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n-Heptane Chemical Mechanism Evaluation for Conterflow Nonpremixed Flame Structure on $1D$ and $2D$ Open Source Codes

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Abstract. *Due environmental and economic reasons the combustion processes that occurs on engines and industrial applications must to be investigated more deeply. The combustion of n-$C7H16$ has been investigated with chemical mechanism for analyses of burning velocities, the structure and extinction of nonpremixed flames for diesel engines*

The number of operations required for solving the chemical kinetics in CFD simulations depends on the number of cells in the mesh and the size of the oxidation mechanism. The size of the mechanism defines the level of complexity to integrate the system of high degree of stiff nonlinear ODE.

Steady, axisymmetric, laminar flow of two counterflowing streams toward a stagnation plane is considered where the a fuel stream made up of prevaporized n-heptane and nitrogen injecteds. The experimental data of conterflow flame non-premixed by Berta *et al.* (2008) are compared with numerical simulations in codes Cantera, with a model one-dimensional, and OpenFoam, with a model two-dimensional and time dependent.

Keywords: *combustion, kinetics reaction mechanisms, flames, counterflow*

1. INTRODUCTION

There is a considerable interest to understanding n-heptane combustion as it is treated as a primary reference fuel for octane rating in compression ignition internal combustion engines. Several investigators have developed chemical-kinetic mechanisms describing the oxidation of n-heptane (Westbrook *et al.*, 1988; Curran *et al.*, 1998). Extensive experimental work has also been performed for validating/developing these detailed mechanisms by Berta *et al.* (2008); Mehl *et al.* (2011). In the present paper two mechanisms developed by LLNL (Lawrence Livermore National Laboratory) with among

159 species were assembled from this detailed LLNL n-heptane mechanism (version 2) (Lu *et al.*, 2009) and 68-species skeletal mechanism for n-heptane, based on the detailed LLNL n-heptane mechanism (version 2) (Lu *et al.*, 2009) are studied into a two-dimensional CFD code, OpenFoam (Open Field Operation and Manipulation)(Greenshields, 2015b,a), and one-dimensional code in Cantera (Goodwin, 2012), is a suite of object-oriented software tools for problems involving chemical kinetics, thermodynamics, and/or transport processes. investigated their ability to predict chemical and thermal structures of nonpremixed flames.

The mechanism LLNL is based on the mechanism of Curran *et al.* (1998) this detailed chemical kinetic mechanism has been developed and validated by comparison to experiments in shock tubes and rapid compression machines. The mechanism performs well at both low and high temperature and over a broad pressure range important for internal combustion engines. The intermediate and the reduced mechanism were used to calculate extinction and autoignition of n-heptane in strained laminar flows. Steady laminar flow of two counterflowing streams toward a stagnation plane was considered by Curran *et al.* (1998). One stream, composed of prevaporized n-heptane and nitrogen, is injected from the fuel boundary and the other stream composed by air, is injected from the oxidizer side. Critical conditions of extinction and autoignition given by the strain rate, temperature, and concentrations of the reactants at the boundaries were calculated (Seiser *et al.*, 2000). Using the dimension reduction strategies (Lu *et al.*, 2009) a reduced mechanism with 52 species was first derived from a detailed mechanism with 561 species.

Detailed chemical-kinetics mechanisms for fuels are generally validated using some specific targets, such as flow reactor data, ignition delay times from shock tube experiments, and laminar flame speeds. The validation process then involves performing zero- and one-dimensional simulations using codes such as RUN1DL (Peters and Rogg, 1993), OPPDIF (Lutz *et al.*, 1996), and CHEMKIN (Kee *et al.*, 1980) and comparing the results with the available experimental data. Extensive experimental data for the intermediate species concentrations are required for obtaining a reasonably built or calibrated kinetics mechanism.

Although the use of multi-dimensional codes are important to the study of flame stability and pollutant formation, the main reason why researchers are restricting themselves to zero- and one-dimensional codes is the limitation of time and computational cost. Although the calculation of multidimensional flames is known since 1960 (Ferri, 1973), the computational time increases significantly with the size of the chemical-kinetics mechanism used, CFD code developments are limited to either simple fuels such as hydrogen.

The objective this work is to compare the chemical kinetics through experimental and numerical numerical by Berta *et al.* (2008) using the 159 species LLNL reduced mechanism kinetic and 68-species skeletal mechanism with $2D$ simulation in OpenFoam simulation and $1D$ simulation Cantera simulation. Once validated the chemical kinetic, can apply it in other numerical simulations as turbulent flames and spray.

2. Test Case

2.1 Nonpremixed Flame Structure

The experimental setup it is sketched in Fig. (1) which the separation distance between the counterflow nozzles of the $10\,mm$. A mixture of the n-heptane and nitrogen fuel it's prevaporized and introduced from the bottom nozzle. A nitrogen

curtain was established through an annular duct surrounding the fuel jet to isolate the flames from ambient disturbances. This nitrogen and combustion products were vented and cooled through another annular duct around the oxidizer nozzle. The velocities of the two streams define the global strain rate (1)

$$a_g = \frac{2|V_O|}{L}\left(1 + \frac{|V_F|}{|V_O|}\sqrt{\frac{\rho_F}{\rho_O}}\right) \tag{1}$$

were, V_F and V_F represent the velocities of fuel and air jets, respectively and ρ_F and ρ_O represent the densities of the respective jets. L is the separation distance between the two nozzles. For model validation purpose the flame established at a moderate strain rate of $150\ s^{-1}$ is considered. Fuel used for this flame contained 15% of the n-heptane and 85% nitrogen. The velocities are $0.3252\,m/s$ and $0.375\,m/s$ for the fuel and air respectively. The temperatures of the fuel and air jets were $300\,K$ and $400\,K$, respectively. The equation Eq. (1) is obtained from an asymptotic theory where the Reynolds numbers of laminar flow at the boundaries are presumed to be large (Seshadri and Williams, 1978).

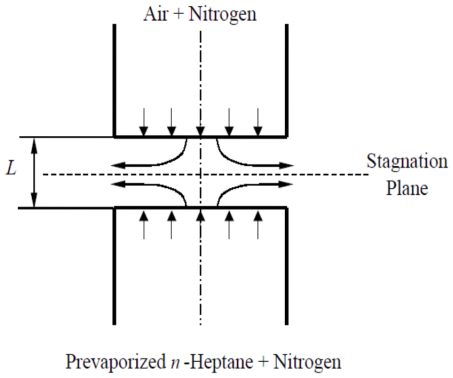

Figure 1. Experimental setup of the counterflow configuration

3. Numerical Simulation

3.1 OpenFoam Simulation

OpenFOAM is an open source object-oriented software package written in C++. It provides a framework to develop numerical solvers in continuum mechanics. Main advantages of the design are the overloaded operators, allowing expressive and versatile syntax for implementations of complex physical models, the extensive pre- and postpro- cessing tools including complex geometry handling and data in-/output and a wide range of implemented discretization schemes and boundary conditions. Additionally, OpenFOAM provides a good parallelization, a high accuracy and is available free of charge. It has been validated many times and is widely used. Fundamental developments are done by the OpenFOAM Foundation with contributions from a large community. The complete source code is licensed under the GNU General Public License (GPL) for free use and customization (Jasak *et al.*, 2007).

In the OpenFOAM simulation here was used solver reactingFoam. The transport equations for species and sensible enthalpy are

$$\frac{\partial(\rho Y_k)}{\partial t} = -\vec{\nabla}.(\rho Y_k \vec{v}) + \vec{\nabla}.(\mu \vec{\nabla} Y_k) + \dot{r_k} \tag{2}$$

$$\frac{\partial(\rho h_s)}{\partial t} = -\vec{\nabla}.(\rho h_s \vec{v}) + \vec{\nabla}.(\frac{\lambda}{c_p}\vec{\nabla} h_s) + \frac{Dp}{Dt} + \dot{\vec{q}}_{reaction} \tag{3}$$

One can see, that Eq . (2) is based on the assumption that the ratio of momentum diffusivity and mass diffusivity is unity. Thus, the dimensionless Schmidt number Sc yields

$$Sc = \frac{\mu}{\rho D} = 1 \rightarrow \rho D = \mu \tag{4}$$

were, the mass diffusivity D has to be same for all species and the species difusion process is entirely controlled by the mixture viscosity, which is calculated from Sutherland's law. Additionally, cross diffusion process based on pressure and temperature gradients are neglected.

In Eq . (3) a unity Lewis number Le as well as the disregards from above are assumed:

$$Le = \frac{\lambda}{D c_p \rho} = 1 \rightarrow \frac{\lambda}{c_p} = \rho D \tag{5}$$

3.2 Cantera Simulation

Cantera is an object oriented software toolkit for problems involving chemical kinetics, thermodynamics and transport processes (Goodwin, 2012). It consists of a kernel written in C++ which is accessible through a wide range of environments like Python and C++. Cantera provides fast, efficient algorithms and is highly customizable.

In Cantera the flames are $1D$ in the sense that, when certain conditions are fulfilled, the governing equations reduce to asystems of equations in the axial coordinate z, where finite-difference flow equations to form a system of nonlinear algebraic equation and the systems of equations are solved using the Newton-Hybrid method. A first solution is found with low solution tolerances and without an energy equation. This is a good approximation because in the experimental case the height of the channel is very small compared to the diameter so the Reynolds number is less than 2300 and we are in the case of laminar,

$$\frac{d}{dz}(\rho u) + 2\rho V = 0 \tag{6}$$

$$\rho \frac{dV}{dt} = \frac{d}{dz}\left(\mu \frac{dV}{dz}\right) - \Lambda - \rho u \frac{dV}{dz} - \rho V^2, \tag{7}$$

$$\rho \frac{dY_k}{dt} = -\rho u \frac{dY_k}{dz} - \frac{dJ_k}{dt} + W_k \dot{\omega}_k, \tag{8}$$

$$\rho c_p \frac{dT}{dt} = -\rho c_p u \frac{dT}{dt} + \frac{d}{dz}\left(\lambda \frac{dT}{dz}\right) - \sum_k W_k \dot{\omega}_k h_k - \sum_k J_k c_{p,k} \frac{dT}{dz}, \tag{9}$$

where, Eq. 6, Eq. (7), Eq. (8) and Eq. (9) are the equations for continuity, radial momentum and species conservation, respectively, and ω_k is net production rate.

3.3 Results and Discussion

The simulations were performed using SGI Altrix 17 compute nodes with 2 CPUs each node, each CPU is Intel Xeon Quad-Core 5540 2.53-GHz, 8MB cache, 5.83 GT / s; 24-GB FBDIMM DDR3 1066MHz memory; 24 GB of RAM per node. The nonpremixed flame (Berta *et al.*, 2008; Seiser *et al.*, 1998), have conducted experiments on this laminar flame and obtained temperature and species measurements along the axis of symmetry (centerline). For balancing the momentums of the gases on the two sides of the stagnation plane (surface along which the axial velocity component is zero) causes opposing-jet nonpremixed flame to curve toward the air jet. Comparing the temperature distributions

shown in Fig. (2) it can be realized all the mechanisms have resulted in flames that are nearly identical in shapes and sizes. Temperature and axial-velocity distributions along the centerline across the flame are shown in Fig. (2). While the computed profiles are shown using lines, temperature measurements obtained by Berta *et al.* (2008) are plotted. Even though the moments of the fuel and air jets were matched, the stagnation point $(U = 0)$ is located $0.004m$, both for the simulation in OpenFOAM as for the simulations in Cantera.

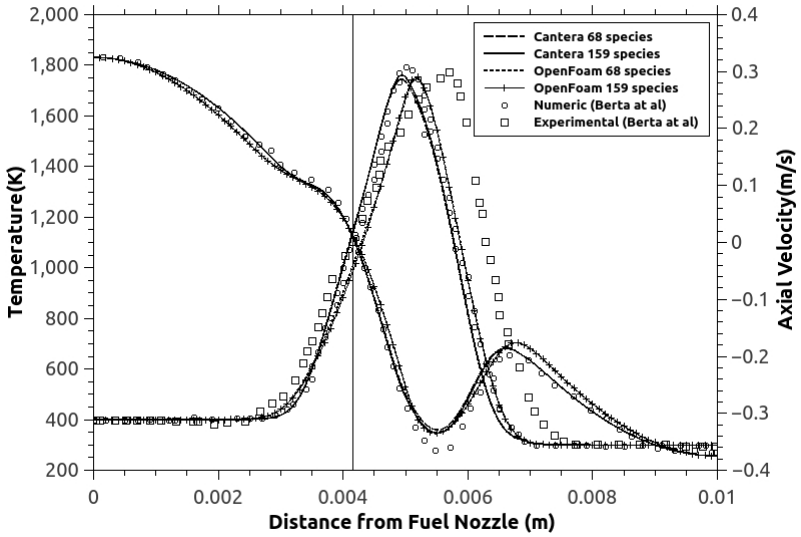

Figure 2. Temperature and axial velocity for n-$C7H16$

We analyze for 2-D temperature profile in OpenFOAM Fig. (3), higher temperature in the region close to the center of the nozzle in accordance with the temperature profile shown in Fig. (2).

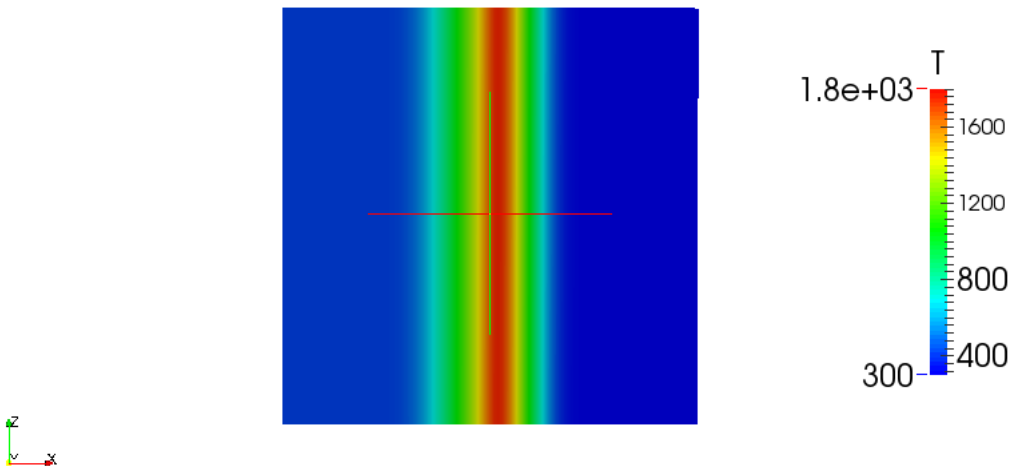

Figure 3. Temperature in OpenFoam 2D simulation

The temperature peak is located at $0.005\,m$ for all simulations in Cantera of $1761\,k$ for distributions between $300\,K$ and $1800\,K$. In OpenFoam simulation the temperature peak is located at $0.0052\,m$ and the value of $1750\,K$. The temperature measurements obtained by Berta *et al.* (2008) the temperature peak is $1798\,K$ in $0.56\,m$. However, as suggested by Seiser *et al.* (1998), flame in the experiment seems to be broader and shifted by $0.05\,m$ toward the air duct. The comparison of minor species profiles with the experimental data shows. The experiment has been performed at $1\,atm$, according to Eq. (1) we have a strain rate of $150s^{-1}$, where the predicted flame speed and strain rate are determined from the stagnation simulation with the same definitions that were applied to the experimental data (minimum velocity for flame speed and maximum preflame gradient for strain). The predicted flame speed and strain rate are determined from the stagnation simulation with the same definitions that were applied to the experimental data (minimum velocity for flame speed and maximum preflame gradient for strain)(Natarajan *et al.*, 2007).

Other details of the configuration can be found in Seiser *et al.* (1998). The oxidizer is air and the fuel is diluted with nitrogen, such that the stoichiometric mixture fraction is $Z_{st} = 0.1$.

In Fig. (4) we can verify the fuel and oxidant along Distance from nozzle fuel. We can see a slight difference in the profile of N_2 for OpenFOAM compared with others profiles. Fuel used for this flame contained 15% heptane and 85% nitorgen, in molar fraction. This is due to the numerical method used in OpenFOAM, which differs from the others.

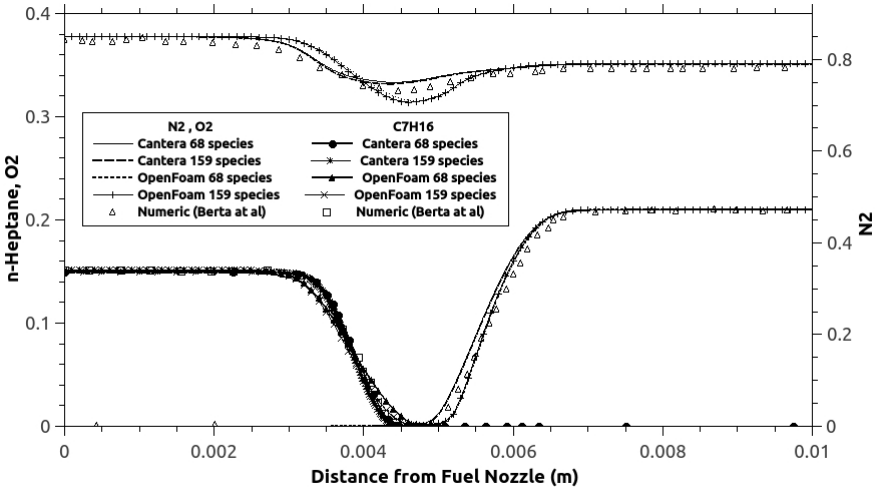

Figure 4. Distributions of fuel, oxygen and N_2 plotted along the ceterline. Lines represent flames computed using different chemical kinetics mechanisms and symbols represent measurements of (Berta *et al.*, 2008) Global strain rate is $150.\ s^{-1}$

In Fig. (5) and Fig. (6) we can see more clearly the results obtained using in OpenFOAM and the compared with experimental cases used Cantera, evidenced by the disagreement of the curves of the OpenFOAM and Cantera in relation numerical results of Berta *et al.* (2008). This is due to different numerical methods used in solvers and differences between grids for each case. Another important factor is associated with the chemical kinetic mechanism adopted in Berta *et al.* (2008) by different of the chemical kinetic mechanism adopted in OpenFOAM and Cantera cases of present work.

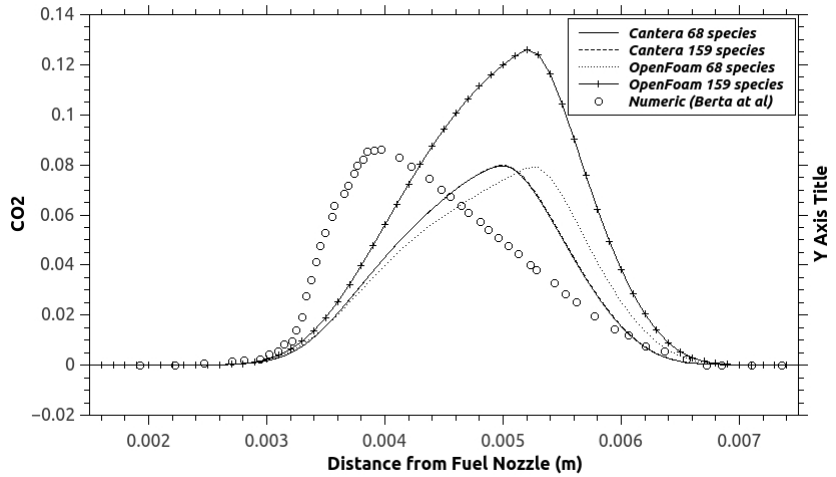

Figure 5. Distributions of CO_2 plotted along the centerline

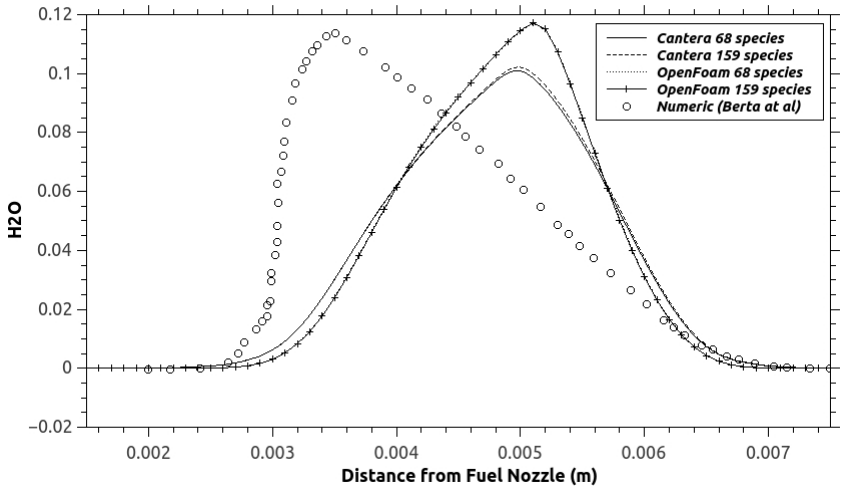

Figure 6. Distributions of H_2O plotted along the centerline

A radical species OH is known to be found in the region between burned and unburned gases in a flame. Planar laser induced fluorescence (PLIF) is a popular, nonintrusive technique for studying flame structure. By tuning the PLIF system to the proper wavelength, OH can be excited and its fluorescence can be imaged, resulting in a map of concentrations. Knowing where OH is located allows the flame front to be defined. Furthermore, if the concentrations of OH can be quantified then this numerical data can be used in theoretical models (Jalbert, 2011). There is a relationship between peak power variation and the concentration of OH, as can be seen in Fig. (7). Where the OH peak region is close to the peak region of the energy variation rate.

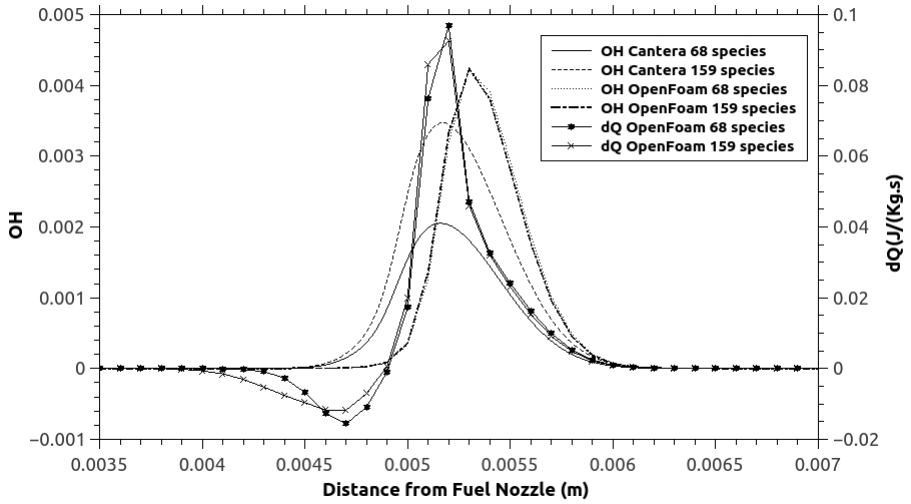

Figure 7. Distributions of HO and dQ plotted along of the distance from fuel fozzle

4. Conclusions

A numerical investigation was performed to examine the structure of N_2 diluted nonpremixed n-heptane/air conterflow flames. For numerical simulation for temperature and species-concentration profiles, including those of major species (n-heptane, O_2, N_2, CO_2, and H_2O), the results in OpenFoam simulation and Cantera simulation for prevaporized n-heptane counterflow flames established at 85% nitrogen dilution and strain rate of the $150\ s^{-1}$, were in accordance with literature suitable for use in other models with turbulent combustion.

The measurements have been compared with simulations performed using reaction mechanism with 159 species for LLNL and 68-species skeletal mechanis. The thermodynamic results were satisfactory compared to the experimental results. However, given the different numerical implementations, the molar concentrations for species H_2O, CO_2, and OH were different, but expected, due different numerical methods used in solvers and differences between grids for each case. This result shows that the chemical kinetics is efficient for future numerical simulations as turbulent flames and sprays. It is expected that there will be a divergence in the molar concentrations of the species H_2O, CO_2, and OH.

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