A. Cuoci\textsuperscript{1}, A. Frassoldati\textsuperscript{1}, T. Faravelli\textsuperscript{1} and F.A. Williams\textsuperscript{2}

Cool flames in microgravity droplet combustion

29\textsuperscript{th} American Society for Gravitational and Space Research
5\textsuperscript{th} International Symposium for Physical Sciences in Space

November 3-8, 2013 – Orlando, Florida (USA)
Outline

1. Introduction
   ✓ Cool flames
   ✓ Low-temperature mechanism

2. Mathematical model
   ✓ Governing equations and numerical methodology
   ✓ Detailed kinetic mechanism

3. Auto-ignited n-decane (C10H22) droplets
   ✓ Comparison with experiments
   ✓ Structure of the cool flame
   ✓ Numerical experiments on n-heptane and n-dodecane

4. Hot-wire ignited n-heptane (NC 7H16) droplets
   ✓ Comparison with experiments
   ✓ Kinetic analysis
   ✓ Comparison between different kinetic mechanisms

5. Conclusions and future works
1. **Introduction**
   - Cool flames
   - Low-temperature mechanism

2. **Mathematical model**
   - Governing equations and numerical methodology
   - Detailed kinetic mechanism

3. **Auto-ignited n-decane (C10H22) droplets**
   - Comparison with experiments
   - Structure of the cool flame
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   - Comparison between different kinetic mechanisms

5. **Conclusions and future works**
Ordinary, visible flames burn at a high temperature between 1500K and 2000K.

Cool flames burn at the relatively low temperature of 500K to 800K, and their chemistry is completely different. Normal flames produce soot, CO₂ and water. Cool flames produce CO and CH₂O.

Jet Stirred Reactor: i-octane/air at 7 bar

The low-temperature (LT) chemistry

**High Temperature Mechanism**

- $\beta$-Decomposition Products
  - $E_{\text{eff}} \approx 30,000 \text{ cal/mol}$
  - $E_{\text{eff}} \approx 19,000 \text{ cal/mol}$
  - $\text{HO}_2\cdot + \text{ alkenes}$
  - $\text{OH}\cdot + \text{ Cyclic Ethers}$
  - $\text{OH}\cdot + \text{ aldehydes + alkanes}$

**Intermediate Temperature Mechanism**

- $E_{\text{eff}} \approx 0 \text{ cal/mol}$
  - $\text{OQOOH} + \text{OH}\cdot$
  - Branching

**Low Temperature Mechanism**

- $R\cdot = \text{alkyl-radical (e.g. C}_7\text{H}_{15})$
- $\text{ROO}\cdot = \text{peroxy radical}$
- $\text{\cdotQOOH} = \text{hydroperoxy-alkyl rad.}$
- $\text{\cdotOOQOOH} = \text{alkyl-hydroperoxy rad.}$
- $\text{OQOOH} = \text{ketohydroperoxyde}$
Cool flames in droplet combustion (I)

Auto-ignition experiments
n-heptane droplets in air ($d_0=0.70$ mm)

Adapted from: Tanabe et al., 26th Symposium (International) on Combustion, p. 1637-1643 (1996)
Cool flames in droplet combustion (II)

Cuoci A., Mehl M., Buzzi-Ferraris G., Manca D., Faravelli T., Ranzi E.,
Autoignition and burning rates of fuel droplets under microgravity,

Fig. 4. Time evolution of the predicted maximum gas-phase temperature for different grid number of points in the gas phase (a); time and radial evolution of the predicted maximum gas-phase temperature (b) (autoignition simulation, n-decane droplet, \(d_0 = 0.91\) mm, \(P = 0.1\) MPa, \(T_G = 633\) K).

1. Better understand the features of cool flames
2. Study the possible formation of cool flames in hot-wire ignitions
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5. Conclusions and future works
Mathematical model

Liquid droplet

Gas phase

Continuous equation
Energy equation
Species equations

Thermodynamic equilibrium
Conservation of fluxes

Interface (liquid/gas)

Spherical symmetry
1D equations
Stretched grid

Ratio between gas and liquid radii: ~120

Equation of state (gas phase): ideal gas


Dufour effect: neglected

Soret effect: accounted for

Cuoci et al., Combustion and Flame 143, p. 211-226 (2005)

Numerical methodology

finite differences in space  Ordinary DAE system

large dimensions of the problem  Numerical difficulties in solving the resulting very stiff DAE system
non linearity of reaction rates and transport properties

The DAE system is structured as a (quasi) tridiagonal block matrix with square and dense submatrices whose dimensions depend on the number of chemical species included in the kinetic scheme.

Example

200 points x 435 species ~ 90,000 equations ~24 h of CPU time

*BzzDAEBloTri*, a specifically conceived numerical solver, allows to efficiently treat the structured sparsity of the Jacobian matrix as well as the stiffness of the DAE system.

http://www.chem.polimi.it/homes/gbuzzi

Detailed kinetic mechanism

Kinetic mechanism of **pyrolysis, oxidation and combustion** of small (C1-C3) and large hydrocarbons up to Diesel and jet fuels (C16) as well as several pollutants

**Hierarchy**  
**Modularity**  
**Generality**

~ 435 chemical species  
~ 13,495 reactions

The kinetic mechanism is freely available in CHEMKIN format at this web address

http://creckmodeling.chem.polimi.it

Frassoldati, A. et al., Combustion and Flame 157(2010), pp. 2-16  
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Autoignition experiments
Experiments performed in either the Japan Microgravity Center (JAMIC) or the NASA Glenn Research Center

Fuel: n-decane (C_{10}H_{22})
Initial diameters: 0.91, 1.22 and 1.57 mm
Pressure: 1 atm
Droplet temperature: 300 K
Gas phase temperature: 633 K
Gas phase composition: air (21% O_2, 79% N_2)
Negligible soot formation
Droplet was suspended using a quartz fiber

If the simulations are performed without considering any reactions in the gas phase, the calculated vaporization rate is smaller than the experimental value.

Only with the inclusion of low temperature (LT) reactions, the numerical simulations are able to correctly reproduce the experimental data.
Dumped cool flames

- Initial dumped cool flame and a successive more stable temperature profile at ~750 K.
- Once the first flame ignites, fuel is consumed and only partially replaced by the vaporization.
- The successive cool flames exhibit a higher frequency, produce less heat and gradually move the system from the cool flame to the slow combustion regime.
**Cool flame structure**

- **Peak temperature ~750K**
- Small amounts of $\text{H}_2\text{O}$ and $\text{CO}_2$ with respect to conventional flames
- No OH radicals
- $d_0 = 1.22$ mm
- Time = 3 s

**Key points**

- Co-existence of fuel ($\text{C}_{10}\text{H}_{22}$) and oxidizer ($\text{O}_2$)
- Large amounts of ketohydroperoxides (e.g. $\text{NC}_{10}\text{H}_{22}\text{-OQOOH}$)
Extension to n-heptane and n-dodecane

**n-heptane**

- $d_0=1.57\, \text{mm}$
- $d_0=1.22\, \text{mm}$
- $d_0=1.57\, \text{mm}$

**n-dodecane**

- $d_0=1.57\, \text{mm}$
- $d_0=1.22\, \text{mm}$
- $d_0=1.57\, \text{mm}$

---

**Cool flames**

- 7 cool flames
- 6 cool flames
- 9 cool flames
- 12 cool flames
- 11 cool flames
- 10 cool flames
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Description of the experiments

**Hot-wire ignition experiments**
Experiments performed on board the International Space Station (ISS) using the multi-User Droplet Combustion Apparatus (MDCA) installed in the Combustion Integrated Rack (CIR) facility as a part of the Flame Extinguishment Experiments (FLEXs)

**Fuel: n-heptane (NC 7H16)**
Initial diameter: 3.91 mm
Pressure: 1 atm
Initial temperature: 300 K
Gas phase composition: air
Negligible soot formation
Droplet tethered by a fine silicon carbide filament

Adapted from Nayagam et al. (2012)

The agreement with the experiments is satisfactory if the LT mechanism is accounted for.

<table>
<thead>
<tr>
<th></th>
<th>Experiment</th>
<th>Simulation</th>
</tr>
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<tbody>
<tr>
<td>1st extinction diameter [mm]</td>
<td>3.28</td>
<td>3.45</td>
</tr>
<tr>
<td>2nd extinction diameter [mm]</td>
<td>1.30</td>
<td>1.10</td>
</tr>
<tr>
<td>mean vaporization rate [mm²/s]</td>
<td>0.368</td>
<td>0.390</td>
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</tbody>
</table>
Flame structures

Hot flame @ 2 s

Cool flame @ 30 s

Temperature

NC\textsubscript{7}H\textsubscript{16}

CO\textsubscript{2} x2

OH x 1000

H\textsubscript{2}O x5

CO x10

O\textsubscript{2}

Temperature

NC\textsubscript{7}H\textsubscript{16}

CO x10

CO\textsubscript{2} x10

H\textsubscript{2}O x20

O\textsubscript{2}

NC\textsubscript{7}H\textsubscript{16}-OQOOH x100

Maximum temperature

1\textsuperscript{st} extinction (hot flame)

2\textsuperscript{nd} extinction (cool flame)

Cool flame at 690-700 K
Path analysis

Hot flame @ 2 s

- \( nC_7H_{16} \)
- \( nC_7H_{15} \)
- \( + O_2 \)
- \( R_7OO \)
  - \( C_4H_9P + C_3H_6 \)
  - \( C_3H_7 + C_4H_8 \)
  - \( C_2H_4 + C_5H_{11} \)
  - \( C_2H_5 + C_5H_{10} \)
  - \( CH_3 + C_6H_{12} \)
  - \( H + C_7H_{14} \)

The thickness of the arrows is proportional to the importance of the corresponding flux.

Transition @ 8 s

- \( nC_7H_{16} \)
- \( nC_7H_{15} \)
- \( + O_2 \)
- \( R_7OO \)
  - \( + O_2 \)
  - \( \bullet Q_7OOH \)
  - \( O_7OOH + OH^\bullet \)
  - \( HO_2^\bullet + nC_7H_{14} \)
  - \( OH^\bullet + Cyclic Ethers \)
  - \( OH^\bullet + R’CHO+C_nH_{2n} \)

Cool flame @ 30 s

- \( nC_7H_{16} \)
- \( nC_7H_{15} \)
- \( + O_2 \)
- \( R_7OO \)
  - \( + O_2 \)
  - \( \bullet Q_7OOH \)
  - \( OH^\bullet + Cyclic Ethers \)
  - \( OH^\bullet + R’CHO+C_nH_{2n} \)

Branching
Global sensitivity coefficients of the vaporization rate during the LT combustion

- NC7-OOQOOH → NC7-QOOH + O2
- NC7-QOOH + O2 → NC7-OOQOOH
- NC7-OOQOOH → NC7-QOOH + OH
- OH + NC7 → H2O + NC7H15
- NC7-QOOH → NC7H14O + OH
- NC7-QOOH → NC7H14 + HO2

Cool flame @ 30 s

- nC7H16
- nC7H15• + O2 → R7OO•
- R7OO• + O2 → HO2• + nC7H14
- HO2• + C7H14O + OH• + Cyclic Ethers
- OH• + nC7H14
- OH• + R’CHO + CnH2n
- OQ7OOH
- OQ7OOH + OH• → Branching
Comparison with other kinetic mechanisms (I)

Several detailed kinetic mechanisms (with Low Temperature chemistry) were tested and compared

**Polimi-C 1C 16T0T (version 1212)**
- Species: 435
- Reactions: 13,495

**Lu-NC7**
- Species: 188
- Reactions: 939

**LLNL-NC7**
- Species: 658
- Reactions: 2,827

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Comparison with other kinetic mechanisms (II)

The results are strongly affected by the ability of the kinetic mechanism to correctly capture the features of the cool flame (i.e. by the accuracy and the reliability of the low-temperature chemistry).
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5. Conclusions and future works
Conclusions

Numerical modeling of auto-ignited and hot-wire ignited isolated droplets in microgravity with detailed kinetic mechanisms were successfully performed.

The formation of cool flames, both for n-decane and n-heptane droplets, was observed, explained and compared with experimental measurements.

**Auto-ignition of n-decane droplets** (experiments performed by Xu et al.)
We demonstrated that the observed vaporization rates can be explained only by the presence of a cool flame around the droplet.

**Hot-wire ignited n-heptane droplets** (experiments performed by Nayagam et al.)
We confirmed the hypothesis that after the first-stage extinction, the vaporization is sustained by a low-temperature, soot-free, “cool-flame” heat release.
Additional simulations of experiments of hot-wire ignition experiments on n-heptane droplets to check the formation of cool flames

Deeper investigations about the chemistry of cool flames

Improvements in the numerical model (radiative heat transfer, numerical methodology, etc.)

Modeling of soot formation through a detailed kinetic mechanism (based on the discrete sectional method)

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**Table 1**

Experimental conditions, measured droplet initial diameter $d_0$, hot-flame extinction diameter $d_{he}$, and the second-stage extinction diameter $d_e$.  

<table>
<thead>
<tr>
<th>Test #</th>
<th>$P$ (atm)</th>
<th>$O_2$ (%)</th>
<th>$CO_2$ (%)</th>
<th>$d_0$ (mm)</th>
<th>$d_{he}$ (mm)</th>
<th>$d_e$ (mm)</th>
<th>$K$ (mm²/s)</th>
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</tbody>
</table>

Adapted from Nayagam et al., Combustion and Flame, 159, p. 3583-3588 (2012)
The authors would like to acknowledge Prof. Eliseo Ranzi (Politecnico di Milano) for his interesting comments and Dr. Daniel L. Dietrich (NASA Glenn Research Center, Cleveland, USA) for the useful discussions and suggestions and the additional details about the hot-wire ignition experiments.

The work at Politecnico di Milano was partially supported by the Italian Government MSE/CNR (Biofuel Project: Utilizzo di biocombustibili liquidi e gassosi per la generazione distribuita di energia elettrica)
CRECK Modeling on the web

All our kinetic schemes can be freely downloaded in CHEMKIN format from our web site:

http://creckmodeling.chem.polimi.it/

Statistics since January 2013
Unique visitors: 3,500
Visits: 6,700 (~25 per day)

Our kinetic schemes were downloaded more than 3,600 times since Jan 2013
Validation of the kinetic mechanism: n-heptane

Polimi C1C16TOT (435 species)

Experimental data from:

Experimental data from:
Veloo P.S., Jahangirian S., Dryer F.L., *An experimental and kinetic modeling study of the two stage auto-ignition kinetic behavior of C7, C10, C12, and C14 n-alkanes*, Spring Technical Meeting of the Central States Section of the Combustion Institute, Dayton, Ohio (2013)

Shock-tube experiments

Princeton Variable Pressure Flow Reactor at temperatures of 500-1000 K and at a pressure of 8 atm
Validation of the kinetic mechanism: n-heptane


Validation of the kinetic mechanism: \textit{n-heptane}

**Shock-tube experiments**

Experimental data from:


**LLNL NC7 (658 species)**

**Princeton Variable Pressure Flow Reactor**

Reactor at temperatures of 500-1000 K and at a pressure of 8 atm

Experimental data from:

Skeletal mechanisms

Polimi-C 1C 16TOT (version 1212)
Species: 435
Reactions: 13,495

Lu-NC7
Species: 188
Reactions: 939
C.S. Yoo et al., Combustion and Flame, 158(9), p.1727–1741 (2011)
Reduction performed by the authors

LNL-NC7
Species: 658
Reactions: 2,827
Reduction performed by the authors

Species: 100
Reactions: 1,567
Reduction factor: 4.35
Stagni A., Lumping and reduction of detailed kinetic schemes: an effective coupling, Submitted to Industrial & Engineering Chemistry Research

Species: 88
Reactions: 387
Reduction factor: 2.13
C.S. Yoo et al., Combustion and Flame, 158(9), p.1727–1741 (2011)

Species: 160
Reactions: 1,540
Reduction factor: 4.11
Validation of the kinetic mechanism: n-heptane

Original mechanism (435 species)

Reduced mechanism (100 species)

Experimental data from:

Experimental data from:
Veloo P.S., Jahangirian S., Dryer F.L., Spring Technical Meeting of the Central States Section of the Combustion Institute, Dayton, Ohio (2013)

Princeton Variable Pressure Flow Reactor at temperatures of 500-1000 K and at a pressure of 8 atm
Validation of the kinetic mechanism: \textit{n}-heptane

- Original mechanism (188 species)
- Reduced mechanism (88 species)

**Experimental data from:**

**Princeton Variable Pressure Flow Reactor**
Reactor at temperatures of 500-1000 K and at a pressure of 8 atm

**Experimental data from:**
Veloo P.S., Jahangirian S., Dryer F.L., Spring Technical Meeting of the Central States Section of the Combustion Institute, Dayton, Ohio (2013)
Validation of the kinetic mechanism: n-heptane

Original mechanism (658 species)
Reduced mechanism (160 species)

Shock-tube experiments

Experimental data from:

Experimental data from:
Veloo P.S., Jahangirian S., Dryer F.L., Spring Technical Meeting of the Central States Section of the Combustion Institute, Dayton, Ohio (2013)