, a brief introduction to the mathematical background is given. The original work should be consulted for more detail.

KH-RT Hybrid Breakup Model

In contrast to the real liquid jet ligaments, the spray is introduced as a collection of discrete droplet parcels and tracked in a Lagrangian fashion. Typically, the droplets are introduced and modeled using primary breakup theory until they reach a model specific switching criterion at which point the secondary breakup equations are applied.

In the KH-RT breakup model, a chain of droplets is introduced with the so-called “blob” method. A common approach would be to define the droplet diameter to be approximately equal to that of the effective nozzle orifice to replicate a liquid core. A discharge coefficient model predicts injection velocity, effective nozzle diameter and spray cone angle based on charge conditions and nozzle geometry. The introduced droplets are tracked and treated with KH instability. This model calculates the diameter of the parent droplet after each time step and at which rate it decreases in size.

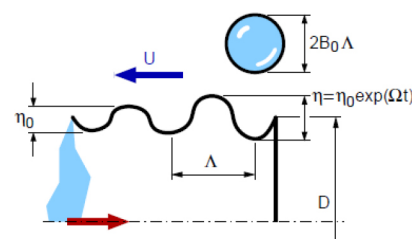


Figure 3. A schematic view of the droplet breakup based on KH instability [22]

For better understanding of the following mathematical equations refer to [Figure 3](#). The characteristic breakup time τ_{KH} is calculated as shown in [equation 1](#), with Ω_{KH} and Λ_{KH} being the maximum wave growth rate and its corresponding wave length. For the sake of brevity, the latter two parameters are not further elaborated.

$$\tau_{KH} = \frac{3.788B_1r}{\Omega_{KH}\Lambda_{KH}} \quad (1)$$

A parent droplet with the radius r breaks up into new child droplets with the radius r_c following [equation 2](#). The tuning constant B_0 can be seen as a multiplier to alter the size of the child droplet.

$$r_c = B_0\Lambda_{KH} \quad (2)$$

These equations show that B_0 and B_1 are the tuning factors responsible for the rate at which the parent droplet shrinks and defines the size of the child droplet.

$$\frac{dr}{dt} = \frac{r - r_c}{\tau_{KH}} \quad (3)$$

The switch between when primary and secondary breakup equations is defined by the breakup length L_b in the Levich model. It is calculated as shown in [equation 4](#). A_{bu} and B_{bu} are user tuning constants. The original authors recommended a value of 5.5 and 0 respectively.

$$L_b = A_{bu}D_n \sqrt{\frac{\rho_l}{\rho_g}} + B_{bu} \quad (4)$$

The RT model is then used in conjunction with KH to predict the secondary breakup of the droplets. The RT model predicts instabilities on the surface of the droplets that grow until a certain characteristic breakup time when the drop finally breaks up. Once waves begin to grow on the surface of the droplet, the wave growth time Ω_{RT} is tracked. This time is then compared to the breakup time. C_{RT} is a non-physical tuning factor and is usually kept at unity.

$$\tau_{RT} = \frac{C_{RT}}{\Omega_{RT}} \quad (5)$$

If the RT waves have been growing for a time greater than the breakup time, the drop is assumed to break up. The approximated diameter D_d of this stable droplet size is influenced by C_3 . This factor is usually kept constant at 5.3.

$$\frac{dD_d}{dt} = -\frac{D_d - 2\pi C_3}{\tau_{RT}K_{RT}} \quad (6)$$

METHODOLOGY

Experimental Data

Offering a particularly rigorous dataset, the ECN provides high quality measurements of important metrics such as liquid and vapor spray penetration and in all but one case, radial temperature and fuel fraction distributions at steady state along the spray plume, at six locations. A match in liquid penetration indicates the droplets are breaking up at the correct distance from the nozzle. Matching vapor length over time indicates the tip of the spray plume propagating at correct speed. The mixture fraction distributions give a good understanding of the instantaneous shape of the spray at a given time. A good correlation in the gas phase temperature distribution suggests an appropriate heat exchange between the charge and the propagating fuel vapor cloud. These latter metrics are important for the future consideration of combusting conditions, where the location, distribution and temperature of the air/fuel mix are key for reliable emission simulations.

The selected Spray A conditions with main characteristics are listed in [Table 3](#). Case 0 was used in single constant swings as well as for model selection and range setting in a test DoE.

Table 3. ECN Spray A conditions [24]

Case	Charge Temperature [K]	Charge Density [kg/m ³]	Inj. Pressure [MPa]	Inj. Duration [ms]
0	900	22.8	150	1.5
1	900	22.8	150	>4
2	1100	15.2	150	>4
3	1400	7.6	150	>4
4	900	22.8	100	>4
5	900	22.8	50	>4

The DoE cases 1 to 5 can be split into two investigated scenarios ([Figure 4](#)). The first is a swing of charge temperatures from 900K up to 1400K. The second scenario is an injection pressure swing from 150MPa down to 50MPa.

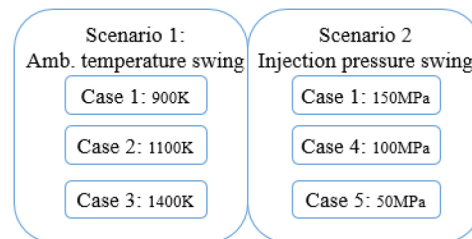


Figure 4. Scenario 1: Charge temperature swing, scenario 2: Injection pressure swing

Semi-Empirical Simulation Models

The five experimental conditions described before are simulated using the VECTIS [25] CFD package. VECTIS is a commercially available package developed by Ricardo Software. The turbulent motion was modelled using the RANS method. The standard $k-\epsilon$ model, based on Jones *et al* [26] with the modified constant of

dissipation, C_2 was selected to solve the governing transport equations. Liquid fuel droplets are injected with the “blob” method and are tracked in a Eulerian-Lagrangian fashion. The droplet breakup was approximated using the KH-RT hybrid breakup model and Levich switching criterion. The Putnam model [27], which assumes spherical droplets was selected to estimate the droplet drag coefficient. Droplet-droplet (collision and coalescence) and droplet-turbulence models options were included to improve the droplet trajectory calculations.

Independence Studies

Mesh Independence

Mesh independence was confirmed by running the same simulation setup and gradually decreasing the size of the mesh size by a set interval (Figure 5). How physically representative the liquid and vapor penetration lengths are plays no role at this stage. The grid was considered independent when the difference in spray penetration at every time step was under 0.5mm for liquid and 1mm for vapor respectively. The grid became independent at cell size of 0.48mm.

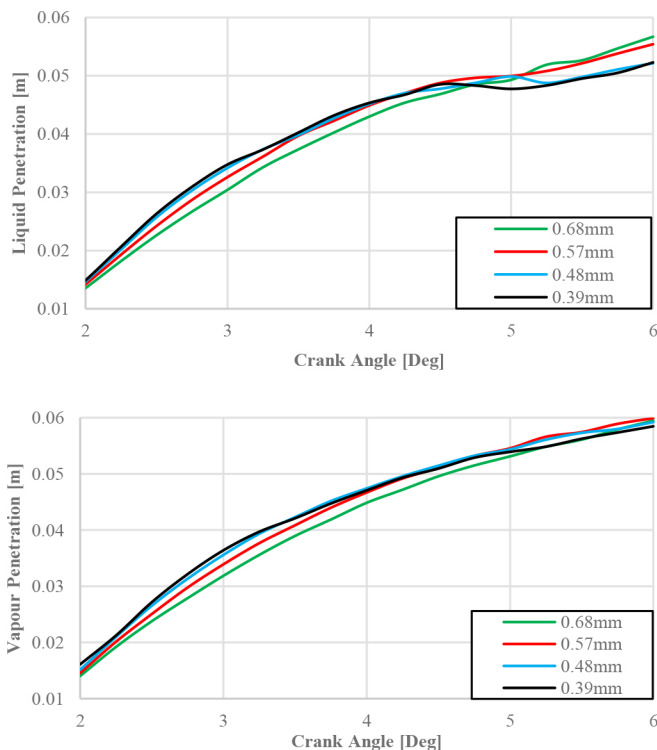


Figure 5. Mesh independence study based on liquid & vapor penetration

The mesh independence study was conducted based on the geometry of the Brighton University Rapid Compression Machine running at ECN Spray A conditions. A subsequent switch to the Sandia quiescent vessel and a repeated mesh independence study confirmed the mesh sizes to still be independent at the selected size (Figure 6). A second approach to confirm mesh independence by calculating the courant number confirmed a mesh size of 0.45mm. Based on these two approaches, a mesh size of 0.45mm was selected. A final level of validation is the comparison to the grid size other ECN participants

have selected. The majority of participants running with the RANS approach reported similar grid sizes. The level of confidence of this grid size is therefore high.

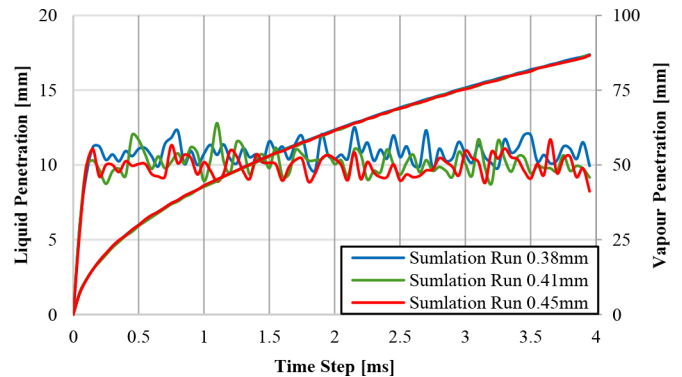


Figure 6. Repeated mesh independence study with the final Sandia Spray A geometry

Parcel Injection Rate Independence

The next step was to study the influence of the parcel introduction rate (PIR) using the previously determined grid size. Droplets are bundled into parcels and treated with the governing equations. Naturally, a higher number of parcels results in a finer resolution of the calculated values. While the effect on liquid and vapor penetration was limited, the assessment showed a greater influence on the spray cone angle. A PIR of 3.6×10^6 was required, with further increases having no affect. The grid independence was checked again with this setup and found to remain within the selected criteria.

Design of Experiments Approach

Traditional experiments are used to identify how a change of input parameters impacts on the output parameters of a system, highlight the systems sensitivity to change or define target values for input parameters to produce a desired output. The DoE method is a statistical approach to reduce experimental effort. The experimental input and corresponding output are key points in a simulation design matrix. Having completed the design matrix a stochastic process model (SPM) can be created, which is capable of modelling multidimensional, nonlinear responses. It is then possible to determine the output of a combination of input parameters deviating from the key points. Like this, the output can be optimized to a distinct target either manually or using an optimizer [28].

The DoE method, which is usually applied in an experimental environment was modified to suit the purpose of investigating computational simulations. The experiments are replaced by simulation runs, input parameters substituted with sub model tuning constants and the output parameters are defined as the calculated root-mean-square-errors (RMSE) between the experimental and simulated liquid and vapor penetrations.

Simulation Design Matrix

The first step in the DoE process is to construct the experimental design matrix. This includes identifying the key input parameters, setting appropriate ranges within the parameters can vary and selecting a statistically relevant number of data points.

Every key point is assigned with an individual combination of the parameters within the ranges shown in Table 4. The simulation design matrix constructed in this project consists of 100 simulation runs. This includes 16 corner points with the parameters at the periphery of the ranges, 2 center points and 82 space filling points. Therefore, a total of 500 simulations were run. The average duration per simulation on 20 cores Intel(R) Xeon(R) CPU E5-2650 v3 CPUs with 2.30GHz is around 2hrs.

Table 4. List of DoE variables, their set ranges and default values

Parameter	Range	Default
Coefficient of Dissipation C_2 [-]	1.7 – 1.85	1.92
Turbulent Schmidt Number	0.6 – 1	0.9
Drag scaling factor A_{drag} [-]	0.05 – 1.5	1
KH B_1 – Constant [-] [18]	1 – 25	13
KH B_0 – Constant [-] [18, 22]	0.3 – 0.8	0.61
Levich A_{bu} – Constant [-] [22]	5.5 – 11	5.5
RT - C_3 – Constant [-] [18]	0.3 – 5.3	5.3
RT C_{RT} – Constant [-] [18]	0.3 – 2	1
Initial Half Cone Angle α [deg]	2.5 – 7.5	-
Initial droplet diameter [μ m]	60 – 84	-

Simulation Comparison Metric

To properly assess the quality of the simulation against the experimental data, it is better to compare the entire propagation curve rather than a single value. The differences between the values at every computational time step are calculated using the RMSE method. To avoid unreasonably high errors, the injection ramp and end of measurements were removed from the calculation (Figure 7).

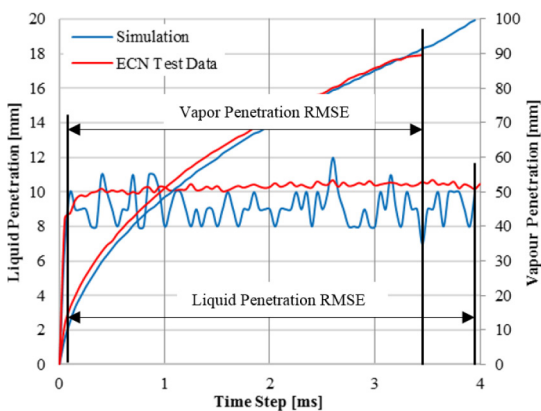


Figure 7. RMSE duration of interest

Mathematically, the RMSE is expressed as shown in eq. 7 and 8 by summing up the squared absolute differences between the measured and simulated spray penetrations x and y (Table 5) at each time step, and averaging the value with the number of comparison points. The root is then the averaged error over the whole curve.

$$RMSE_{liq} = \sqrt{\frac{\sum_{t=1}^n (x_{1,t} - x_{2,t})^2}{n}} \quad (7)$$

$$RMSE_{vap} = \sqrt{\frac{\sum_{t=1}^n (y_{1,t} - y_{2,t})^2}{n}} \quad (8)$$

Table 5. Calculation parameters for RMSE

Case	Time step	Liquid Penetration	Vapor Penetration
Test	t	$x_{1,t}$	$y_{1,t}$
CFD		$x_{2,t}$	$y_{2,t}$

RESULTS AND DISCUSSION

Before commencing the DoE runs at the five selected conditions, a test DoE run against ECN data, termed case 0 was conducted to justify appropriate range setting and sub-model selection. In this study, it became apparent that the changes of the selected parameters (Table 6) would not have a considerable influence on the vapor penetration (Figure 8). Most notably, the gradient always remained unchanged.

Table 6. Input variables of randomly selected runs used in test DoE

Run No.	11	30	38
Initial Blob Size [μ m]	84.2	84.2	83.5
Switching Criterion	5.5	11	6
Drag scaling constant - A_{drag}	1.5	1.5	0.63
B_1 – Constant	60	1	27.62
B_0 – Constant	0.3	0.8	0.78
C_{RT} – Constant	0.3	0.3	2.1
C_3 – Constant	0.3	2	0.92
Fuel Temperature [K]	403	343	347

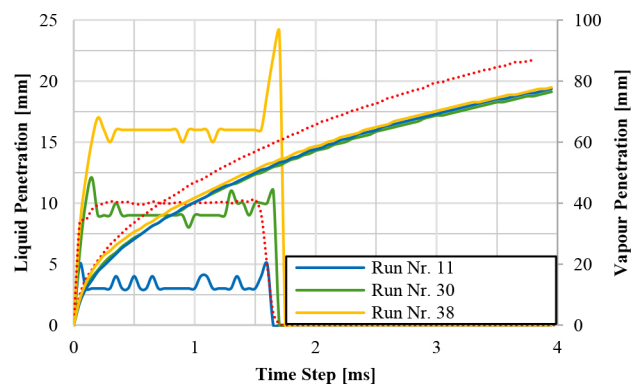


Figure 8. Influence of sub model constants on test DoE