Uncertainty estimation in determining liquid and vapor penetration lengths for Diesel like spray injection

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I declare that this written submission represents my ideas in my own words, and where others' ideas or words have been included, I have adequately cited and referenced the original sources. I also declare that I have adhered to all principles of academic idea/data/fact/source in my submission. I understand that any violation of the above will be a cause for disciplinary action by the Institute and can also evoke penal action from the sources that have thus not been properly cited, or from whom proper permission has not been taken when needed.

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(ME10B14M000008)

Approval Sheet

This thesis entitled Uncertainty estimation of liquid and vapor penetration length of diesel like spray simulations by Sumit Jadhav is approved for the degree of Master of Technology from IIT Hyderabad.

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I am thankful to my family and well-wishers for their constant enduring towards my betterment.

Dedicated to

I C Engine Lab IIT Hyderabad

Abstract

Uncertainty estimation in Computational Fluid Dynamics (CFD) simulation is becoming increasingly important as CFD is being extensively used as a design tool. Performance prediction from CFD along with an uncertainty band is expected to give a designer an estimation of the overall performance of a design within a defined confidence level.

In a numerical approach, there are two sources of errors: (a) modelling errors and (b) numerical errors. Modelling error arises due to the assumptions and approximations in the mathematical representation of the physical problem. Numerical error are due to numerical solution of the mathematical equations.

In this project, an attempt will be made to establish the procedure to estimate both sources of uncertainty in a typical CFD study. Diesel like spray simulation will be taken as an illustrative example to establish the procedure. Hence, as a major deliverable in this proposed project proposal, a general guideline will be established to determine uncertainty from a CFD study.

Contents

1. Motivation and Introduction

(a) Motivation

Numerical modelling and simulation of a physical problem has been in use for many decades and developed extensively with time. The techniques have established itself in many spheres of fluid mechanics and used extensively for everyday applications like aerospace, refinery, automotive etc. Simulation has helped to decrease the time and cost of experimentation in the iterative process of trial and error. Seldom though the experiment is exactly as per the predictions of simulations. This is mainly caused by the approximation of the actual physics and the non-ideal real life systems.

(b) Introduction to uncertainty analysis

The present study aims to quantify this mismatch between the numerical predicted output and the real life measurements. Often the experiment itself on repetition is varying in its measured output. The uncertainties are both numerical and experimental. The experimental setup involves instruments with its own uncertainty and setup which is not as per the ideal conditions like ambient air has varying humidity, composition, etc. Numerical uncertainty is the focus of the present study. The numerical uncertainties of different types are studied, analyzed and quantified accordingly to predict the final uncertainty.

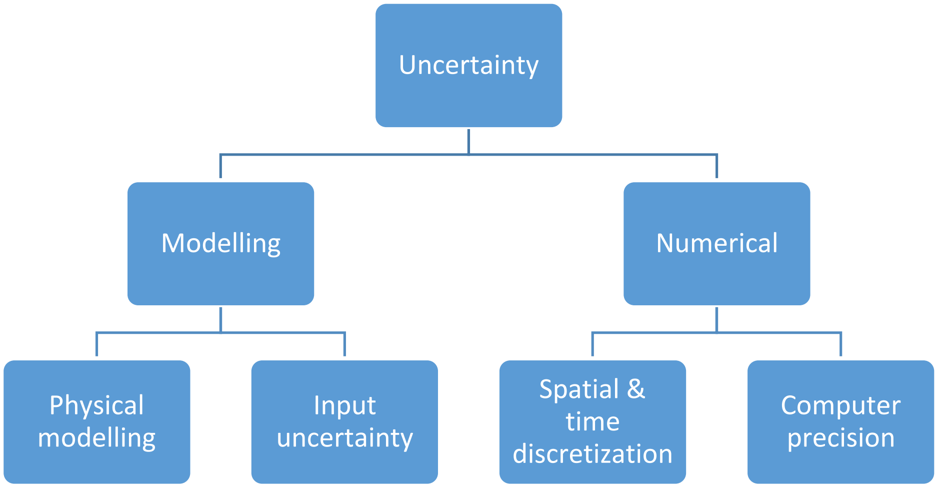


Figure 1. Uncertainty and its categorization

Uncertainty in numerical simulations arise due to two sources [1]:

(a) Modeling errors:

Modelling errors arise due to the assumptions made in representing a particular physical phenomenon in mathematical form. The governing equations inherit assumptions in its derivation as a governing ordinary or partial differential equation. These governing differential equations are numerically discretized and solved, this involves truncating the equations after a particular order, resulting in truncation error. Higher the order lesser is the truncation error.

The input and/or initial conditions are again involving uncertainty in real life as opposed to the fixed values given in the numerical simulations. The geometrical or manufacturing uncertainty of the system under consideration causes the difference in the modelling of the actual experimental setup.

(b) Numerical errors:

Numerical errors arise due to the numerical solution of the mathematical equations. The discretization of the physical equation is performed in any Computational Fluid Mechanics (CFD) problem. It necessarily involves spatial discretization and may also have time discretization for a transient problem. This discretization causes equation to be evaluated at certain discreet points and not exactly in a continuous way, leading to errors which keeps adding up with every iteration.

The computer has its own range for storing the numbers, double precision is a general practice which has the least count of10^{-308}, and the error caused on rounding off also keeps adding up at every iteration. As it can be understood this uncertainty is the most insignificant of all the other sources of uncertainty and hence not included in the present study.

As an example, consider the incompressible Navier Stoke's equation used for a flow over a cylinder problem:-

Navier Stoke's incompressible equation:

$$\rho \frac{\partial u}{\partial t} + \rho(u \cdot \nabla)u - \mu\nabla^2 u = -\nabla P + \rho g \quad (1)$$

Where,

u is the velocity of the fluid,

t is the time,

μ is the dynamic viscosity,

ρ is the density,

P is the pressure,

g is the acceleration caused due to earth

Modelling uncertainty:

1. The equation has an assumption of 'continuum hypothesis' which is applicable when the non-dimensional Knudsen number is less than 1.
2. A first or second order scheme would be used on discretization which would result in the corresponding truncation error.
3. The input flowrate of the fluid and its ambient parameters like temperature, pressure etc. would have uncertainty as opposed to the simulation.
4. The geometry of the cylinder and the boundaries includes the manufacturing tolerances as opposed to the perfect lines and curves in simulation.

Numerical uncertainty:

5. The geometry would be further meshed. The flow field would converge to a particular solution as the mesh gets finer and finer.
6. Same as the mesh size, the flow field would converge to a particular solution as the time stepping keeps on decreasing.

(c) Why Uncertainty in spray like simulations

Spray simulations is composed using coupled Eulerian-Lagrangian approach. The physical equations have continuum assumptions which tend to be invalid as and how the scale of mass, volume etc. decrease. Spray like problems are an involving certain extremes like extreme velocities, pressure and temperature. To compensate, many empirical models are developed which would need fine tuning as per every particular case. This empirical nature further adds to the already caused uncertainties by turbulence model, discretization and input uncertainty. Hence the study is performed involving spray like problem.

2. Literature review

The literature study can be split into two categories, one to understand the spray modelling and the other to understand uncertainty analysis.

(a) Spray modelling:

Rayleigh was a pioneer to understand jet behavior. Since then jet modelling has been studied extensively. The jet is further atomized which is again modelled in many different ways. There are many models developed so far to model different sprays belonging to low or high pressure applications [1][2]. For a high pressure liquid jet the kelvin Helmholtz instabilities are commonly used at the liquid – gas interface [2]. Taylor analogy breakup (TAB) model is also another commonly used model wherein the drop behavior is compared to the spring-mass system [search on net]. The KH wave model is combined with TAB or the newer Rayleigh-Taylor instability model (e.g., Patterson and Reitz [2]). Modifications to these is often the subject of many published studies.

Rietz and Bracco [3] evaluated a number of proposed jet atomization theories. Comparing these with the experimental data they concluded the inadequacy of the models when used alone. They further concluded that the atomization is due to the aerodynamic effect of the gas on the injected liquid as well as nozzle geometry effects. Reitz and Bracco [3] described the aerodynamic interaction between gas and liquid as well as the nozzle geometry effects. They mention briefly the existence of a length of intact liquid near the nozzle of a jet. Hiroyusa [4] experimentally concluded the strong dependence of breakup length on nozzle geometry effects and the velocity.

Intact core modelling is described by Bracco [5]. Reitz and Diwakar [6] simulated the intact core by injecting drops with an initial SMR equal to the effective nozzle radius. As an actual continuous liquid volume cannot be modelled in ‘discrete particle spray models’ instead large closely packed ‘blobs’ were used to represent the intact core. Reitz [7] used the ‘blob’ injection model and incorporated a wave model based on the KH instability to predict secondary drop breakup. Beale and Reitz [8] modelled secondary breakup of the individual drops with Kelvin-Helmholtz model in conjunction with the Rayleigh-Taylor (RT) accelerative instability model. A modification was made to the KH-RT hybrid model that allowed the RT accelerative instabilities to affect all drops outside the intact liquid core of the jet.

(b) Uncertainty analysis:

Numerous papers have appeared in the Computational Fluid Dynamics (CFD) literature addressing the subject of credible CFD simulations [9]–[21]. The AIAA Journal devoted a special section on this topic, one of the aspects being sources of uncertainty. Summary from Oberkampf and Blottner [17] for the source of uncertainty and error in CFD

Source	Examples
Physical Modelling (assumptions in the PDE)	Inviscid flow Viscous flow Incompressible flow Chemical reacting gas Transitional /Turbulent flow
Auxiliary Physical Models	Equation of state Thermodynamic properties Transport properties Chemical models, reactions, and rates Turbulent model
Boundary conditions	Wall, e.g. roughness Open, e.g. far-field Free surface Geometry representation
Discretization & solution	Truncation error – spatial and temporal Iterative convergence – steady state Iterative convergence – time dependent Geometry representation
Round-off error	Finite – precision arithmetic

Table 1 – summary for the source of uncertainty and error in CFD Simulations

Turbulence model, geometric uncertainty and discretization error is found to cause major sources of uncertainty and cause significant scatter of experimental data with reference to simulation [10] .Discretization error has been estimated by various methods (e.g. [23][21]). Grid adaptation use such techniques to improve the base grid. ASME has benchmarked this grid uncertainty [24]and considers this as the standard way to quantify the same. Geometric uncertainties and their effect of output functions have been studied by[25][26]. Michele has modelled geometric parameters as input parameters and studied the propagation of these in the output uncertainties using sensitivity derivatives. Very less work has been carried out for exclusively quantifying the turbulence modelling uncertainty relatively.

Pie and Som [27] studied uncertainty for different output functions of injection sprays. They varied 32 parameters using Monte Carlo technique and identified the sensitive parameters to any specific output function. Further quantification was not carried out though.

The methods to study uncertainty in CFD can further be classified into 4 categories [28]:

(i) Interval analysis

If the parameter is bound to vary but the range is known, a simple technique can be used to assess the range of output function. All the probable values are simulated and the maximum and minimum of the output function is the range for uncertainty caused by the given uncertainty in the input parameter.

(ii) Propagation of error using sensitivity derivatives

The output function under consideration can be seen as a function of several parameters including the ones involving uncertainty. If the function is continuous with respect to the parameter, it can be approximated with the Taylor series in the uncertain domain thus estimating the propagated uncertainty to the output.

If u is a fnction of ξ_i where ξ_i is the ith independent variable with error $\Delta\xi_i$ associated with it then a deterministic approximation given to the error is Δu,

$$\Delta u = \left[\sum_{i=1}^{n} \left(\frac{\partial u}{\partial \xi_i} \right)^2 \Delta_{\xi_i}^2 \right]^{\frac{1}{2}}$$

(iii) Monte Carlo

For a multivariate problem, (like Pie and Som [27]), to study statistically the output dependence on the different input parameters Monte Carlo method is very helpful. It most importantly helps to maintain the input distribution as equally scattered and equally probable as possible. It is basically a tool to improve quality of statistical analysis while minimizing the computational cost inquired.

Basic procedure consists of:

1. Sample input random variables from their known or assumed probabilities
2. Compute deterministic output for each input
3. Determine statistics of the output distribution, i.e. mean variance, skewness

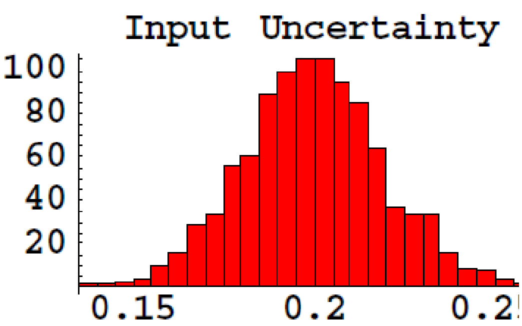


Figure 2– example input uncertainty

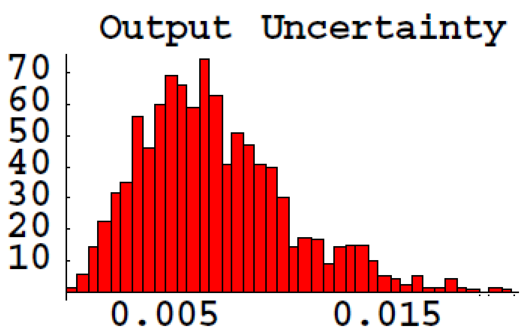


Figure 3 - example output uncertainty

(iv) Moments method

Statistical determination of the error due to truncation of the Taylor series is the Moments Method. It is a statistical method which estimates the variance in the output from the variance in the input which is a function of the derivatives of the output with respect to the inputs.

For example consider a function $u(\xi)$ expanded about the point$(\bar{\xi})$:

First order accurate approximation

$$E_{FO}[u(\xi)] = u(\bar{\xi})$$

Second order accurate approximation

$$E_{SO}[u(\xi)] = u(\bar{\xi}) + \frac{1}{2} Var(\xi) \frac{\partial^2 u}{\partial \xi^2} |_{\bar{\xi}}$$

First order accurate approximation of the variance

$$Var_{FO} u[(\xi)] = \left(\frac{\partial u}{\partial \xi} |_{\bar{\xi}} \right)^2 Var(\xi)$$

Second order accurate approximate of the variance

$$Var_{SO}[u(\xi)] = \left(\frac{\partial u}{\partial \xi} |_{\bar{\xi}} \right)^2 Var(\xi) + \frac{1}{2} \left(\frac{\partial^2 u}{\partial \xi^2} |_{\bar{\xi}} Var(\xi) \right)^2$$

3. Scope and specifications of the study

(a) Essentials

The Solver needs to be tested for against an experimentally quantified problem. This establishes the solver credibility. The solver inherently may have sources of error and hence this needs to be assessed beforehand. The empirical nature of spray simulations need a tuning of the hydrodynamic constants to get the flow as per the experimentally measured data. Ansys Fluent v13 was used in this study. Experimental data for dodecane spray under “Spray-A” condition provided on Engine Combustion Network (ECN) website (http://www.sandia.gov/ecn/) was used for validation.

To have consistency of results all the study was conducted on the v13 as a version change also reflected in sharp deviations from the experimental data or in other words needed redoing the tuning of the hydrodynamic constants.

System Configuration:

The system as 6 Giga Byte Random Access Memory, 64 bit Intel Zeon quad core processor. With all the simulations running on double precision accuracy.

(b) Problem description

Transient CFD simulations to perform and calculate the penetration length of liquid and vapor spray. A 50mm x 50 mm x 100mm cube is the control chamber which is uniformly meshed for cell sizes of 1mm x 1mm x 1mm. The liquid penetration length is estimated by the length from the nozzle tip such that 90% of the ejected mass is contained within. The vapor penetration length is the farthest length containing all the vapor from the nozzle tip. No slip boundary condition on all the walls and pressure outlet condition on the exit

- Injection was carried out for 1 ms
- Injected fuel mass flow rate and velocity was determined from the data provided on the ECN website
- Liquid penetration length and vapour penetration length were used to characterise the spray
- Liquid penetration length was defined as the average liquid length achieved between 0.8 – 1.0 ms

- Vapour penetration length was defined as the vapour length achieved at 1 ms

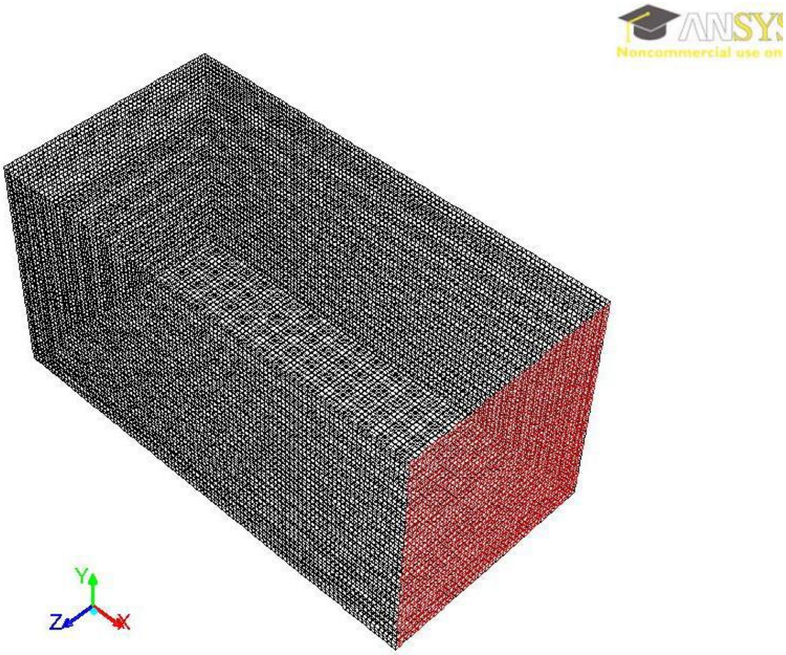


Figure 4 – Control volume of the spray chamber

Parameter	Value
Time of injection	1 ms
Mass of fuel injected	3.5 g
Nozzle diameter	0.1 mm
Fuel inlet temperature	363 K
Ambient temperature	900 K
Ambient pressure	6 MPa
Cone angle	8.7º

Table 2 – specifications of the simulation

(c) KH-RT parameters

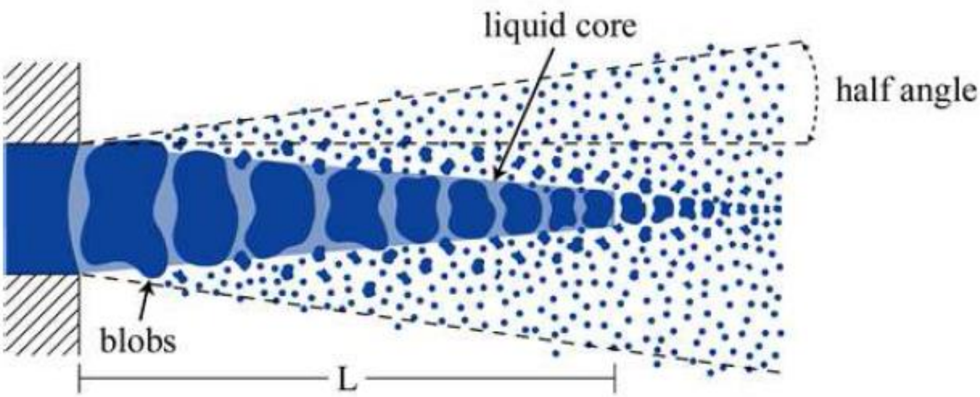


Figure 5 – Jet breakup

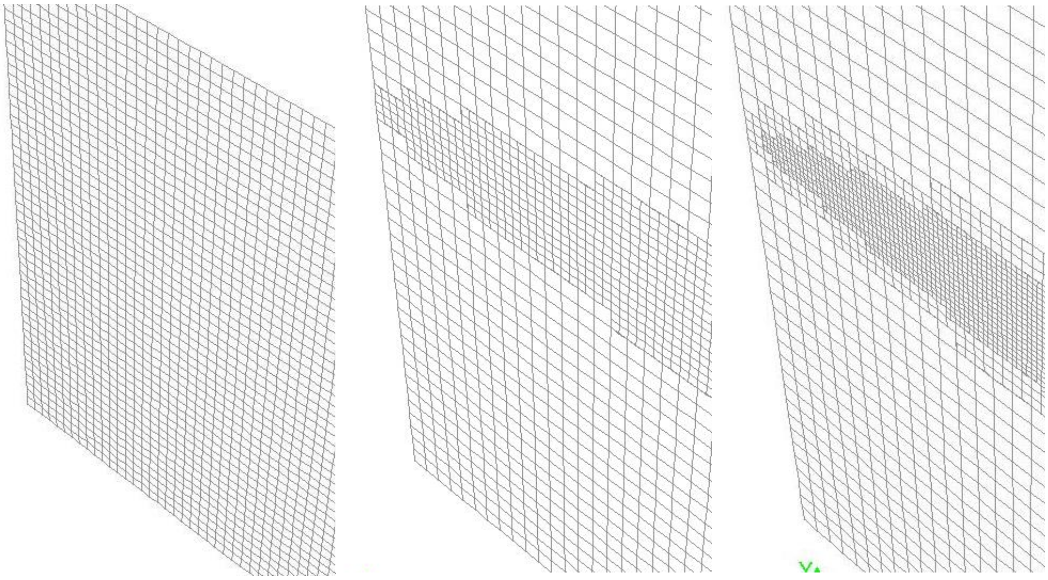
- KH-RT model is a hybridization of two breakup models – primary breakup of the incoming blobs and secondary forming the child drops.
- It assumes that a liquid core exists in the near nozzle region
- Droplet breakup within liquid core is due to aerodynamic breakup which is described by Kelvin-Helmholtz instability
- Child droplets are shed from the liquid core
- Rayleigh-Taylor instability is dominant on these child droplets when subjected to sudden acceleration

B_o	$r_c = B_0\varphi_{KH}$	Child radius for KH instability
B_1	$\tau_{KH} = \frac{3.726B_1 r}{\omega_{KH}\varphi_{KH}}$	Time constant for KH
C_τ	$\tau_{RT} = \frac{C_\tau}{\omega_{RT}}$	Time constant for RT
C_{RT}	$r_c = \frac{\pi C_{RT}}{K_{RT}}$	Child radius for RT instability
C_l	$L_b = C_b d_0 \sqrt{\frac{\rho_f}{\rho_a}}$	Liquid core length

Table 3 – KH-RT parameter and significance

- The length of the liquid core is obtained from Levich theory.
- Where φ_{KH} is the wavelength corresponding to the KH wave with the maximum growth rate ω_{KH} , which are functions of surface tension, density, temperature, weber and Re number and orifice diameter.
- ω_{RT} is the frequency of fastest growing wave in the RT model wave instability which is a function of surface tension, densities and acceleration.
- K_{RT} is the corresponding wave number.

(d) Adaptive Mesh refinement (AMR)



Refinement level-0 Refinement level-1 Refinement level-2

Figure 6 – AMR refinement

The jet like spray is highly dynamic in nature. The droplets vary significantly in sizes and keep varying dynamically.

As and how the grid size decreases the final output, liquid and vapour penetration length also converge. At the same time the refined mesh proportionately increase the time taken to compute as the number of cells it needs to perform computation on increases.

Adaptive mesh refinement is a smart solution for the same. It can intelligently refine mesh only where required for each time step. The criteria for defining need of refinement can be gradient of any property like density, temperature etc. In the spray like simulations it is appropriate to use gradient of the density. The present study refines the mesh if the gradient is more than 0.2 and coarsens the mesh if it is less than 0.05.

Fluent v13 has two options to control the mesh refinement dynamically. The first one is to limit the number of refinement levels and the other is to limit the least cell volume that can be allowed before refinement. As the study involves uncertainty in output function due to mesh refinement it is binding to understand the software's algorithm on performing AMR. The following figure describes the same.

Algorithm:

1. **Check for Dynamic mesh enable**
2. **If yes check for minimum cell volume**
3. **If no then no refinement.**
4. **If yes then check for the maximum level of refinement**
5. **If maximum level not reached then refine further.**
6. **If the maximum level reached already then stop further refinement**

Thus it can be seen that the final refined least cell volume might be less than the minimum cell volume specified.

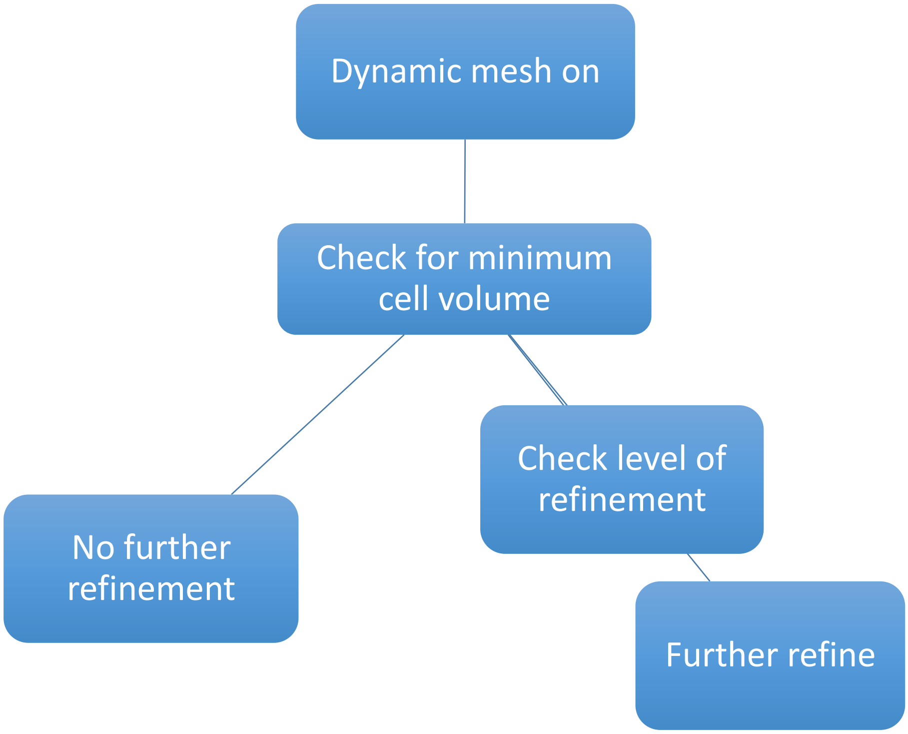


Figure 7 – Fluent v13 refinement algorithm

(e) Nominal case

A 50x50x100mm parallelepiped was meshed for 1x1x1mm cell size. The resultant is a quarter million cell mesh. This is the base mesh for the simulation. The injector model was used from ‘define’ utilities. The nozzle is positioned at 1 mm from the inlet and along the z axis. The material properties used for Dodecane have been extensively gathered from Perry’s handbook and other sources mentioned in appendix -1. AMR is further used over the geometry

The problem was modelled in Ansys fluent v13 as mentioned previously. Second order upwind schemes in solution methodologies. And 50 iterations per time step. The KH-RT parameters were fine tuned to get the output as close to the experimental data as possible.

- Rectangular cross-section of 50mm×50mm and 100mm length
- Baseline mesh of 1×1×1 mm^3
- Two levels of Adaptive Mesh Refinement (AMR) based on vapour concentration gradient
    - Min. cell size 0.25×0.25 ×0.25 mm^3
- Time step size $\Delta t = 1 \times 10^{-6}$ sec
- k-ε turbulence model

B_o	0.2	0.8
B_1	5	80
C_τ	0.5	1.5
C_{RT}	0.05	0.15
C_l	5	80

Table 4 – KH-RT parameters with their range for tuning

The liquid penetration length increases initially and stays more or less constant thereafter. Vapour penetration length though continuously increases as the liquid is constantly vaporising and adding to the total vapour content.

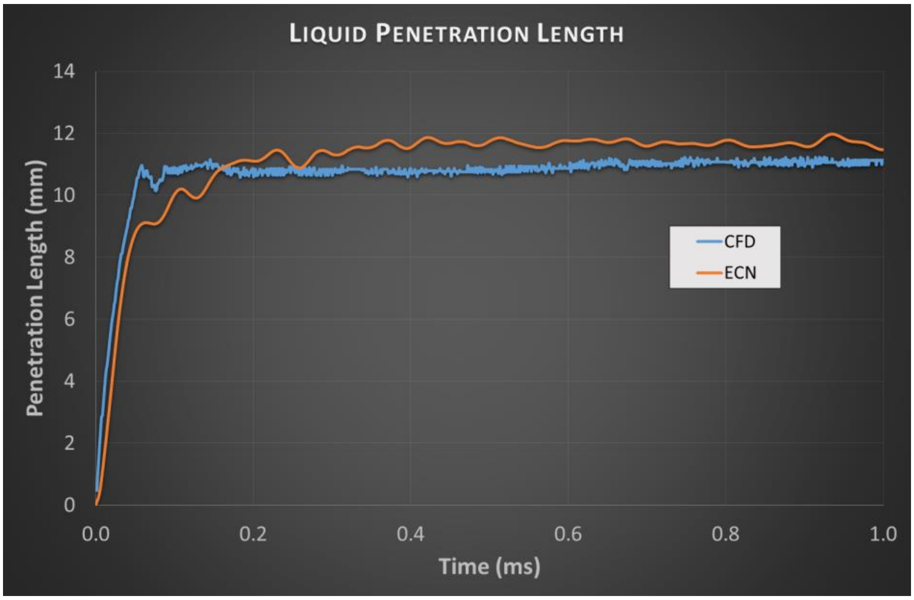


Figure 8- Liquid penetration length vs time for the nominal case and ECN

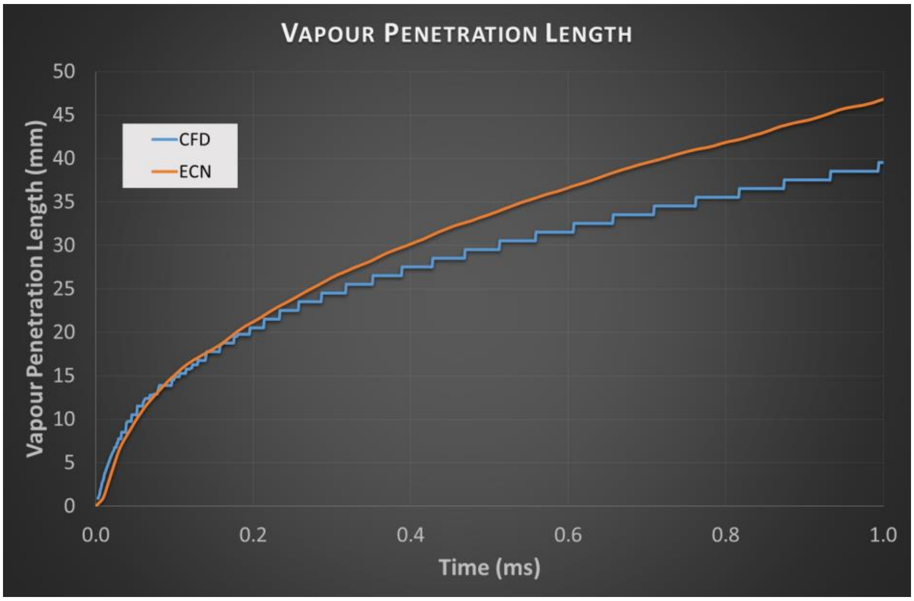


Figure 9-Vapor penetration length vs time for the nominal case and ECN

Penetration Length	ECN (mm)	CFD (mm)	% Error
Liquid	11.68	11.07	- 5.22%
Vapour	46.81	39.5	- 15.61%

Table 5 – Nominal simulation results

B_o	0.6
B_1	20
C_τ	1
C_{RT}	0.1
C_l	20

Table 6– KH-RT parameters after tuning

The results are in close agreement with that of the experimental data and thus this set of input was finalized as the nominal case for the study. All the uncertainty calculations are with respect to this benchmarked results.

4. Uncertainty quantification methodology

The objective of the study is to quantify the uncertainty that may be found from an actual experimentally measured quantity compared to the predicted numerical simulation value. At the same time we need to keep in mind the time intensive nature of the 'numerical prediction'. The methodology evolved over the period of study. Some mistakes helped further improvise on the methodology to make it robust in nature for future implementation on any other CFD problem.

(a) Initial approach:

The study involved a 3 step approach:-

- Identify the parameters to perform uncertainty analysis.
- Perform a Monte Carlo methods study.

(b) Identify the parameters –

The physical problem at hand, spray simulation of diesel like fuels, was studied and existing significant dependence of the desired output, liquid and vapor penetration length, on the many parameters input to the simulation were considered in identifying the parameters to be studied for. The limits of the same were as per the existing research had been carried on over. If no exact range was found a 10% limit above and over the nominal value was considered in th study. The parameters were considered based on the classification of the uncertainty in CFD. The modelling uncertainty in this study is comprised primarily from the turbulence models used and the KH-RT spray modelling. The input uncertainty is caused by the input parameters namely temperature and pressure of the chamber, injector temperature, cone angle of the injector, mass flow rate of the spray. The discretization errors due to the spatial and time discretization. All of the parameters were considered for the next stage of study.

1	**Turbulence**	$k - \in$
2		$k - \omega$
3		RNG
4		RSM
5	KHRT	B_0
6		B_1
7		C_τ
8		C_{rt}
9		Cl
10	Time	dt
11	Grid	AMR
12	Input uncertainties	Inlet temp
13		Inlet Mass flow rate
14		Inlet pressure
15		Cone angle

Table 7 - the parameters included in the study

(c) Monte Carlo methods study –

(i) Introduction to Monte Carlo methods

Monte Carlo methods (or Monte Carlo experiments) are a broad class of computational algorithms that rely on repeated random sampling to obtain numerical results. They are often used in physical and mathematical problems and are most useful when it is difficult or impossible to use other mathematical methods. Monte Carlo methods are mainly used in three distinct problem classes: optimization, numerical integration, and generating draws from a probability distribution (as in this study).

(ii) Requirement for Monte Carlo Methods

The problem at hand has multiple parameters to study for uncertainty. Uncertainty can be estimated by knowing the gradients of the physical problem by relating variance in the output as a function of the input variance and its gradients. But as we don't have gradients from a governing equation we need to calculate the gradients numerically i.e. perturbing the simulations and calculating the gradient based on the difference in the input and output values.

The parameters need to have as many points equally distributed among the domain to perturb to get better numerically approximated gradients over the domain. Also the multiple parameters arise accordingly many permutations and combinations in the domain. For example a 5 parameter set with 5 points each in the perturbing domain would result in 5^5 which is 3125 combinations to simulate. Since the time required for each simulation is 10 hours approximately on the system configuration mentioned in the previous chapter, 3125 simulations would require around 31250 hours which is close to 3.56 years for a single system to carry out. Hence we need to reduce the number of simulations with keeping the distribution as equally spaced as possible. Monte Carlo methods fulfill these requirements and hence used for the study.

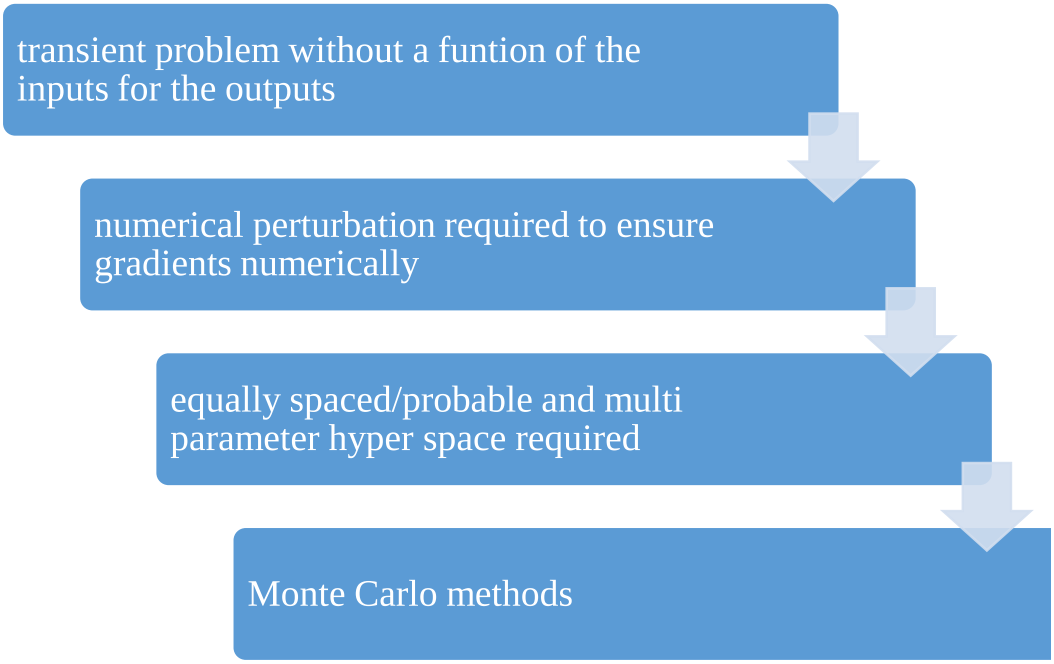


Figure 10 - Need for Monte Carlo Methods

(iii) Procedure to generate the Monte Carlo distribution –

A code was developed to generate equally probable and equally distributed sample space. The following example illustrates the process:-

Example: A random distribution of 50 samples between 5 and 80 is required for the parameter C_l

1. The code is given the 4 values namely, lower bound, higher bound, the sample size required and the number of discrete points the sample has to be divided into. If no discrete distribution required then the sample size can be entered as the number of discrete points required.
2. The sample is then divided into the discrete values based on the number of intervals required, in this case the sample would be generated by dividing 5 to 80 into 50 values including 5 and 80.
3. Each of the values is assigned a value from 1 to 50 (number of samples)
4. A random generator 'rand' built in Matlab 2013b is used to generate a random number 0 to 1 which is then multiplied by 50 (sample size)
5. The number corresponding to this number is taken as the final sample input.
6. If the number has already been taken as input the random number generator is called again.
7. After 50 (sample size) inputs are generated the code ceases.

If the number of discrete values is less than that of the sample size multiple copies are generated. For example if 50 sample inputs of 5 discrete values is required, then 5 copies of each input would be generated each assigned a value from 1 to 50. If it isn't a perfect multiple, then a rough spread is maintained over the range. For example 53 samples are required from 5 discrete values, then 6 copies of 1st, 3rd and 5th value would be generated and 5 copies of 2nd and 4th value each assigned a value from 1 to 53.

A key feature is the non-repeatability of the spread i.e. every single time we run the code we get a different combination of the sample

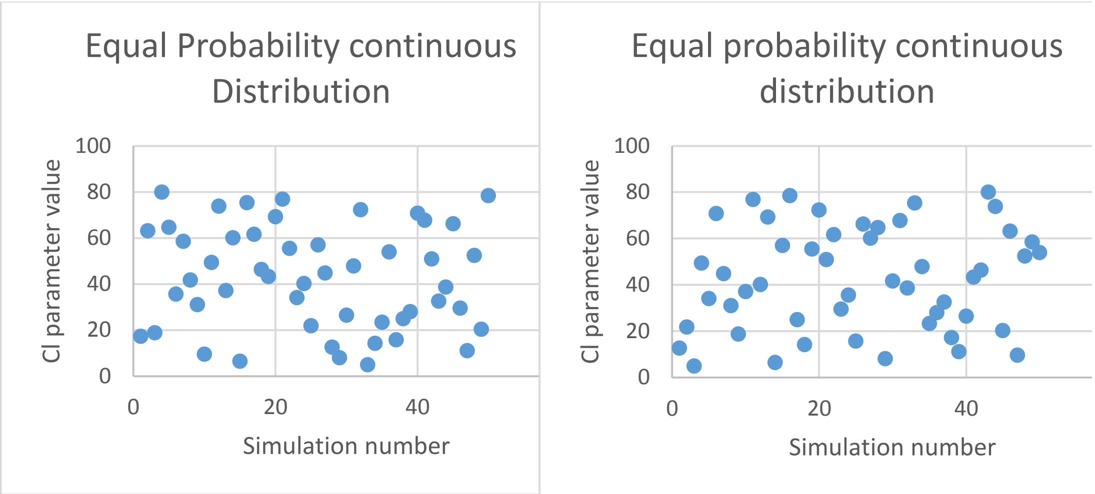


Figure 11 - Different pattern generated on repetition of the code for equal probability continuous distribution

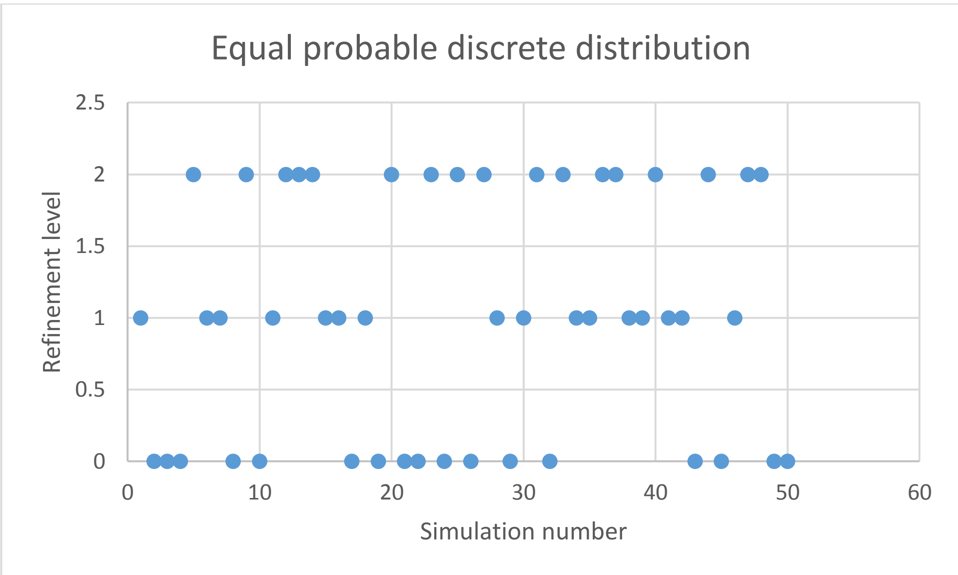


Figure 12 - pattern generated by the code for equal probability discrete distribution

(d) Need for improvisation

During the study the above procedure was undertaken. The 15 parameters where considered for the study. Accordingly the code was used to generate the Monte Carlo based samples. The simulation would take anywhere between 10 minimum (no other computational process ongoing on the system) to 48 hours (heavy computation running parallel). Thus the study was considered to be carried out only for 50 samples.

The parameter to simulation ratio was nearly 1:3.33 (15 parameters and 50 simulations). There was no empirical thumb rule found in literature for the threshold ratio required. The ratio seemed quite inadequate though. Also the number of simulations may need to vary dynamically, i.e. the number of simulations may be increased later or the 50 simulations may not be possible to simulate in time. Also the manual process of changing each parameter for every simulation had an inherent error possible due to human error.

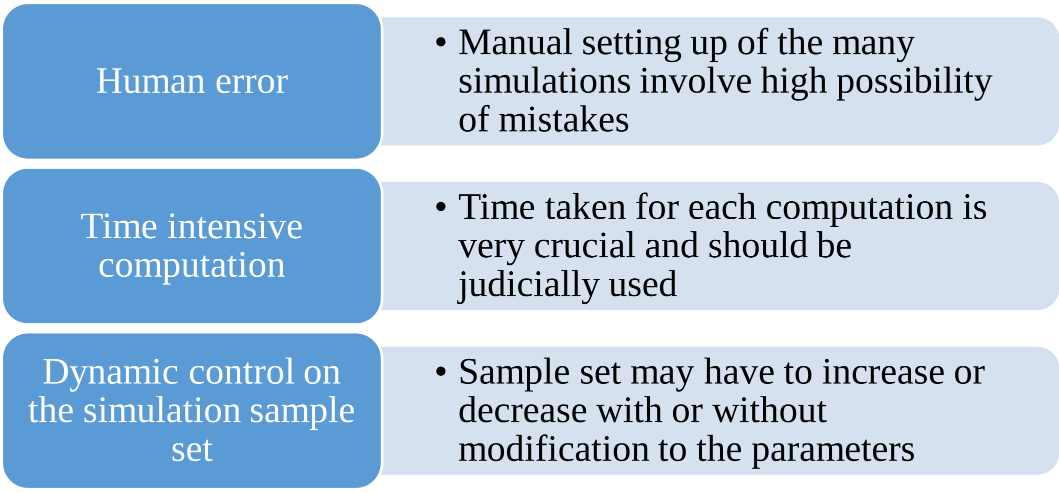


Figure 13- Considerations for the study

(e) Improvisations

The considerations were individually addressed. As the objective of the study is to establish a standard methodology for estimating uncertainty in CFD applications, a robust methodology is very much required. Three of the improvisations made are as follows:

(i) Automation

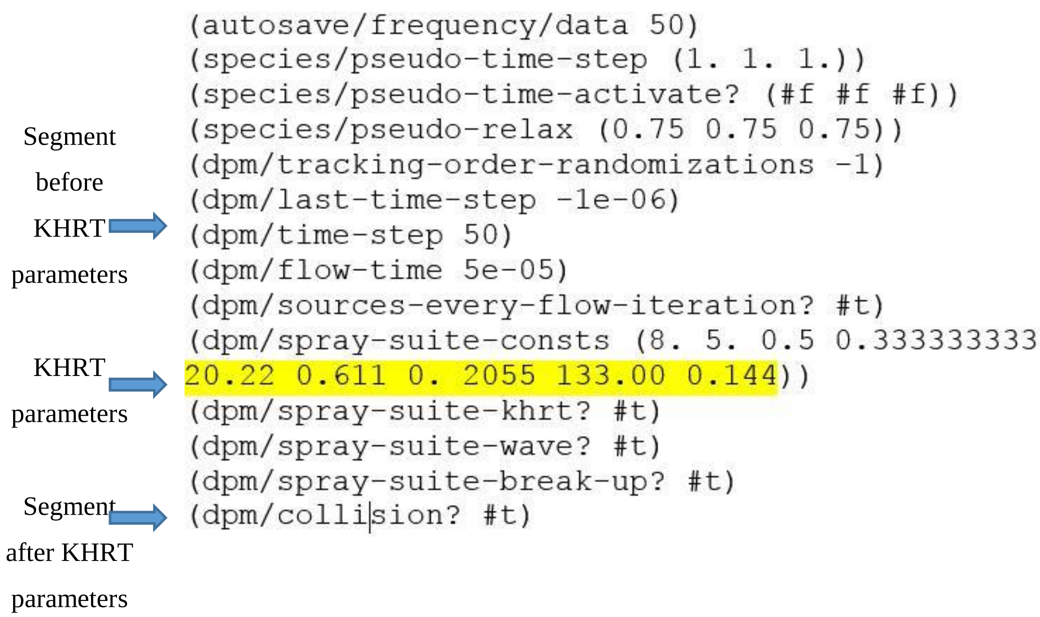


Figure 14 -automatic file stitching

Ansys Fluent v13 has a feature of ‘input boundary condition’ file which is basically recording all the input values given for the case to be simulated in a text file. This file can be generated for the simulation and saved onto the workspace. The input file can be edited manually or by a program, which on reading by the Ansys Fluent v13 would accordingly reflect upon the changes.

1) The code for automation uses the input file generated from the nominal case file.
2) The parameters in the study are located on the input file.
3) The input file is sliced into various segments leaving the parameters value.
4) The segments are read by a code and pasted in a new file one after the other with every value being written in between the segments.

Thus the format is maintained with modified values for each case. This input file is used as input for all the simulations to perform.

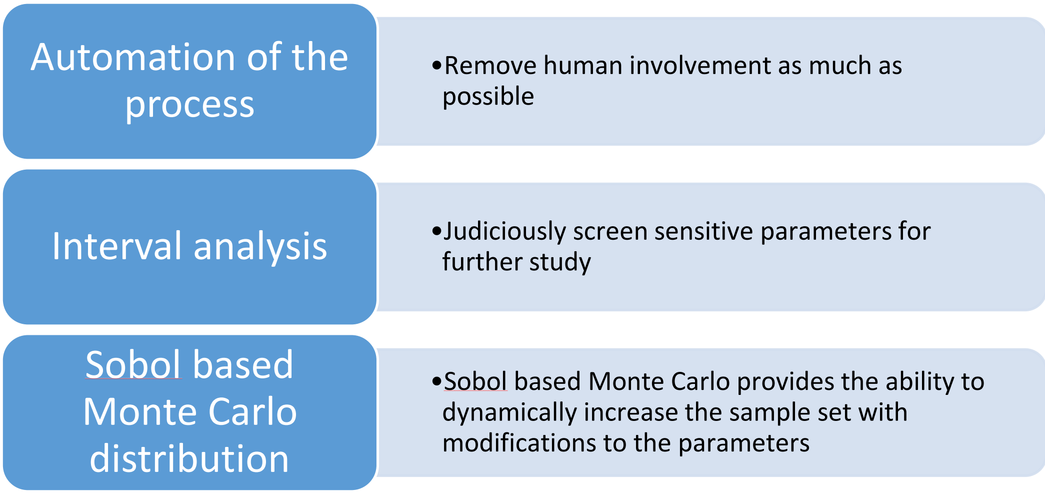


Figure 14 - Improvisations in the study

(ii) Interval Analysis

The ratio of parameter to number of simulations can be improvised if we focus on the parameters which are sensitive to the concerned output. This can be estimated by individually perturbing he parameters one after another, keeping all the rest constant. Interval Analysis has been used in uncertainty estimation of CFD applications. The interval analysis is basically a tool which can be used to estimate the maximum and minimum value of the output for the entire range of inputs available. All the possible values the input can take is simulated and output of all is recorded. The maximum and minimum among these is the interval for the output function to take.

The parameters were then decided to be perturbed individually by a constant deviation of 10% from the nominal value. Parameters from each type of uncertainty namely, modelling, input and discretization were to be shortlisted for further Monte Carlo methods.

(iii) Sobol based Monte Carlo Methods

Sobol sequences (also called LPτ sequences or (t, s) sequences in base 2) are an example of quasi-random low-discrepancy sequences. They were first introduced by the Russian mathematician I. M. Sobol in 1967. Low-discrepancy sequences are also called quasi-random or sub-random sequences, due to their common use as a replacement of uniformly distributed random numbers.

The discrepancy of a sequence is low if the proportion of points in the sequence falling into an arbitrary set B is close to proportional to the measure of B, as would happen on average (but not for particular samples) in the case of an equidistributed sequence. Specific definitions of discrepancy differ regarding the choice of B (hyperspheres, hypercubes, etc.) and how the discrepancy for every B is computed (usually normalized) and combined (usually by taking the worst value).

Key feature of Sobol sequence for which it is incorporated are:

1) Constant values on every time we generate the sample.

The code used in the study is built in function of Matlab 2013 named 'sobolset(input number of parameters)'. The function gives a point to the set of values generated by the Sobol method. From which the required amount of values can be recorded. These values remain constant every time we generate the values.

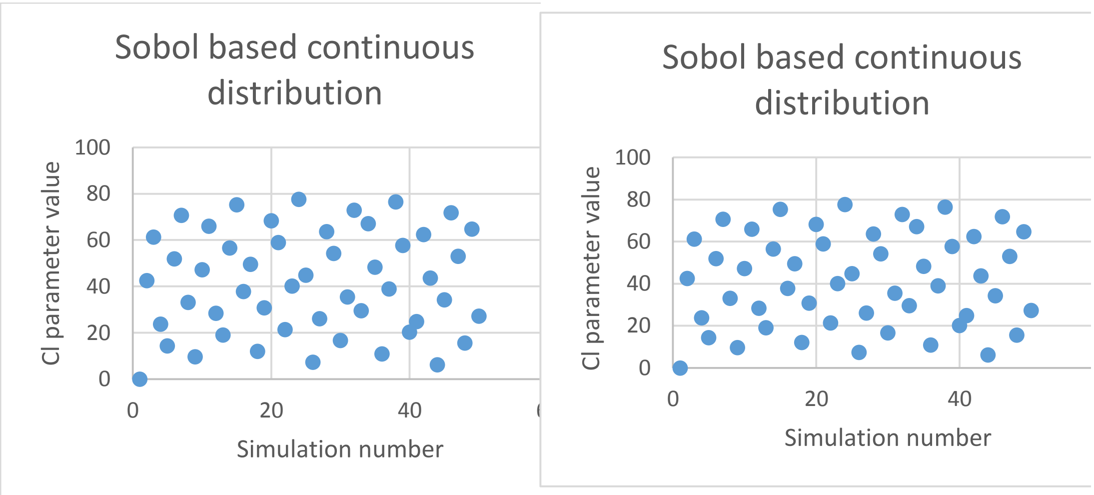


Figure 15- Same distribution on repetitive use of Sobol sequence

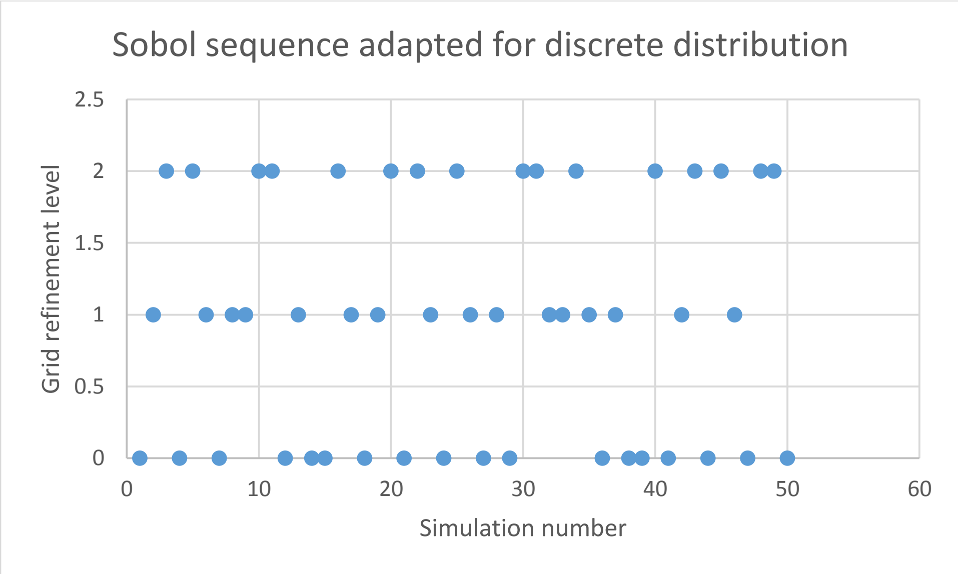


Figure 16 - Pattern when Sobol sequence adapted for discreet distribution

2) Low discrepancy distribution

The distribution tends to be distributed equally more or less. This doesn't depend on the number of samples taken. The more the sample size the more is it equally distributed. Morris and Mitchell developed a method to quantify the distribution of the sample termed as "mmphi index". The smaller the index the better is the distribution. The Sobol based distribution lowers the mmphi index significantly as can also visually experienced.

Mmphi index = 429.2955

*normalized for the range (0,1)

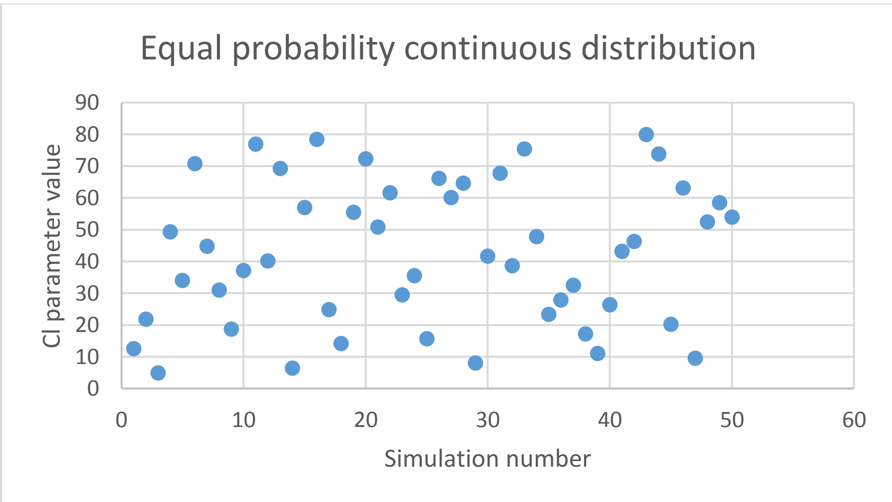


Figure 17 - mmphi index for equal probability continuous distribution

Mmphi index = 485.4272

*normalized for the range (0,1)

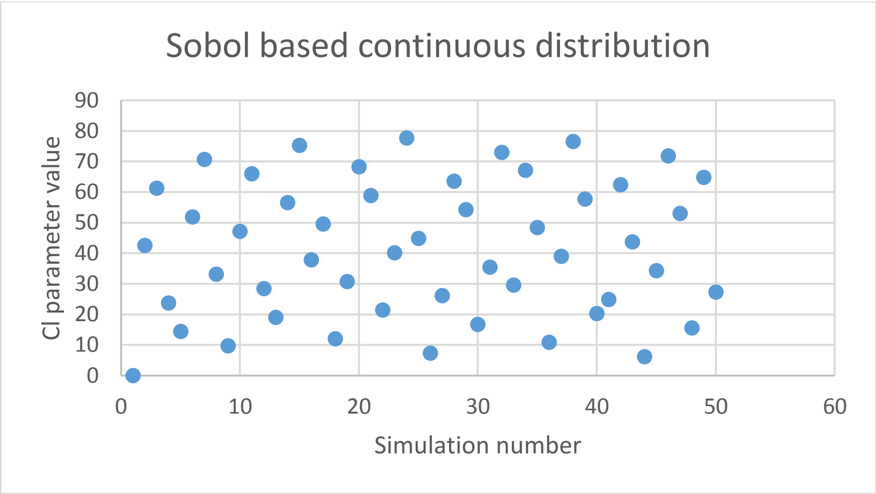


Figure 18 - mmphi index for Sobol continuous distribution

The inputs should be taken from the start of the Sobol sequence to the number of inputs required. For the above two requirements to hold consistent.

(f) Moments Method

Statistical determination of the error due to truncation of the Taylor series is the Moments Method. It is a statistical method which estimates the variance in the output from the variance in the input which is a function of the derivatives of the output with respect to the inputs.

For example consider a function $u(\xi)$ expanded about the point $(\bar{\xi})$:

- First order accurate approximation

$$E_{FO}[u(\xi)] = u(\bar{\xi})$$

- Second order accurate approximation

$$E_{SO}[u(\xi)] = u(\bar{\xi}) + \frac{1}{2}Var(\xi)\frac{\partial^2 u}{\partial \xi^2}|_{\bar{\xi}}$$

- First order accurate approximation of the variance

$$Var_{FO}u[(\xi)] = \left(\frac{\partial u}{\partial \xi}|_{\bar{\xi}}\right)^2 Var(\xi)$$

- Second order accurate approximate of the variance

$$Var_{SO}[u(\xi)] = \left(\frac{\partial u}{\partial \xi}|_{\bar{\xi}}\right)^2 Var(\xi) + \frac{1}{2}\left(\frac{\partial^2 u}{\partial \xi^2}|_{\bar{\xi}} Var(\xi)\right)^2$$

For a similar Multivariate problem it would be:

- For first order accurate approximations

$$E_{FO}[u(\xi_1, \xi_2)] = u(\overline{\xi_1}, \overline{\xi_2})$$

- First order accurate approximation of the variance

$$Var_{FO}[u(\xi_1, \xi_2)] = \left(\frac{\partial u}{\partial \xi_1}|_{\bar{\xi}_1}\right)^2 \sigma_{\xi_1}^2 +$$

$$\left(\frac{\partial u}{\partial \xi_2}|_{\bar{\xi}_2}\right)^2 \sigma_{\xi_2}^2 + 2\left(\frac{\partial u}{\partial \xi_1}|_{\bar{\xi}_1}\right)\left(\frac{\partial u}{\partial \xi_2}|_{\bar{\xi}_2}\right)$$

The Variance being the final band of uncertainty. Thus the Moments method is the last step in estimation of the uncertainty. The problem existing though is that there is no direct governing function between the input and the output. The gradients can be estimated numerically though. The study uses least squares fit method to acesses the gradients.

(g) Modified least square fits

The method of least squares is a standard approach in regression analysis to the approximate solution of overdetermined systems, i.e., sets of equations in which there are more equations than unknowns. "Least squares" means that the overall solution minimizes the sum of the squares of the errors made in the results of every single equation.

The most important application is in data fitting. The best fit in the least-squares sense minimizes the sum of squared residuals, a residual being the difference between an observed value and the fitted value provided by a model. When the problem has substantial uncertainties in the independent variable (the x variable), then simple regression and least squares methods have problems; in such cases, the methodology required for fitting errors-in-variables models may be considered instead of that for least squares.

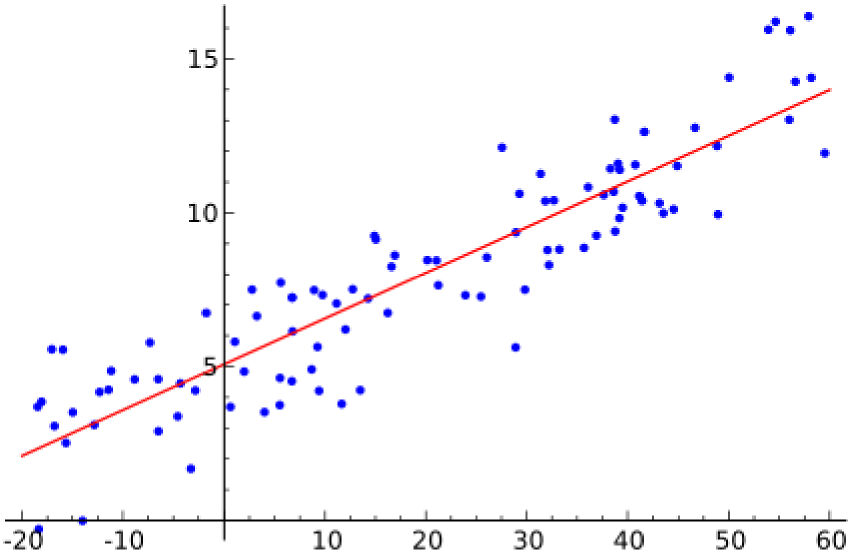


Figure 19– linear least square fit through randomly generated data (source: internet)

As the study has 7 parameters to study uncertainty for the minimizing second order function according to standard least square fit technique is:

$$\Sigma j = 1: (sample\ size) \left(V_j - \Sigma i = 1: 7\left(a_{ij}x_{ij} + b_{ij}x_{ij}^2\right)\right)^2$$

Where,

$$a_{ij} = f',\ b_{ij} = \frac{f''}{2!}$$

The study at hand has a complexity of two sets of parameters:

1. Continuous domain interval (KH-RT parameters, temperature, pressure)
2. Discreet domain interval (AMR refinement level, turbulence model, time stepping,)

The continuous domain interval could be easily estimated with a standard least square approach whereas the discreet domain cannot as there is no physical significance for derivatives in that case. Hence the need to modify the least square fit to accommodate the discreet domain. The modification assigns a constant value to each of the possible discreet values.

Minimizing function modified accordingly is then:

$$\Sigma j = 1:(sample\ size)\begin{pmatrix} V_j - \Sigma i = 1:4\left(a_{ij}x_{ij} + b_{ij}x_{ij}^2\right) + \\ ((C_1 + C_2 + C_3)|_{turb} + (C_4 + C_5)|_{mesh} + C_6|_{\Delta t} \end{pmatrix}^2$$

C_1	k-ω turbulence model
C_2	RNG k-ε turbulence model
C_3	RSM turbulence model
C_4	Level 0 mesh refinement
C_5	Level 1 mesh refinement
C_6	$\Delta t = 10^{-5}$ sec

This equation is then repeatedly differentiated with respect to every unknown parameter in the equation and equated with zero, thus resulting in:

10 unknowns & 10 equations	-For 1st order least square fit
14 unknowns & 14 equations	-For 2nd order least square fit
18 unknowns & 18 equations	-For 3rd order least square fit
26 unknowns & 26 equations	-For 5th order least square fit

These set of simultaneous linear equations are then solved to estimate the gradients and constants.

These gradients are later then used in the Moments Method to estimate the Uncertainty.

5. Results and discussions

(a) Sensitivity analysis

To reduce the parameters studied in the extensive probabilistic approach the Interval study is carried out. The sensitivity is then estimated from the same. The sensitivities are calculated with respect to the nominal value. For parameters other than the discreet values 10% deviation in the input was carried out. The higher bound is the nominal +10% value and the lower bound is the nominal -10% value. Sensitivity is calculated as follows:

$$S = \frac{Output\ value - (nominal\ output\ value)}{nominal\ input\ value} \Bigg/ \frac{Input\ value - (nominal\ input\ value)}{nominal\ outut\ value}$$

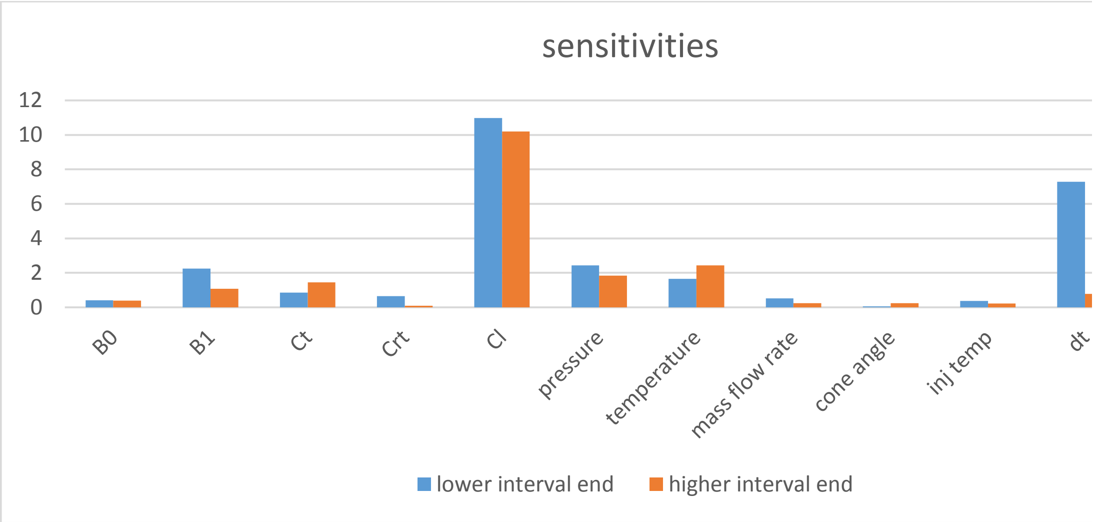


Figure 20 – Liquid penetration length sensitivity with respect to the parameters

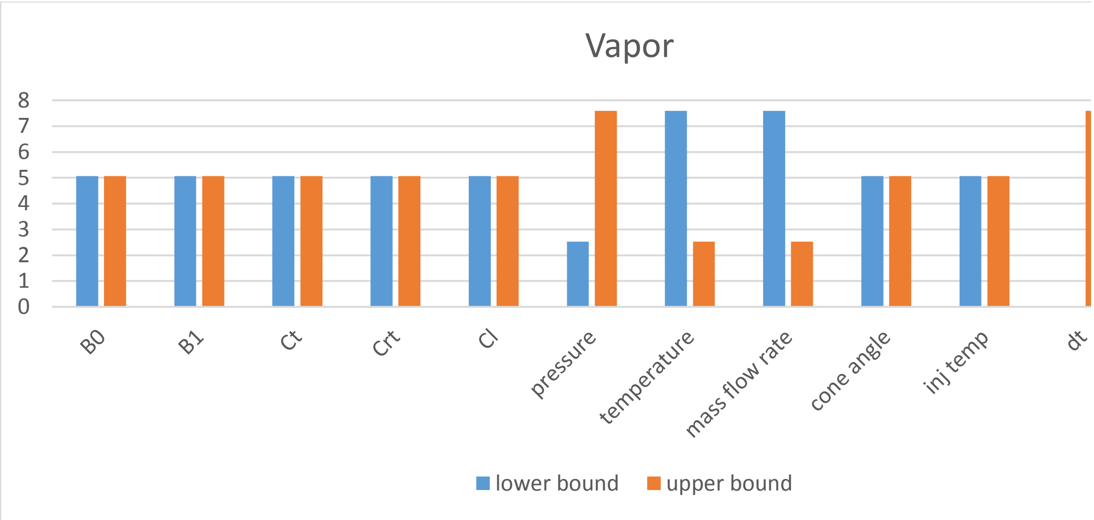


Figure 21 – Vapor penetration length sensitivity with respect to the parameters

Based on the Interval study six parameters were screened for a further analysis using Monte Carlo simulations with 4 turbulence models added as the seventh parameter.

1. B_1
2. C_L
3. Ambient Temperature
4. Ambient pressure
5. Mesh size
6. Time step size
7. Turbulence models

(b) Sobol based Monte Carlo Methods

The screened seven parameters are now generated using Sobol based Monte Carlo sampling. A sample set of 50 values was generated and executed the simulation run. On which 47 converged and 3 diverged. The intervals for the KH-RT inputs is set as the domain encompassing all the range found in literature for the same. For the input parameters approximate range was specified. For the discreet valued parameters the discreet values itself as range were taken.

#	Name	Lower limit	Upper limit
1	Model	1	4
2	B1	5	80
3	Cl	5	80
4	Pressure	5MPa	7MPa
5	Temperature	800 Kelvin	1000 Kelvin
6	Grid refinement	0 level	2 level
7	Time stepping	1.00E-05	1.00E-04

Table 8 – Limits for each parameter for the Sobol based Monte Carlo study

The inputs are as follows:

#	Input							Output	
	Model	*B1*	*Cl*	*pressure*	*temperature*	*AMR*	*dt*	*Liquid penetration length*	*Vapor penetration length*
1	1	5	5	5400000	810	0	1.00E-05	3.69E-03	4.25E-02
2	3	42.5	42.5	6000000	900	1	1.00E-06	2.327E-02	3.15E-02
3	2	23.75	61.25	6300000	855	2	1.00E-06	3.25E-02	4.68E-02
4	3	61.25	23.75	5700000	945	0	1.00E-05	1.40E-02	3.05E-02
5	1	70.625	14.375	6150000	967.5	2	1.00E-05	8.37E-03	4.55E-02
6	3	33.125	51.875	5550000	877.5	1	1.00E-06	2.04E-02	2.95E-02
7	2	51.875	70.625	5850000	922.5	0	1.00E-06	4.26E-02	4.93E-02
8	4	14.375	33.125	6450000	832.5	1	1.00E-05	1.87E-02	4.65E-02
9	1	56.5625	9.6875	5475000	843.75	1	1.00E-05	5.64E-03	4.45E-02
10	3	19.0625	47.1875	6075000	933.75	2	1.00E-06	1.51E-02	2.55E-02
11	2	75.3125	65.9375	6375000	888.75	2	1.00E-06	3.62E-02	5.15E-02

12	1	28.4375	19.0625	6225000	956.25	1	1.00E-05	1.03E-02	4.65E-02
13	3	65.9375	56.5625	5625000	866.25	0	1.00E-06	2.84E-02	3.55E-02
14	2	9.6875	75.3125	5925000	911.25	0	1.00E-06	3.43E-02	5.15E-02
15	4	47.1875	37.8125	6525000	821.25	2	1.00E-05	2.02E-02	4.85E-02
16	1	35.46875	49.53125	5962500	973.125	1	1.00E-06	2.87E-02	3.65E-02
17	3	72.96875	12.03125	6562500	883.125	0	1.00E-05	6.44E-03	2.35E-02
18	2	16.71875	30.78125	6262500	928.125	1	1.00E-05	2.85E-02	5.45E-02
19	4	54.21875	68.28125	5662500	838.125	2	1.00E-06	3.49E-02	4.65E-02
20	1	44.84375	58.90625	6412500	815.625	0	1.00E-06	3.22E-02	3.98E-02
21	3	7.34375	21.40625	5812500	905.625	2	1.00E-05	5.81E-03	2.25E-02
22	2	63.59375	40.15625	5512500	860.625	1	1.00E-05	2.36E-02	2.55E-02
23	4	26.09375	77.65625	6112500	950.625	0	1.00E-06	3.45E-02	4.85E-02
24	1	68.28125	44.84375	5887500	961.875	2	1.00E-06	2.65E-02	4.15E-02
25	3	30.78125	7.34375	6487500	871.875	1	1.00E-05	3.82E-03	2.25E-02
26	2	49.53125	26.09375	6187500	916.875	0	1.00E-05	1.53E-02	5.45E-02
27	4	12.03125	63.59375	5587500	826.875	1	1.00E-06	2.56E-02	4.95E-02
28	1	21.40625	54.21875	6337500	849.375	0	1.00E-06	2.59E-02	3.95E-02
29	3	58.90625	16.71875	5737500	939.375	2	1.00E-05	9.44E-03	2.75E-02
30	2	40.15625	35.46875	5437500	894.375	2	1.00E-05	2.30E-02	5.65E-02
31	4	77.65625	72.96875	6037500	984.375	1	1.00E-06	4.20E-02	5.45E-02
32	1	76.48438	29.60938	6543750	829.6875	1	1.00E-06	1.50E-02	3.35E-02

33	3	38.98438	67.10938	5943750	919.6875	2	1.00E-05	2.13E-02	2.85E-02
34	2	57.73438	48.35938	5643750	874.6875	1	1.00E-05	3.00E-02	5.75E-02
35	1	10.85938	38.98438	5793750	987.1875	1	1.00E-06	1.65E-02	3.65E-02
36	2	29.60938	57.73438	6093750	942.1875	0	1.00E-05	2.87E-02	5.35E-02
37	4	67.10938	20.23438	5493750	852.1875	2	1.00E-06	1.13E-02	4.45E-02
38	1	24.92188	24.92188	6468750	840.9375	0	1.00E-06	1.31E-02	3.75E-02
39	3	62.42188	62.42188	5868750	930.9375	1	1.00E-05	2.77E-02	3.35E-02
40	2	6.171875	43.67188	5568750	885.9375	2	1.00E-05	2.92E-02	5.15E-02
41	4	43.67188	6.171875	6168750	975.9375	0	1.00E-06	5.22E-03	4.55E-02
42	1	53.04688	34.29688	5718750	953.4375	2	1.00E-06	1.96E-02	4.05E-02
43	3	15.54688	71.79688	6318750	863.4375	1	1.00E-05	9.52E-03	2.25E-02
44	2	71.79688	53.04688	6018750	908.4375	0	1.00E-05	3.19E-02	5.35E-02
45	4	34.29688	15.54688	5418750	818.4375	2	1.00E-06	8.38E-03	4.35E-02
46	1	50.70313	64.76563	6056250	981.5625	2	1.00E-05	3.42E-02	4.75E-02
47	3	13.20313	27.26563	5456250	891.5625	0	1.00E-06	1.14E-02	2.45E-02

Table 9 – Input values

Model number	
1	Standard **k-** ϵ
2	Standard k- ω
3	RANS
4	RSM

Table 10 – Model number and associated turbulence model

The associated scatter plot of the outputs is as follows:

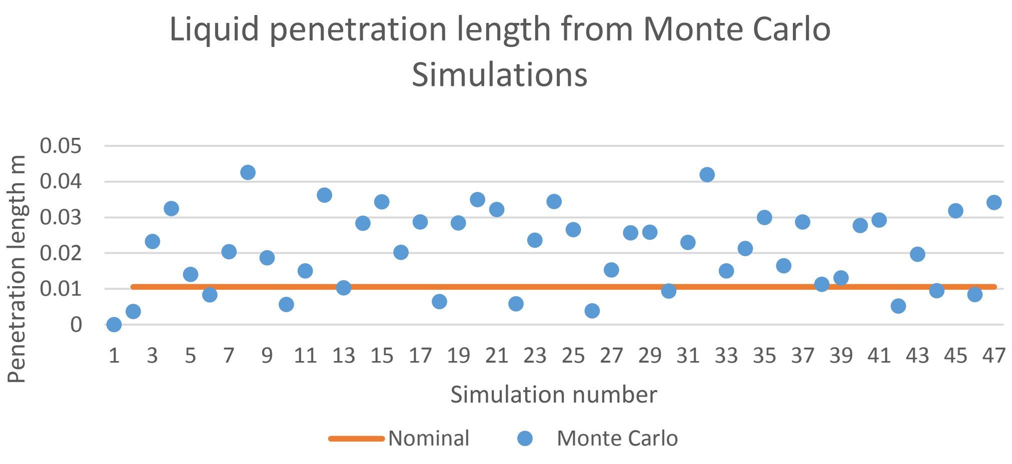


Figure 22 - Liquid penetration length

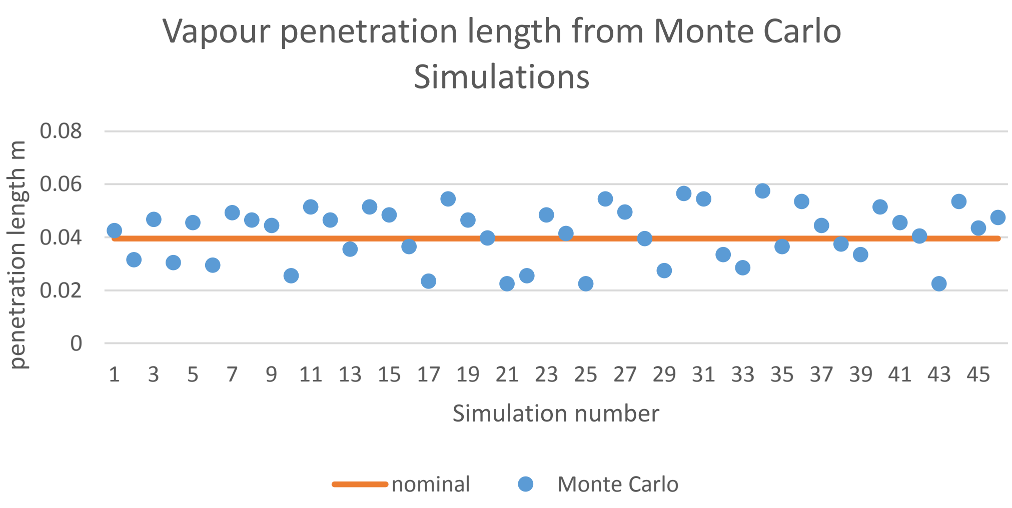


Figure 23 - Vapor penetration length

The spread is very wide for the Liquid penetration length compared to the vapor penetration length. As the liquid penetration length is computed using Lagrange approach, it is expected to be more sensitive than the vapor penetration length computed using the Euler approach.

(c) Modified least square fit

The output data from the Sobol based Monte Carlo study is used to estimate gradients and constants of the modified least square fit equation. 1st and 2nd order comparison states that the parameters have more or less a monotonic relation over the parameters. To further ensure accuracy of the curve fit higher order equations like 3rd order and 5th order were also computed.

(i) 1st order curve fit

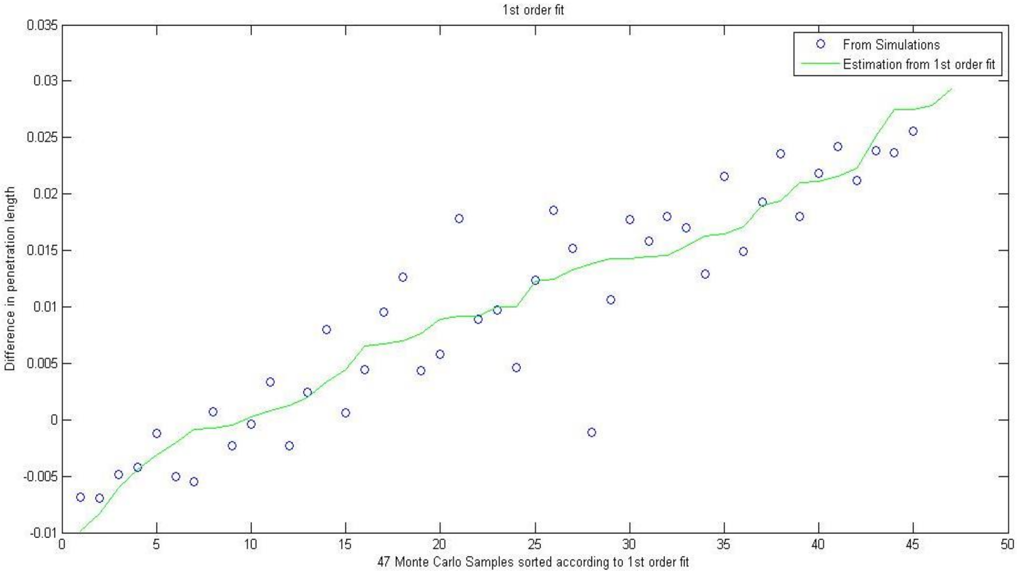


Figure 24 – 1st order curve fit for the 47 simulations liquid penetration length

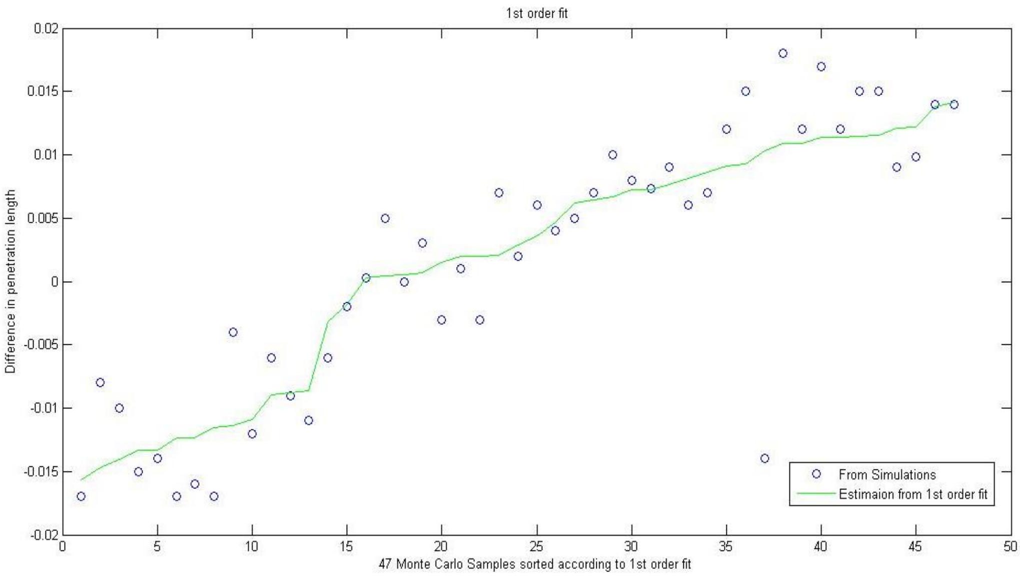


Figure 25– 1st order curve fit for the 47 simulations vapor penetration length

The gradients and constants are used to compute the estimated values for each of the 47 output values. And are compared. The 5th order fit is slightly better than the 1st order. 1st order curve fit is considered close enough and used for further calculations.

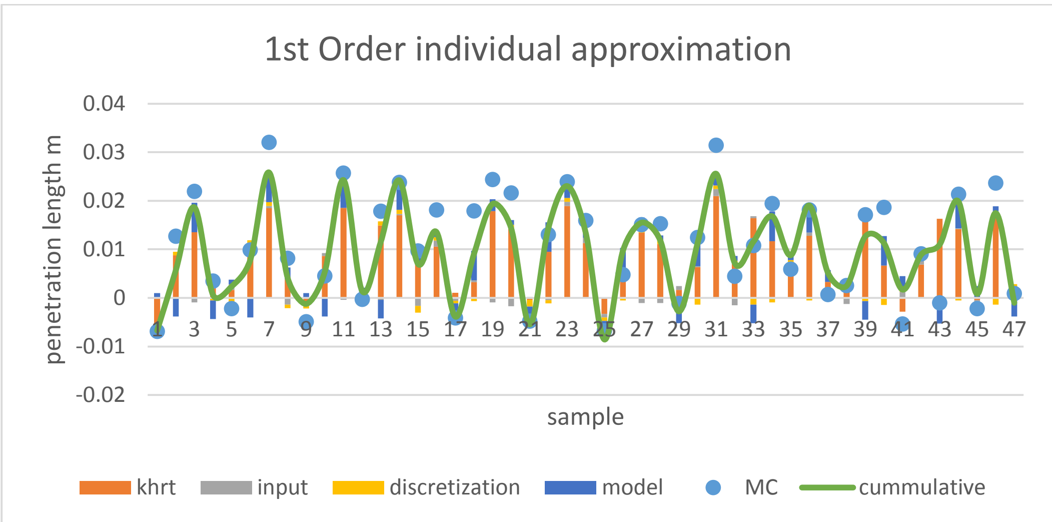


Figure 26– Approximation using 1st order curve fit gradients for liquid penetration length

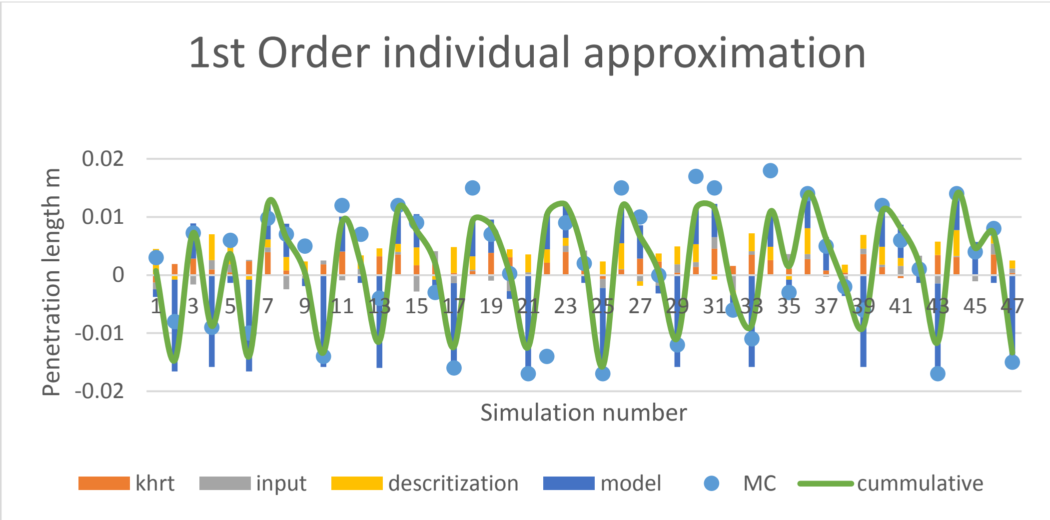


Figure 27– Approximation using 1st order curve fit gradients for vapor penetration length

(ii) 2nd order curve fit

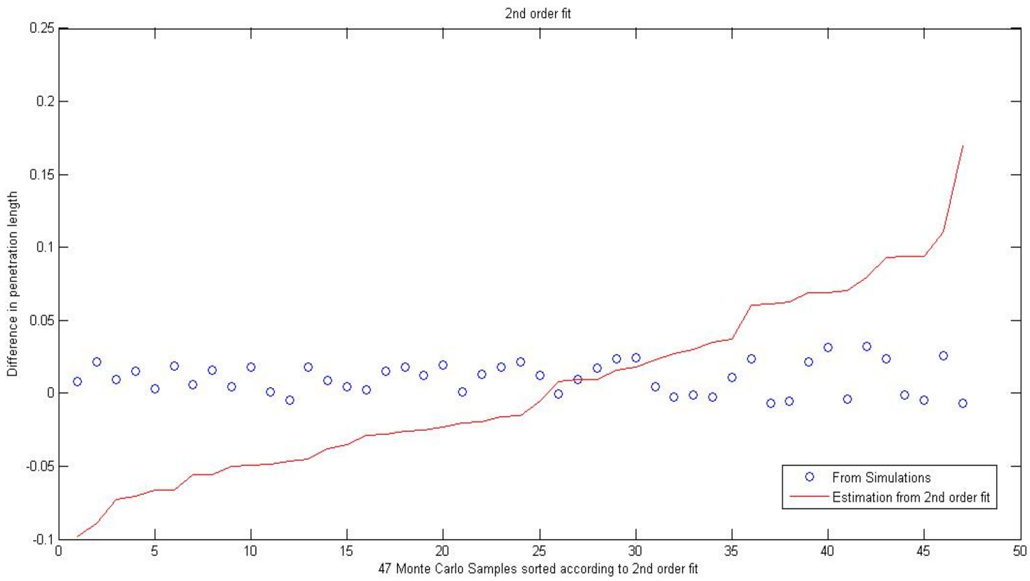


Figure 28– 2nd order curve fit for the 47 simulations liquid penetration length

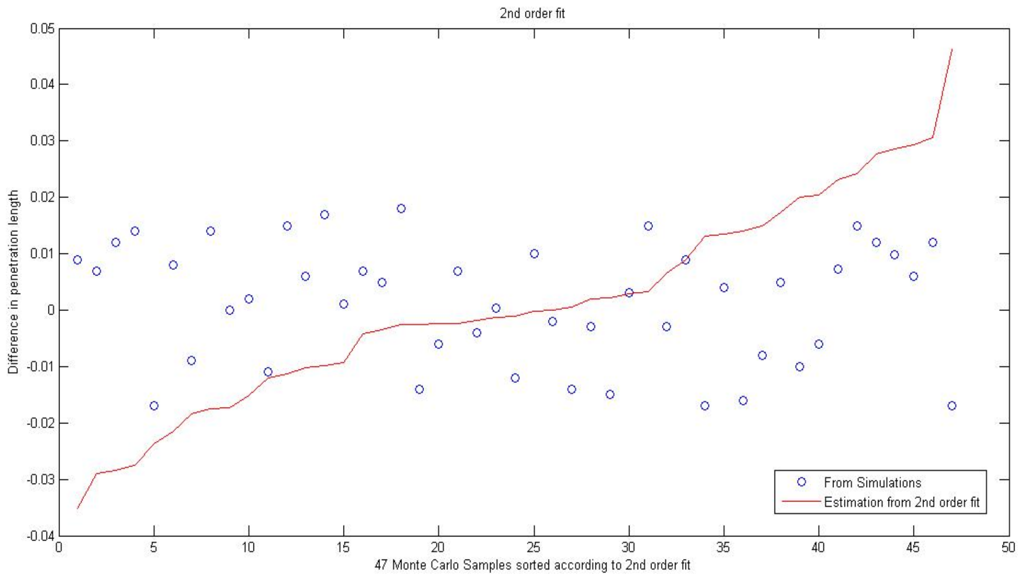


Figure 29– 2^{nd} order curve fit for the 47 simulations vapor penetration length

The trend of the output to input relation is best mimicked by 1^{st} order compared to 2^{nd} order least square fit, implying an odd degree relationship more or less like that of monotonically increasing or decreasing dependence.

To further ensure the approximation is well approximated 5^{th} order curve fit is also computed.

(iii) 5^{th} order curve fit

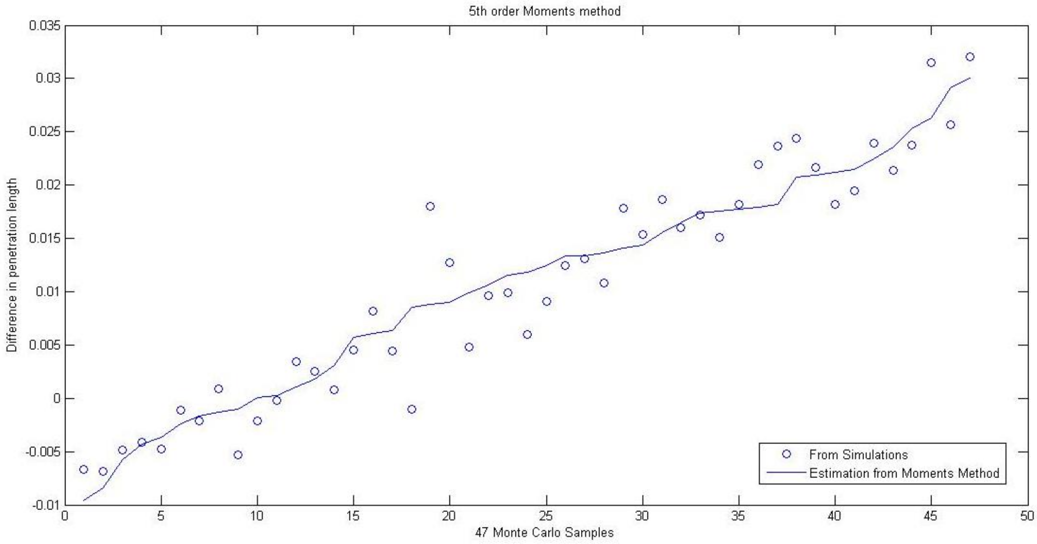


Figure 30– 5^{th} order curve fit for the 47 simulations liquid penetration length

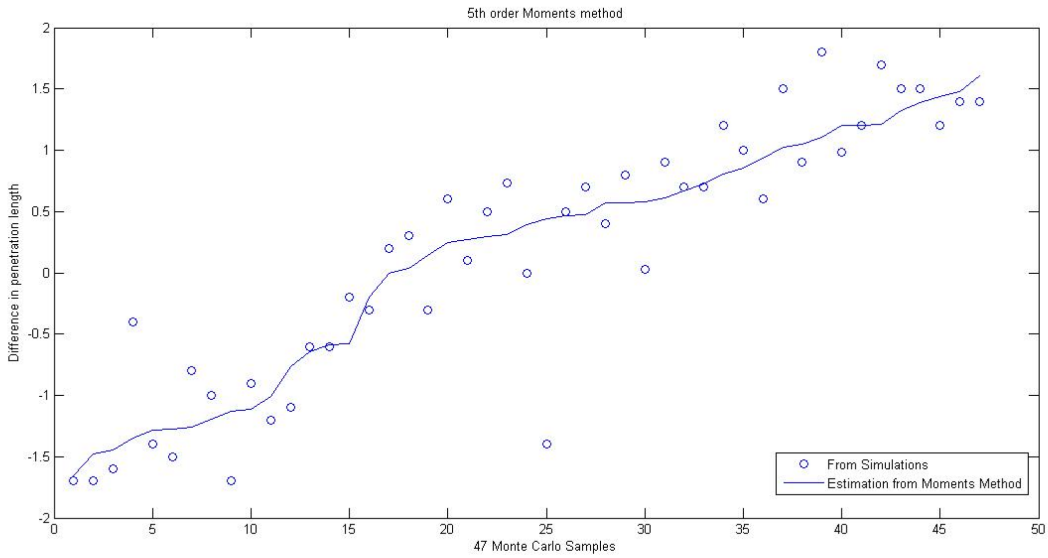


Figure 31– 5^{th} order curve fit for the 47 simulations vapor penetration length

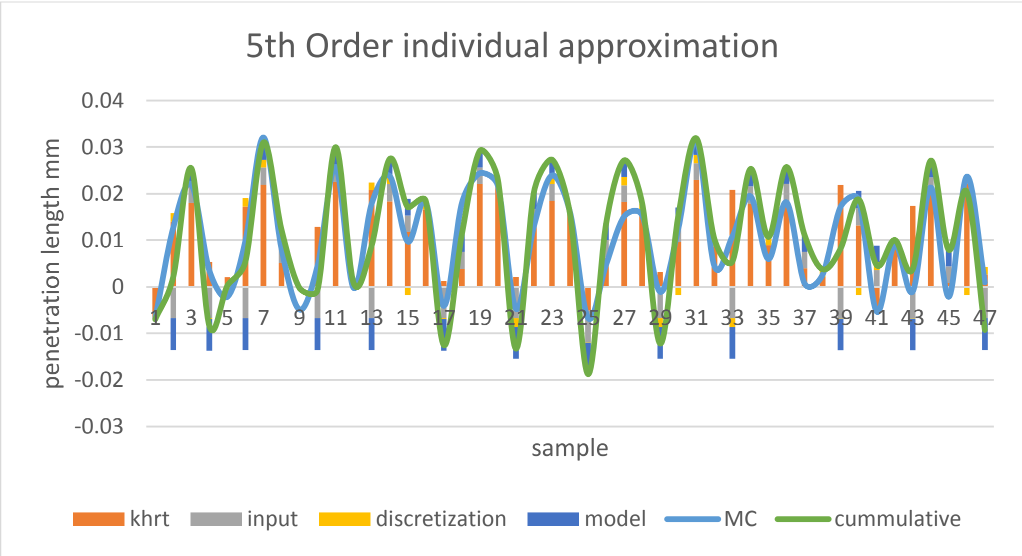


Figure 32– Approximation using 5th order curve fit gradients for liquid penetration length

(iv) Additional 10 simulations

As the 50 simulations conducted for Sobol based Monte Carlo study involved the KHRT parameters uncertainty a wide spread of liquid and vapor penetration length was detected. This uncertainty is basically uncertainty in characterization of the injector. An injector has its own peculiar nozzle geometry and surface properties which has significance in the jet breakup. To quantify this breakup one needs to fine tune the KHRT parameters to match with the experimentally measured output. Once done the KHRT parameters are the characterized constants for the given nozzle specifications.

Thus there are 2 types of uncertainty that are of interest with respect to diesel like sprays:

1. Without the injector characterization
2. With injector characterization.

The former can be studied from the already performed 50 simulations. For the latter we need to fix the KHRT parameter values to its nominal values and repeat the process. As the system is Sobol based the number of sampling could be dynamically controlled. 10 further simulation sampling was therefore generated and simulated.

The results of which are as follows:

(9 on the simulations converged and 1 diverged)

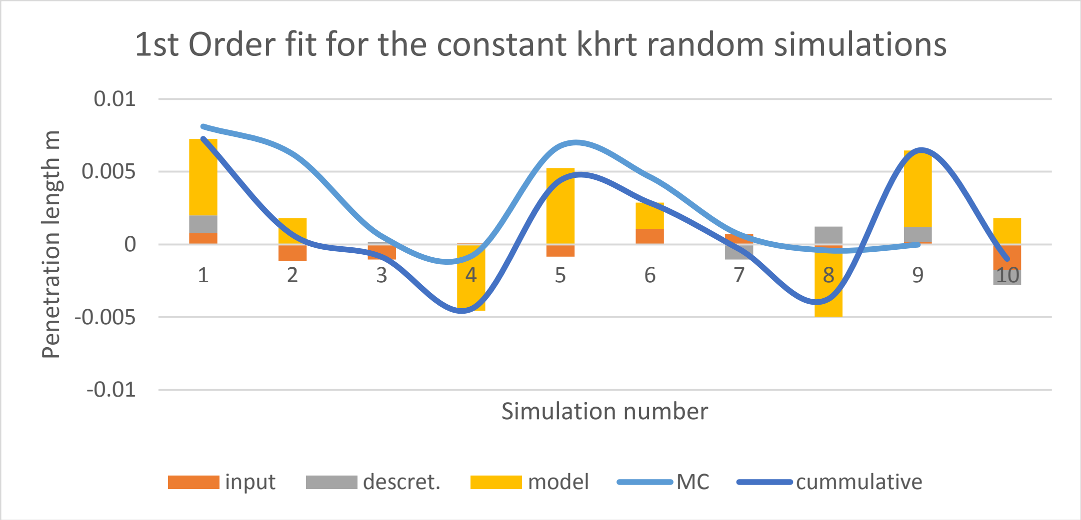


Figure 33– Estimated values using 1st order gradients for liquid penetration length

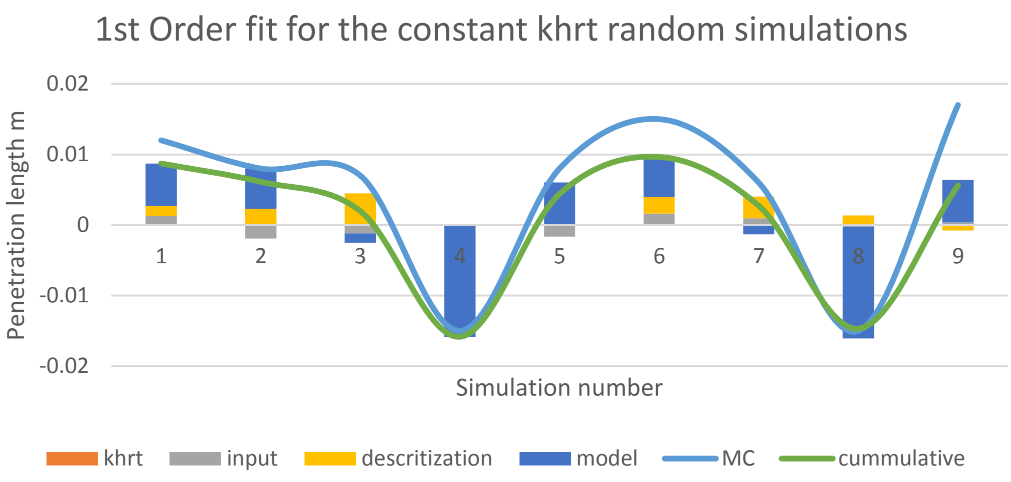


Figure 34– Estimated values using 1st order gradients for Vapor penetration length

(d) Moments Method

The gradients and constants are finally used to estimate the uncertainty. The parameters are assumed to be mutually independent i.e. the co-variance terms are zero. The assumption is aimed to simplify the study though it would not be as accurate.

The variance in the output due to each input is computed with the help of the 1st order gradients which are added for the continuous domain parameters. Among the constants maximum and minimum values are calculated for each namely, Turbulence model, time discretization and grid discretization. The upper bound of uncertainty is estimated by the total variance from all the gradients and adding the maximum value of constants among each of the 3 categories. Similarly the lower bound computed by deducting the total sum of all the variance and the minimum value of constants.

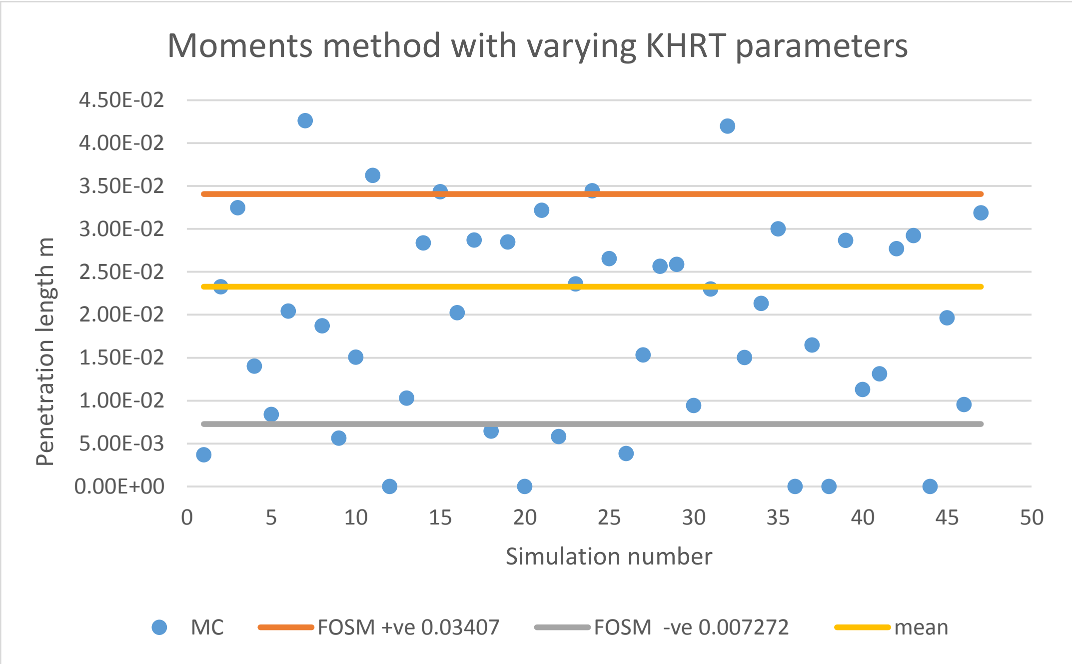


Figure 35– Uncertainty band for liquid penetration length without injector characterization

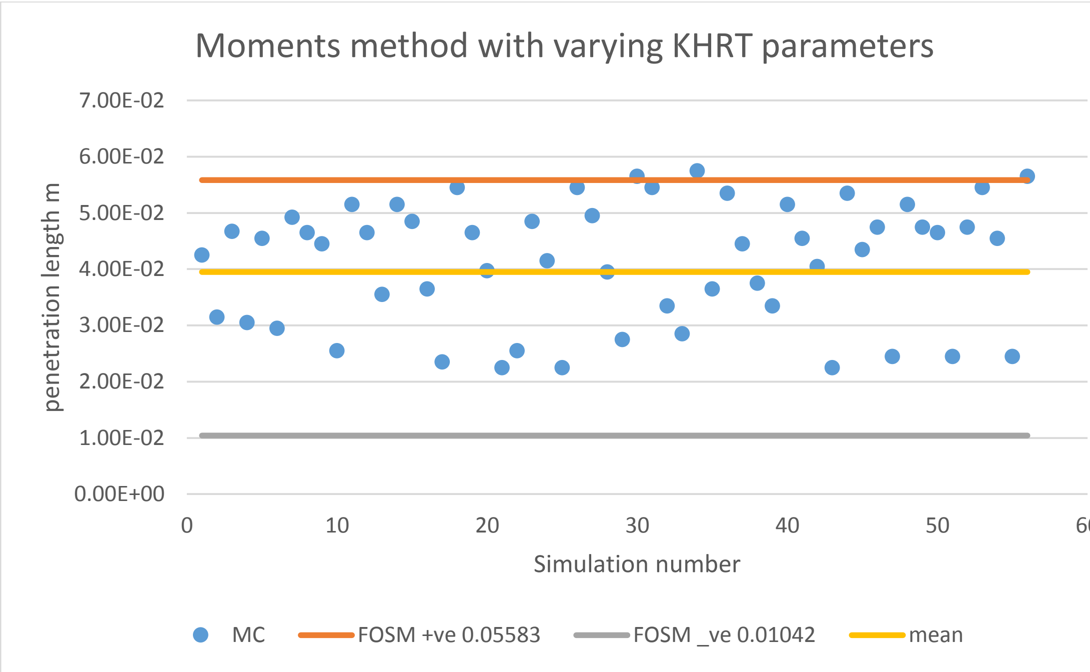


Figure 36– Uncertainty band for vapor penetration length without injector characterization

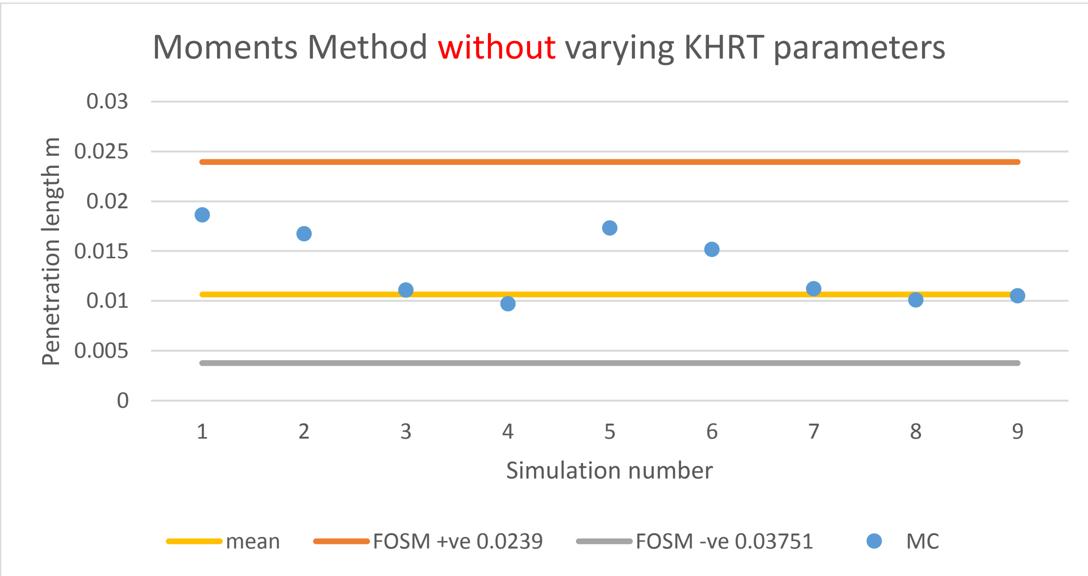


Figure 37– Uncertainty band for liquid penetration length with injector characterization

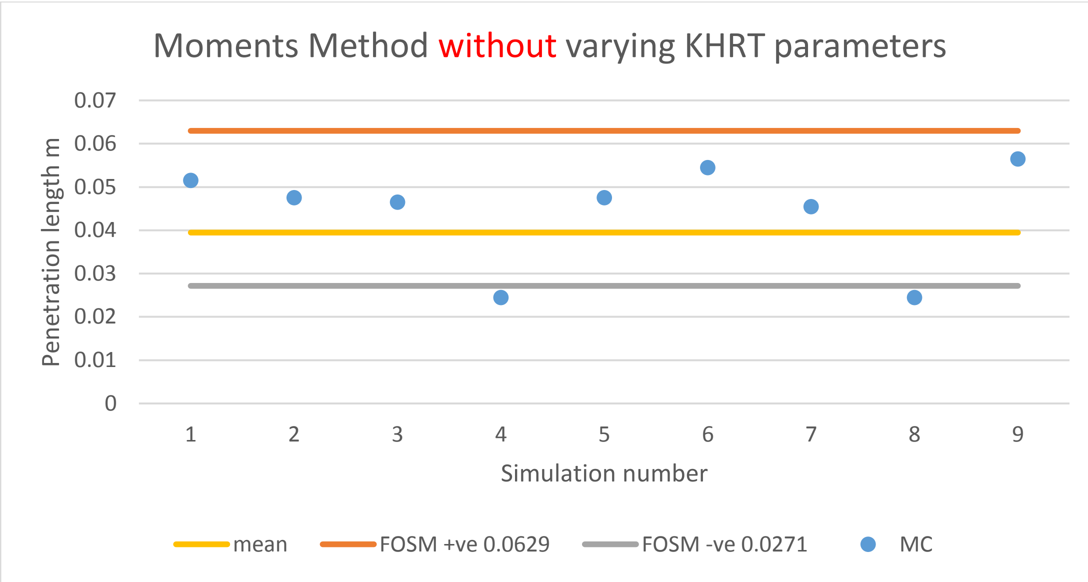


Figure 38– Uncertainty band for vapor penetration length with injector characterization

Type	Liquid penetration uncertainty band length	Vapor penetration uncertainty band length
Without injector characterization	38.65 mm	45.41 mm
With injector characterization	13.57 mm	35.8 mm

Table 11 – Summary of the uncertainty band

6. Conclusions & future scope

The uncertainty band is extremely sensitive to injector characterization. The uncertainty is estimated for the 10 simulations based on the gradients received from the 1^{st} order curve fitting the initial 47 simulations. It should be noted that the uncertainty study is based on Taylor series expansion around the nominal value. As much as the interval closer to the interval used to compute the gradients, better approximate uncertainty estimation can be expected.

The uncertainty is considerably reduced with the injector characterisations, 25.08 mm for liquid and 9.6 mm for vapour penetration length.

A systematic methodology established and executed for a computationally intensive problem. The technique does need improved uncertainty quantification for modified least square technique needed to solve. The current study estimates uncertainty in a crude way of adding the maximum and minimum bounds of all the discreet domain parameters.

The study included injector cone angle as the only geometrical input parameter. The parameter did not though require to redo the geometry and meshing. Which would not always be the case. Most of the times the geometry being simulated would have to be redone each time. In such case automation is extremely complicated but even more important. A process to do the same is very much required.

The parameters are assumed to have no mutual dependence on each other. Considering a system with mutual dependence would improvise on the accuracy of the model.

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