Chemical Reactors and Autoignition

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

1. Improve your understanding of chemical kinetics and chemical mechanisms, in the context of autoignition.
2. Provide you with experience using chemical kinetic modeling tools.

Report Format

Follow the guidelines at: http://seitzman.gatech.edu/classes/ae6766/projectformat.html. 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

You will determine constant-pressure induction times (also known as **autoignition delays**) as a function of initial mixture temperature and pressure for at least two fuel-air[1] systems: one fuel must be propane, the other can be ethane or ethene. You will need to explain how you defined the autoignition delay times reported in your results.[2]

At a minimum, find how the induction time varies with temperature and pressure at three equivalence ratios[3]: 0.4, 1.0, and 2.0.[4] We are only interested in cases where the autoignition delay is less than a second; in most combustion systems - that is an "eternity".[5] Your pressure range must include (at least) 0.5-10 atm results, and your initial temperatures should extend up to 1500 K.

For a "long" induction delay case and a "short" delay case for each fuel, provide some time-histories of the temperature leading up to the ignition "event", as well as the species concentrations of some important intermediates during the induction delay and ignition (rapid) event.

For at least one of your fuels, examine the sensitivity of the delay to changes in oxidizer composition. At a minimum, pick a case with ϕ=0.4 where the delay was between 10 and 100 ms, and replace the air[6] with the following oxidizers (so you will have 3 new oxidizer cases):

1) χ_{O_2}=0.21, χ_{Ar}=0.79 (*fake air replacing N_2 with Ar*)
2) χ_{O_2}=1.0 (*pure oxygen*)
3) χ_{O_2}=0.20975, χ_{N_2}=0.78984, χ_{O}=4.1×10^{-4} (air with ~0.1% of the O_2 dissociated)

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[1]Use synthetic air.

[2]You cannot just pull them off a graph "by eye", you need a quantitative definition.

[3]Suggestion: use the built-in "Equivalence Ratio" option in Chemkin to set up the reactants.

[4]These parameter sweeps can be conveniently done using Chemkin's parameter study capability.

[5]Room temperature mixtures will NEVER ignite on this time scale – start with sufficiently high initial temperatures, likely somewhere above 750 K; note, it is also NOT interesting if most of your cases have very short delays, e.g., less than 100 μs.

[6]Make sure the "Complete Combustion Products" are correct given the composition of the new oxidizer.

Software

For this problem, you will need to use a software tool to model a chemical reactor; the tool will require you to supply a chemical mechanism for the reaction rate calculations, as well as thermochemical data for the species. You will use the USC (Ver.2) mechanism; the data files (USCII.cks, gas phase kinetics, thermodynamics and transport properties) can be downloaded from Canvas (see Files).

I suggest you use the **ANSYS Chemkin** software package for these calculations, which is available at GT (if you have access to a different package, e.g., Cantera, you are free to use it instead). You can get access to Chemkin using the virtual PC's on Georgia Tech's Mycloud:

1. Log in at https://mycloud.gatech.edu/vpn using your Georgia Tech login credentials (if prompted, you may have to install the Citrix client on your host computer).

2. Select either the virtual machine named AE-2019 (this one has Chemkin as an icon on the desktop) or COE-2020 (will need to locate Ansys Chemkin in the ANSYS folder in the Windows Start menu).

Before starting Chemkin, you should upload the USCII files to a folder on your Prism drive (P:) drive. You will also need to store your output data on the P: drive, which you can then download to your own computer (if you wish); otherwise you will lose data when you log off the virtual machine.