STATISTICAL APPROACH ON VISUALIZING MULTI-VARIABLE INTERACTIONS IN A HYBRID BREAKUP MODEL UNDER ECN SPRAY CONDITIONS

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1. Introduction
   • Challenge & Objectives

2. Methodology
   • Approach
   • ECN Spray A
   • Design of Experiments (DoE)

3. Results & Discussion
   • Case specific best matches provided by Stochastic Process Model (SPM)
   • Performance of a single set of parameters in all conditions

4. Conclusions
Introduction – Industry is calling for computationally efficient and predictive CFD in-cylinder simulations

Current main approaches for CFD simulations are:

<table>
<thead>
<tr>
<th>DNS</th>
<th>LES</th>
<th>RANS</th>
</tr>
</thead>
<tbody>
<tr>
<td>No tuning required</td>
<td>Some tuning is required</td>
<td>Highly dependent on tuning</td>
</tr>
<tr>
<td>Highest level of physical accuracy</td>
<td>Good level of physical accuracy</td>
<td>Lowest level of physical accuracy</td>
</tr>
<tr>
<td>Very computationally expensive</td>
<td>Computationally expensive</td>
<td>Computationally efficient</td>
</tr>
</tbody>
</table>

BUT, what if we could reduce tuning effort and simultaneously increase accuracy in the RANS approach?
With appropriate tuning it is possible to get very accurate spray simulations using a RANS approach

Challenge:
Selecting appropriate simulation models and defining their tuning constants

Objective:
1. Visualize multivariable interactions using DoE
2. Find set of constants for a spray match for 5 conditions
3. Find a single set of constants for all 5 conditions
Methodology – Approach

Selection of experimental data

Independence studies

Discrete model selection trials

Minimize RMSE for each case

Produce Stochastic process models (SPM's)

Minimize RMSE over all cases

DoE constant range setting
Methodology – Experimental data selection – Engine Combustion Network (ECN) and Spray A

Spray A
- Utilizes a vertical, single hole injector
- The condition represents
  - light duty DI injection
  - moderate EGR rates
- Reliable measurements are provided for
  - Liquid & vapour penetration
  - Steady state radial & axial mass fraction and charge temperature distributions

Engine Combustion Network (ECN)

<table>
<thead>
<tr>
<th>Spray A Nozzle</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel injector nominal nozzle outlet diameter</td>
<td>90µm</td>
</tr>
<tr>
<td>Nozzle K factor</td>
<td>1.5</td>
</tr>
<tr>
<td>Discharge coefficient</td>
<td>0.86</td>
</tr>
<tr>
<td>Fuel</td>
<td>n-dodecane</td>
</tr>
<tr>
<td>Fuel temperature at nozzle</td>
<td>363K (90°C)</td>
</tr>
</tbody>
</table>
Methodology – Experimental data selection – The test matrix

<table>
<thead>
<tr>
<th>Case</th>
<th>Charge Temperature [K]</th>
<th>Charge Density [kg/m³]</th>
<th>Inj. Pressure [bar]</th>
<th>Inj. Duration [ms]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>900</td>
<td>22.8</td>
<td>1500</td>
<td>&gt;4</td>
</tr>
<tr>
<td>2</td>
<td>1100</td>
<td>15.2</td>
<td>1500</td>
<td>&gt;4</td>
</tr>
<tr>
<td>3</td>
<td>1400</td>
<td>7.6</td>
<td>1500</td>
<td>&gt;4</td>
</tr>
<tr>
<td>4</td>
<td>900</td>
<td>22.8</td>
<td>1000</td>
<td>&gt;4</td>
</tr>
<tr>
<td>5</td>
<td>900</td>
<td>22.8</td>
<td>500</td>
<td>&gt;4</td>
</tr>
</tbody>
</table>

Decreasing injection pressure
Increasing charge temperature and decreasing charge density

Case 1
Case 2
Case 4
Case 3
Case 5
## Methodology – Selected sub models

<table>
<thead>
<tr>
<th>Software</th>
<th>VECTIS by Ricardo Software</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turbulence Model</td>
<td>Standard k-ε</td>
</tr>
<tr>
<td>Droplet Breakup Model</td>
<td>Kelvin-Helmholtz / Rayleigh-Taylor (KH-RT)</td>
</tr>
<tr>
<td>Spray Injection Method</td>
<td>Blob (Table distribution)</td>
</tr>
<tr>
<td>Droplet Drag Model</td>
<td>Putnam</td>
</tr>
<tr>
<td>Droplet Collision &amp; Coalescence</td>
<td>Cell based interaction</td>
</tr>
<tr>
<td>Droplet/Turbulence Interaction</td>
<td>Stochastic Model following Shuen, Chen and Faeth</td>
</tr>
<tr>
<td>Evaporation Model</td>
<td>Spalding</td>
</tr>
<tr>
<td>Grid type</td>
<td>Cartesian</td>
</tr>
<tr>
<td>Grid size</td>
<td>0.45mm</td>
</tr>
<tr>
<td>Grid dimensionality</td>
<td>3D – Axisymmetric</td>
</tr>
<tr>
<td>Time-step size [µs]</td>
<td>0.5</td>
</tr>
</tbody>
</table>
## Methodology – Design of Experiment

Model Selection & Range Setting (Simulation Design Matrix)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Range</th>
<th>Default</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coefficient of Dissipation $C_2$ [-]</td>
<td>1.7 – 1.85</td>
<td>1.92</td>
</tr>
<tr>
<td>Turbulent Schmidt Number</td>
<td>0.6 – 1</td>
<td>0.9</td>
</tr>
<tr>
<td>Drag scaling factor $A_{drag}$ [-]</td>
<td>0.5 – 1.5</td>
<td>1</td>
</tr>
<tr>
<td>KH $B_1$ – Constant [-]</td>
<td>1 – 25</td>
<td>13</td>
</tr>
<tr>
<td>KH $B_0$ – Constant [-]</td>
<td>0.3 – 0.8</td>
<td>0.61</td>
</tr>
<tr>
<td>RT $C_3$ – Constant [-]</td>
<td>0.3 – 5.3</td>
<td>5.3</td>
</tr>
<tr>
<td>RT $C_{RT}$ – Constant [-]</td>
<td>0.3 – 2</td>
<td>1</td>
</tr>
<tr>
<td>Levich $A_{bu}$ – Constant [-]</td>
<td>5.5 – 11</td>
<td>5.5</td>
</tr>
<tr>
<td>Initial Half Cone Angle $\alpha$ [deg]</td>
<td>2.5 – 7.5</td>
<td>-</td>
</tr>
<tr>
<td>Largest droplet diameter [μm]</td>
<td>60 – 84</td>
<td>-</td>
</tr>
</tbody>
</table>
Methodology – The Design of Experiment approach with Root-Mean-Square-Error comparing simulated spray penetrations to ECN Spray A measurements

10 Simulation Constants as DoE variables
Response model for key metrics as a function of model constants (SPM)
Optimizer to minimize RMSE between simulation and experiment
Analyse parameter sets for patterns
Results & Discussion – Charge temperature and density swing
All cases show good correlations

All cases:
Liquid & vapour penetration match well

Charge temperature: 900K

- Case 1 Best Match
- ECN Test Data - Case 1

RMSE: 0.63

Vapour: 1.59

Charge temperature: 1400K

- Case 3 Best Match
- ECN Test Data - Case 3

RMSE: 0.64

Vapour: 1.2

Charge temperature: 1100K

- Case 2 Best Match
- ECN Test Data - Case 2

RMSE: 0.54

Vapour: 1.5
Charge temperature swing

![Graph 1](image1)

- **Case 1 Best Match**
- **ECN Test Data - Case 1**

![Graph 2](image2)

- **Case 2 Best Match**
- **ECN Test Data - Case 2**

![Graph 3](image3)

- **Gas Phase Temperature [K]**
- **Distance to Sprayaxis [mm]**

![Graph 4](image4)

- **Mixture Fraction [-]**
- **Axial Distance to Nozzle Exit [mm]**
Results & Discussion – Charge temperature and density swing
All cases show good correlations

<table>
<thead>
<tr>
<th>Pattern</th>
<th>Physical Implication</th>
</tr>
</thead>
<tbody>
<tr>
<td>Generally high $B_1$ (Primary atomization time constant)</td>
<td>Parent droplets decrease slowly in size</td>
</tr>
<tr>
<td>Decreasing $B_0$ values (Primary atomization size constant)</td>
<td>Child droplets in primary breakup are smaller</td>
</tr>
<tr>
<td>Increasing $A_{drag}$ values (Droplet drag force scaling)</td>
<td>Liquid-to-gas phase momentum transfer increases</td>
</tr>
<tr>
<td>Constant of destruction of dissipation $C_2$ highly sensitive</td>
<td>Affects turbulent dissipation</td>
</tr>
</tbody>
</table>

Charge temperature: 900K

Charge temperature: 1100K

Charge temperature: 1400K
Cases 1 & 4
• Liquid and vapour propagations lie mostly within experimental error

Case 5
• Liquid penetration matches well, vapour under-penetrates over most of the simulation duration
Inj. Pressure swing

**Case 1 Best Match**
ECN Test Data - Case 1

**Case 4 Best Match**
ECN Test Data - Case 4

**Case 5 Best Match**
ECN Test Data - Case 5
Results & Discussion – Injection pressure swing
Cases 1 & 4 match well, Case 5 shows some shortcomings in vapor penetration

<table>
<thead>
<tr>
<th>Pattern</th>
<th>Physical Implication</th>
</tr>
</thead>
<tbody>
<tr>
<td>Generally low $A_{\text{drag}}$ (Droplet drag force scaling)</td>
<td>Liquid-to-gas phase momentum transfer decreased</td>
</tr>
<tr>
<td>Decreasing $B_0$ (Primary atomization size constant)</td>
<td>Child droplets in primary breakup are smaller</td>
</tr>
<tr>
<td>Decreasing $B_1$ (Primary atomization time constant)</td>
<td>Parent droplets decrease faster in size</td>
</tr>
<tr>
<td>Constant of destruction of dissipation $C_2$ highly sensitive</td>
<td>Affects turbulent dissipation</td>
</tr>
</tbody>
</table>

### Injection pressure: 1500bar

- **Case 1 Best Match**
- **ECN Test Data - Case 1**

Liquid RMSE: 0.63
Vapor RMSE: 1.59

### Injection pressure: 1000bar

- **Case 4 Best Match**
- **ECN Test Data - Case 4**

Liquid RMSE: 0.85
Vapor RMSE: 1.03

### Injection pressure: 500bar

- **Case 5 Best Match**
- **ECN Test Data - Case 5**

Liquid RMSE: 0.74
Vapor RMSE: 2.52
Conclusion

1. The constant of destruction of dissipation $C_2$ in the Standard k-ε model and the drag scaling coefficient $A_{\text{drag}}$ are highly sensitive key tuning parameters.

2. At lower injection pressures matching both liquid and vapor penetration became more challenging.

3. Depending on the condition, the breakup constants in the hybrid spray breakup model (KH-RT) model tend to assemble in a distinct spectrum of the investigated range.
Results & Discussion – Proposed set of parameters for multiple conditions
Charge temperature and density change

Approach:
Use case SPM’s to minimize RMSE over all 5 cases

Results
• Both cases of elevated temperature show an under-penetration of liquid
Results & Discussion – Proposed set of parameters for multiple conditions
Charge temperature and density change – The most apparent patterns

<table>
<thead>
<tr>
<th>Overall match shows following pattern</th>
<th>Physical Implication</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lower $B_1$ values (Primary atomization time constant)</td>
<td>Parent droplets decrease faster in size</td>
</tr>
<tr>
<td>Lower $B_0$ values (Primary atomization size constant)</td>
<td>Child droplets in primary breakup are larger</td>
</tr>
<tr>
<td>Injected droplets are larger</td>
<td>Shorter liquid penetrations</td>
</tr>
</tbody>
</table>

- **Charge temperature: 900K**
  - Overall match: Liquid RMSE: 1.19, Vapor RMSE: 1.78

- **Charge temperature: 1100K**
  - Overall match: Liquid RMSE: 2.16, Vapor RMSE: 1.97

- **Charge temperature: 1400K**
  - Overall match: Liquid RMSE: 3.26, Vapor RMSE: 2.36
Results

- Cases 1 & 4 remain roughly unchanged due to the new set of constants not being very different
- Case 5 shows significant over-penetration of liquid penetration

Injection pressure swing

- Injection pressure: 500bar
- Injection pressure: 1000bar
- Injection pressure: 1500bar
Results & Discussion – Proposed set of parameters for multiple conditions
Injection pressure swing – The most apparent differences

<table>
<thead>
<tr>
<th>Injection pressure: 1500bar</th>
<th>Injection pressure: 1000bar</th>
<th>Injection pressure: 500bar</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid Penetration [mm]</td>
<td>Liquid Penetration [mm]</td>
<td>Liquid Penetration [mm]</td>
</tr>
<tr>
<td>Time [ms]</td>
<td>Time [ms]</td>
<td>Time [ms]</td>
</tr>
</tbody>
</table>

- **Overall match shows following pattern**
  - Injected droplets were smaller

- **Physical Implication**
  - Longer liquid penetrations
Conclusions:

• It was found that if the vapor phase is the metric of interest, the simulation constants may be held constant across all five conditions.

• Otherwise it is recommended to adjust other tuning constants.

• It was mostly possible to explain the shortcomings of the generalized simulation with the physical expression of the changed constants.
This investigation will be soon extended to ..

- Multicomponent diesel
- Multi-hole commercially available injectors

.. and in long term extended to reacting case and emission simulations using same methodology.
Acknowledgements

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