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SUBJECT: Annual Progress Report
PROJECT NUMBER: 413LUB0136A
PROJECT TITLE: CFD Study of Important Flare Operating Parameters
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Project Description
Current EPA regulations (40CFR60.18) require smokeless flaring, which motivates flare operators to over-steam or over-air to suppress smoke at the expense of combustion efficiency (CE). It is also well known that incipient smoke point (ISP) is a good indicator for good combustion, but the phenomena is neither well understood nor scientifically defined [1-7]. Further, many factors affect soot emission and unburned/produced VOC emissions [2-4,8]. In this project, computational fluid dynamics (CFD) methods based on CHEMKIN CFD-FLUENT [9-10] will be used to study important flare operating parameters such as composition, combustion zone heating value (CZHV), combustion zone lower flammability (CZLFL), exit velocity, and crosswind [2-4,8,11].

Lamar University has developed a series of 50-species mechanisms for C1-C3 hydrocarbon combustion that were validated with key performance indicators like laminar flame speeds, adiabatic flame temperature, ignition delay tests [11,12]. In this project, a new mechanism that contains soot precursors and C4 species, LU3.0.1, was developed and validated with experimental data. Lamar’s CFD modeling has been validated with several laboratory flame (e.g., Berkeley flame, Sandia flame, and McKenna flat flame) data sets having detailed VOC composition profiles [8]. Currently, CFD methodology is used to model soot yield and combustion efficiency for 2010 TCEQ flare tests data. Further, response surface models were developed based on controlled flare tests data sponsored by EPA (1983, 1984) and TCEQ (2010) for which both soot and CE/DRE data are available [2-6]. After simulating various flare scenarios, the data base will be used to develop correlations/response surfaces for emission inventory and flare optimization applications.

Objectives

The proposed project will

1) Study important flare operating parameters by varying CZHV, exit velocity, tip diameter, crosswind, and vent gas species.
2) Implement soot models in the CFD simulation.
3) Develop easy-to-use response surface models to estimate DRE/CE and speciated emissions including soot.

Methodology

Computational Fluid Dynamics (CFD)

A computational fluid dynamics simulation is based on the application of fundamental physics along with turbulence and chemistry models. A CFD package such as FLUENT follows the finite volume approach to solve the governing transport equations for temperature, pressure, mole fraction and other
fluxes [8-11]. Basically, the Navier-Stokes equations together with equations for mass, energy, and species transport need to be solved.

Mechanism Development using CHEMKIN

CHEMKIN, a reaction engineering software package, was used to develop the reaction mechanism files for use in the CFD software FLUENT. The complete combustion mechanisms are usually too complicated and have to be reduced to a maximum of 50 species to be used in certain Fluent models (such as EDC) and to save computation time [8-12]. Chemical kinetic mechanisms, LU 1.0, 1.1, and 2.0 for the combustion of C1-C3 hydrocarbons have been generated and validated with data of key performance indicators like laminar flame speeds, adiabatic flame temperature, ignition delay tests using Chemkin. The results for the validation of the LU 1.0, 1.1, and LU 2.0 were published in the literature [8,11].

Flare Operating Variables and Polynomial / Exponential Correlations

The variables known to influence flare efficiencies (CZH, LFL, exit velocity, tip diameter, crosswind, and vent gas species) will be studied for the DRE/CE/emissions data base [2-8]. Generalized response surface models can be established with Minitab, MATLAB statistics toolbox, and Microsoft Excel spreadsheets [13-14]. Some closed form equations (e.g., sigmoid function) and others may also be explored.

Accomplishments/Problems

Mechanism Development using CHEMKIN

A new reduced reaction mechanism LU 3.0.1 was built upon earlier mechanisms (LU 1.0, LU 1.1, and LU 2.0) geared for C1-C3 hydrocarbons. LU 3.0.1 contains important soot precursor species and can handle C2-C4 hydrocarbons. The C5-species included are n-butane, 1-butene and 1,3-butadiene. Soot precursors species (acetylene, ethylene and benzene) employed in ANSYS Fluent (e.g., Moss-Brookes-Hall) soot models are also included. This selection, which implemented the reaction path analyzer in CHEMKIN and conducted reaction rate analysis, leads to a new mechanism, LU3.0.1, with 50 species and 310 reactions. LU3.0.1 has been compared to the full USC II mechanism and earlier combustion mechanisms for its accuracy, Table I. LU3.0.1 has been validated successfully against experimental performance indicators like laminar flame speed, ignition delay and adiabatic flame temperature using CHEMKIN, Fig. 1. LU3.0.1 has been used in conjunction with in the Moss-Brooks soot model built in ANSYS Fluent to predict black carbon emission in sooty flames (2010 flare study data provided by Aerodyne Research, Inc. [4-6]).
Table I Comparison of prediction errors of reduced mechanisms for mole fraction of major species at residence time of 1 sec for C\textsubscript{3}H\textsubscript{6} fuel

<table>
<thead>
<tr>
<th>Species</th>
<th>USC I</th>
<th>LU 3.0.1</th>
<th>Abs. error %</th>
<th>LU 1.0</th>
<th>Abs. error %</th>
<th>LU 2.0</th>
<th>Abs. error %</th>
</tr>
</thead>
<tbody>
<tr>
<td>C\textsubscript{2}H\textsubscript{2}</td>
<td>1.46E-06</td>
<td>1.32E-06</td>
<td>9.72</td>
<td>1.19E-06</td>
<td>18.53</td>
<td>1.21E-06</td>
<td>17.23</td>
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<tr>
<td>CH\textsubscript{4}</td>
<td>3.01E-07</td>
<td>3.02E-07</td>
<td>0.23</td>
<td>3.30E-07</td>
<td>9.68</td>
<td>3.91E-07</td>
<td>30.07</td>
</tr>
<tr>
<td>CO</td>
<td>5.59E-03</td>
<td>5.70E-03</td>
<td>1.97</td>
<td>6.24E-03</td>
<td>11.68</td>
<td>5.98E-03</td>
<td>7.06</td>
</tr>
<tr>
<td>CO\textsubscript{2}</td>
<td>1.21E-01</td>
<td>1.21E-01</td>
<td>0.20</td>
<td>1.20E-01</td>
<td>0.64</td>
<td>1.21E-01</td>
<td>0.35</td>
</tr>
<tr>
<td>H\textsubscript{2}</td>
<td>1.35E-03</td>
<td>1.37E-03</td>
<td>2.10</td>
<td>1.51E-03</td>
<td>12.31</td>
<td>1.45E-03</td>
<td>7.41</td>
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<tr>
<td>Average abs. error %</td>
<td>2.84</td>
<td>10.57</td>
<td>12.42</td>
<td></td>
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</tr>
</tbody>
</table>

CFD Simulation of 2010 Flare Study

Computational fluid dynamics (CFD) analysis of soot yield and combustion efficiency have been performed on controlled flare tests for which DRE/CE/soot data are available. LU3.0.1 is used in conjunction with turbulence-chemistry models like non-premixed model in Ansys FLUENT 13 to simulate air assisted flare tests in 2010 study. Probability Density Function (PDF) turbulence-chemistry interaction approach has been adopted to simulate these flare tests. For 2010 study data, the PDF model provided good predictions for soot yield and CE, Figure 2 and Table II. However, the VOC yields are nearly non-existent when PDF model is used.

Fig. 2 Measured vs. Predicted black carbon

Table II Simulated (PDF) and experimental combustion efficiency of air-assisted flares in 2010 flare study

<table>
<thead>
<tr>
<th>Case no.</th>
<th>CE Exp. %</th>
<th>CE Simu. %</th>
<th>% error</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1.1</td>
<td>96.9</td>
<td>96.93</td>
<td>0.03</td>
</tr>
<tr>
<td>A2.1</td>
<td>95.9</td>
<td>95.09</td>
<td>0.84</td>
</tr>
<tr>
<td>A3.1</td>
<td>98.3</td>
<td>98.88</td>
<td>0.59</td>
</tr>
<tr>
<td>A4.1</td>
<td>97.1</td>
<td>99.23</td>
<td>2.19</td>
</tr>
<tr>
<td>A5.1</td>
<td>95.9</td>
<td>99.37</td>
<td>3.62</td>
</tr>
<tr>
<td>A6.1</td>
<td>99.4</td>
<td>92.9</td>
<td>6.54</td>
</tr>
<tr>
<td>Avg.</td>
<td></td>
<td></td>
<td>2.3</td>
</tr>
</tbody>
</table>
Response Surface Models

Since soot emission was not considered for the CE calculations in the 1983/1984/2010 flare studies, corrections were made based on soot data provided by ARI and designated as "corrected CE" or CCE [2-6]. In this work, quadratic response surface (RS) models between DRE/CE/soot emission and the design/operating parameters were developed based on the 2010 TCEQ flare study and 1983/1984 EPA test data using Minitab and MATLAB statistics toolbox [2-6,13-14]. The following response surface models were developed:

a. log BC versus LHV, VG, S, DB (steam assist flares)

\[
\log \text{BC} = -2.567 + 0.002904 \text{LHV} - 0.4747 \text{S} - 0.1679 \text{VG} + 4.321 \text{DB} + 0.4575 \text{S*DB} \\
\text{Eq. 1}
\]

b. log BC versus LHV, V, A, D, DB (air assist flares)

\[
\log \text{BC} = -2.350 - 0.000001 \text{LHV*LHV} + 0.0501 \text{A*A} + 0.000115 \text{LHV*D} + 0.000187 \text{LHV*A} - 0.01579 \text{D*A} - 0.01203 \text{D*V} + 0.07571 \text{D*DB} - 0.1208 \text{A*V} \\
\text{Eq. 2}
\]

c. CCE vs. S, LHV, V, VG, and D (steam assist flares)

\[
\text{CCE} = 98.78 + 0.1088 \text{S} - 0.001152 \text{LHV} - 0.00771 \text{V} + 0.0862 \text{VG} - 0.023 \text{D} - 0.000169 \text{LHV*D} \\
\text{Eq. 3}
\]

d. CCE vs. A, LHV, VG, and DB (air assist flares)

\[
\text{CCE} = 107.24 - 0.04917 \text{LHV} - 3.18 \text{A} + 1.773 \text{VG} - 6.79 \text{DB} + 0.000021 \text{LHV*LHV} - 1.396 \text{A*A} - 0.000980 \text{LHV*VG} - 5.66 \text{A*DB} \\
\text{Eq. 4}
\]

e. DRE vs. LHV, S, VG and D (steam assist flares)

\[
\text{DRE} = 99.561 - 0.000708 \text{LHV} + 0.0363 \text{S} + 0.0287 \text{VG} - 0.0860 \text{D} - 0.000448 \text{S*S} + 0.000429 \text{LHV*D} - 0.000740 \text{S*VG} \\
\text{Eq. 5}
\]

f. DRE vs. LHV, A, and VG (air assist flares)

\[
\text{DRE} = 92.835 + 0.002843 \text{LHV} - 5.192 \text{A} - 0.1971 \text{VG} + 0.000983 \text{LHV*A} \\
\text{Eq. 6}
\]

where LHV: Vent gas lower heating value (BTU/scf), D: Flare tip Dia (inch); A: Air assist flow (lb/MMBTU), S: Steam assist flow (lb/MMBTU), DB: Double bond (0/1), V: Exit velocity (ft/s), BC: Soot yield (lb/MMBTU), VG: Vent gas heat flow (MMBTU/hr), CCE: Corrected Combustion Efficiency (%), DRE: Destruction and Removal Efficiency (%).

**Future Work**

- Work on Geometry/Meshing for steam/air assisted flares.
- Continue to simulate 2010 JZ data (Propylene/Propane) and 1983/1984 EPA data (with Propane) with PDF & EDC models.
- Inverse response models of S (or A, VG, LHV) as a function of Log BC and DRE.
- Use Dimensionless Variables in Response Surface Models
- Study the effect of H2 and propene vs. propane on soot yield and CE

**List of Publications and Presentations**

- Hitesh S. Vaid, Kanwar Devesh Singh, Helen H. Lou, Daniel Chen, Peyton Richmond, "A Run Time Combustion Zoning Technique towards the EDC Approach in Large-Scale


References


