**ME382R**

**Fa 2023**

**Homework #2: Kinetics**

In the following problems, we will use various reaction mechanisms to study constant pressure adiabatic explosions.

Goal: To learn how to use Cantera for constant pressure explosions and to observe the variation in species, particularly radical species, as the reaction proceeds to completion.

As a part of your assignment, select one case, focus on the reaction zone, and examine the variation of species as the explosion takes place. Identify when the initial breakdown of the fuel takes place, when the radical production peaks, and when the heat release peaks. Do CO and NO form on different time scales?

H2/air or H2/O2

1. Study the explosion characteristics of stoichiometric H2/air for various initial temperatures from 1000 to 2000K and pressures between 0.1 and 100 atm. Plot the temperature vs. time. The time axis will need to be a log scale to cover the range of interest. Determine the induction time. Identify the S-curve. Compare to experimental values.

CH4/air or CH4/O2

2. Determine the explosion characteristics of a stoichiometric CH4/air mixture for various initial temperatures from 1000 to 2000K and pressures between 0.1 and 100 atm. Plot the temperature vs. time. The time axis will need to be a log scale to cover the range of interest. Determine the induction time. Compare to experimental values.

C3H8/air or C3H8/O2

1. Determine the explosion characteristics of a stoichiometric C3H8/air mixture for various initial temperatures from 1000 to 2000K and pressures between 0.1 and 100 atm. Plot the temperature vs. time. The time axis will need to be a log scale to cover the range of interest. Determine the induction time. Identify the cool flame region. Compare to experimental values.

Any fuel/ox

4. Determine the effect of radicals to initiate a reaction and compare to different temperatures. How efficient are radicals vs. increased temperature in promoting reaction? Find relevant technologies that use one or both of these methods and discuss.

Grade: Powerpoint presentation to class (50% calculations, 50% presentation)

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| Quinten, Joshua, Robert | 1 |
| Tullie, Ameya, Gabriel | 2 |
| Isha, Caelix, Ganesh | 3 |
| Ty, Ethan | 4 |