Chemical Equilibrium Project Outline

11/17/2022

# Purpose

Create a chemical equilibrium solver for H2-O2 combustion at various , combustor pressures, and implementing Neon to lower flame temperature. NOx concentrations should be recorded at all conditions. Validate temperature and chemical composition with GasEq for validation.

# Problem Description

**Scenario 1:**

Elements of interest:

* Assume only H2 and air injected
* Add inert gas, Ne, to equation for consistency with Scenario 4

Temperatures

* Inlet air: 500K
* Inlet H2: 298K

Vary equivalence ratio:

Combustor pressure: 20 atm

**Scenario 2:**

Same but…

Combustor pressure: 10 atm

**Scenario 3:**

Same but…

Combustor pressure: 2 atm

**Scenario 4:**

Same but…

Combustor pressure: 20 atm

, choose such that is equivalent to case when

# Equations

**Unknowns:** for M species, M-1 concentrations, , T, and P

So 11 unknowns. M = 8, R = 3, M-R=5

**Formation Reaction Equations:**

Make 5 equations from reactants to products, must be *independent!*

Form formation reaction equations from above chemical formulas

**Atom Conservation:**

so write 4 atom conservation equations.

Multiply all equations by

Remove by dividing by

**Given P (constant Pressure) and guess T, thus 9 Equations + 2 knowns!**

**Adiabatic Flame Temperature:**

Or

# Code Layout

* JANAF files for all elements
* Code to open JANAF files and read/save tables of element properties at various conditions
* Code to solve