# Planar Detonations

Goals of the Project (do not use these for the motivation in your report)

- 1. Improve <u>your</u> understanding of the sensitivity of detonation properties to initial reactant conditions.
- 2. Allow <u>you</u> to investigate chemical kinetic behavior behind the leading shock in a planar detonation.

## **Report Format**

Your report should be complete but <u>concise</u>. Please follow the course's report guidelines : <u>http://seitzman.gatech.edu/classes/ae6766/projectformat.html</u>.

However since you have already described how an equilibrium solver determines equilibrium compositions, and how a kinetics solver determines autoignition delays in previous projects, be brief about these issues in your Methods section, rather focus more on the new ways you are using your tools to address the unique aspects of the current project.

Remember that the project description below only lists the required calculations; your report needs to draw meaning/insight into combustion phenomena from the results.

## **Project Description**

At a minimum, you are to examine the following.

#### **C-J DETONATIONS**

Using an appropriate chemical equilibrium tool (see below), determine the following properties for a Chapman-Jouguet detonation as a function of fuel mole fraction in the reactants:

- detonation speed
- product temperature

- detonation Mach number
- product/reactant pressure ratio
- product specific heat ratio (γ)
- product/reactant density ratio
- product velocity (in the wave frame of reference)

At a minimum, determine these values for ethane-air and propane-air mixtures ranging from 2.0% to 10.0% fuel (mole fraction) for at least the following three sets of initial reactant conditions:

• 300 K, 1 atm • 300 K, 10 atm • 600 K, 1 atm

Compare your detailed C-J detonation speed results for the conditions that give a product temperature of ~2700 K to estimates of the detonation speed using the simplified approximation given in class

$$D \cong \frac{\gamma_2 + 1}{\gamma_2} \sqrt{\gamma_2 \frac{\overline{R}}{\overline{W_2}} T_2} \quad .$$

You should be able to produce 2 cases (lean and rich) for each reactant,p,T combination that give this post-detonation temperature. For these estimated detonation

speeds, use values for the specific heat ratio and molecular weight based solely on N<sub>2</sub> properties at high temperatures, i.e.,  $\gamma_{N_2} \approx 1.29$  and  $\overline{W}_{N_2} = 28$ .

#### DETONATION LIMITS

Experimentally, it has been found that stable quasi-planar detonations of propane-air mixtures in a long pipe (70mm diam, L/D=240), initially at ~300 K and 1 atm, do not exist for mixtures outside a range of fuel mole fractions, i.e., less than ~2.5% C<sub>3</sub>H<sub>8</sub> (the lean or lower detonation limit, LDL) and more than ~9% C<sub>3</sub>H<sub>8</sub> (the rich or upper detonation limit, UDL).

In order to investigate the cause of the detonation limits, assume these detonations follow the ZND structure. So first, use some appropriate tool to calculate the temperature, pressure and velocity (in the appropriate reference frame) upstream of the subsonic heat release zone (i.e., after the leading shock)<sup>1</sup> at a few fuel-air ratios close to the LDL (but both above and below the limit) and a few close to the UDL (again, both above and below UDL). Then calculate the induction (time) delays and the corresponding distances behind the shock before significant heat release would occur (*assuming* constant pressure and velocity in the induction zone).

### **Tools Needed**

- 1) You will need to use a chemical equilibrium software package that can calculate C-J detonation properties and a tool to calculate non-reacting (i.e., frozen), but calorically imperfect, post-shock properties. GasEq, Cantera (with the appropriate toolbox) and CEA can do both.
- 2) You will also need to use a chemical kinetics solver (e.g., ANSYS Chemkin or Cantera) to calculate autoignition delays. As in project 2, use the USC-II mechanism for these calculations.

<sup>&</sup>lt;sup>1</sup> Hint: you will need to use the detonation speeds calculated in the first part of the project.