Numerical and Experimental Investigation of Mixing Quality for Pulsed Mixing Flows with Application to Diesel Aftertreatment

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Outline

- Literature Review and Motivation
  - Aftertreatment Mixing, LNT, RPR Mixing Requirement

- Preliminary Mixer Design and Analysis

- Experimental Study

- Test results and Discussion

- Numerical Analysis

- Conclusion and Future Work
Mixing uniformity is important for many Diesel Aftertreatment Methods [1-4]. Different Designs have been used, both experimental and numerical (CFD) studies [2,5,6].

- DPF Regenerations

Cone Mixer [2]
Stage Mixer [2]
Mixer Tube Geometry [3]  
*Zheng et al.*

Injection Orientation [4]

Flapper [4]
Twister [4]  
*Gardner et al.*
Greater mixing challenge occurs with a process referred to as: Rapidly Pulsed Reductants (RPR)

Reductants injected as high frequency ($\sim 1\text{Hz}$) pulses ahead of a LNT

Improved NOx conversion - Expanded the operating window of LNT to higher temperatures and SV [7-9]

Challenge:

Uniform radial mixing, and well separated rectangular pulses in the axial direction (i.e. minimal axial mixing)

NOx conversion vs Temperature [9]

Bisaiji et al. Toyota
Literature review and Motivation

Preliminary Mixer Design and Analysis

Mixer Design and Simulation, Uniformity Index for RPR

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Preliminary Mixer Design

A design based on radial reductant jet and generation of Counter Rotating Vortices (CRV) to form plug flow. Different designs were investigated using 3D unsteady two-phase flow simulation of mixing.
**Stoichiometric Area Index (SAI)**

\[ S_{AI} = \frac{\text{Surface area within acceptable mole fraction}}{\text{Total surface area}} \times 100 \]

Usually, used in SCR [10]

**Mixing quality**

\[ \gamma = (1 - \sigma/T) \times 100 \]

Used in EGR [11]

where: \( \sigma \) – Standard deviation of temperature at a cross section

\( T \) - Mass weighted average temperature at a cross section

**Uniformity index (UI)**

Usually defined over the inlet face of the catalyst [12]

\[ (\phi) = 1 - \sum \phi f - \phi \int A f / 2 \phi \sum A f \]

Since, axial distribution is also important

For RPR, we define:

\[ \phi = 1 / \lambda \]

\[ UI (\phi) = 1 - \int \phi f - \phi - \phi \]

**Figures of merit for mixing**
Literature review and Motivation

Preliminary Mixer Design and Analysis

➤ Experimental Study
  ○ Method, Uniformity Index Measurement
  ○ Test Condition
  ○ Parameters and Measurement Procedure

Test results and Discussion

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Conclusion and Future Work
Using a DOC, two Fast Flame Ionization Detector (f FID) channels upstream and downstream of DOC. HC concentrations were measured with 200Hz frequency. Using the axial distribution of HC (upstream probe) and HC break through (downstream probe) pulse characteristics defined.
The lean portion (A2)

Equal amount of injected HC and HC breakthrough:

Mixing quality of (a) is better $t\downarrow 1, t\downarrow 2 \neq t\downarrow inj$ (due to axial mixing) data from upstream probe.

$$UI (\phi) = 1 - \left( \int_{\text{down}}^{\text{down}} (\phi - \phi) dv \right) \downarrow \text{lean} + \left( \int_{\text{down}}^{\text{down}} (\phi - \phi) dv \right) \downarrow \text{rich} / 2 \phi V$$
Literature review and Motivation

Preliminary Mixer Design and Analysis

Experimental Study

- Method, Uniformity Index Measurement
- Test Condition
  1-DOC Temperature, 2-Oxygen Concentration, 3-Probe Location, 4-Space Velocity
- Parameters and Measurement Procedure

Test Results and Discussion

Numerical Analysis

Conclusion and Future Work
C Temperature

DOC light-off temperature: **175°C**

Mixing tests were performed at **300°C** to ensure HC conversion.

2- Oxygen Concentration (Flammability Limits)

- Flammability limits not available (i.e. diluted and elevated T)
- Steady PSR simulation was performed in CHEMKIN
- Deflagration flame was initiated from glowing DOC
- Oxygen concentration was reduced from 6.8% to 4%

Zhao, F
**stream probe location:** The effect of eccentricity (e) of upstream Fast FID probe was investigated.

Eccentricity (e) was limited to **4.5 mm** by catalyst feature. The difference in measured uniformity index was very low (difference in UI was **1.8%**). Eccentricity of 4.5mm was chosen for experiments.
Surface Velocity

A breakthrough was observed to be dependent on SV

Experiments done with constant $SV = \frac{31000}{h}$ using DOC samples with different volume (constant SV)

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**Ideal Pulse**
Literature review and Motivation

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Parameters for Mixing:

**Reynolds Number**: Determines the turbulence intensity of the jet flow. \[ Re_{Jet} = \frac{\rho_{Jet} V_{Jet}}{\mu_{Jet}} \]

**Momentum Ratio**: Determines the length of jet penetration in the main flow, \[ mr = \frac{\rho_{Jet} V_{Jet}}{\rho_{main} V_{main}} \]

Whether it hits the outer tube walls or not.

### Experimental Parameters

<table>
<thead>
<tr>
<th>Jet Reynolds number</th>
<th>Momentum Ratio, by d1</th>
<th>Mixer to DOC distance d2 (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9000</td>
<td>6.3</td>
<td>20</td>
</tr>
<tr>
<td>18000</td>
<td>12.6</td>
<td>40</td>
</tr>
<tr>
<td>27000</td>
<td>25.3</td>
<td>60</td>
</tr>
</tbody>
</table>
Three level full factorial experiments
Concentrations of HC upstream and downstream of DOC were recorded with 200 Hz sampling rate.
For each test point 5 consecutive pulses were measured. Measurements were averaged and uniformity index was calculated using the following formula:

\[
\text{Uniformity Index (UIC)} = 1 - \frac{\int_{\theta}^{\theta} |\phi - \phi| \, dv}{2\phi} \]

For lean and rich conditions:

\[
V_{\text{lean}} = 1 - \left( \int_{\theta}^{\theta} (\phi - \phi) \, dv \right) \]

\[
V_{\text{rich}} = 1 - \left( \int_{\theta}^{\theta} (\phi - \phi) \, dv \right) \]

Polynomial response surface was fitted to data, to investigate the optimum mixing condition.
Literature review and Motivation
Preliminary Mixer Design and Analysis
Experimental Study
➢ Test Results and Discussion
Numerical Analysis
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Response Surface for $d_{\downarrow 2} = 20 \text{mm}$

Maximum UI was found on this surface; however, the region is sharp and the UI is sensitive to Jet Re number and to a lesser extent momentum ratio.
Response Surface for $d^2 = 40 \text{ mm}^2$

near maximum efficiency, and a flat region of surface, gives robust mixing over a wide range of operating conditions.
Response Surface for $d^2 = 60 \text{mm}$
Selected Mixing Conditions

- Near rectangular pulses with near zero HC breakthrough
- Provides a broad range of operating condition: Low to moderate jet Re number/momentum ratio/d2

**Experimental Results**

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Literature review and Motivation

Preliminary Mixer Design and Analysis

Experimental Study

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Numerical Analysis

- Models and Results

Conclusion and Future Work
Numerical Analysis

Conducted at Experimental Condition

Dissipation model and turbulent transport parameters have a significant effect on the spatial and temporal distribution of species in the flow field.

RANS (Reynolds Ave. N.S.) models $k-\varepsilon$ RNG [14] and RNG

Turbulent Schmidt number $Sc\downarrow t$ [13] $Sc\downarrow t = \frac{v\downarrow t}{D\downarrow t}$

For general applications $Sc\downarrow t = 0.7 - 0.9$

For cross flow jets $Sc\downarrow t = 0.2 - 1.5$ lower range is recommended
Numerical Results

- ε RNG results for $Sc_{\text{t}} = 0.2, 0.7, 2.0$

The ε RNG model underestimated mixing due to calculation of only one component of Reynolds stress tensor.

[16 CPU hours]
**NUMERICAL RESULTS**

**RSM results for $Sc = 0.2, 0.7, 2.0$**

In the tail part of the diagram, mixing is still underestimated, since turbulence is not resolved in RANS models.
for rectangular pulses with $U_I \approx 0.7$ over a broad range of operating condition using new mixer design.

Low to Moderate Re number, momentum ratio and mixer distance to catalyst gives the best Uniformity.

**Omega–RSM** model with low $Sc_{\downarrow t}$ good agreement with reasonable computation cost.

### Effect of Mixing on NOx Conversion

The effect of Radial and axial mixing uniformity is being investigated separately on the NOx conversion of the conventional LNT.


Thanks for your attention
Questions?