ASSIGNMENT 5 (help sheet)

Files needed for running FlameMaster laminar flame speed code:

1) mechanism file (xyz.mech),
2) thermodynamic property data file (thermo.dat),
3) transport property data file (trans.dat),
4) initial profile data file (abc) and
5) FlameMaster input file (FlameMaster.input)

1. Mechanism file (example: ch4.mech)

```
let allowed atoms be  O, H, C, N, AR.
let additional species be N2, AR.
let temperature exponent be n_k.
let order of reaction be n.
let units for A be [ cm^(3(n-1)) / ( s * mole^(n-1) * K^n_k ) ].
let units for E be [ kJ / mole ].

1f:    2 O + M1 -> O2 + M1     { a = 1.200E+17 n = -1.000 E =   0.000 }
2f:    O + H + M2 -> OH + M2   { a = 5.000E+17 n = -1.000 E =   0.000 }
3f:    O + H2 -> H + OH        { a = 3.870E+04 n = 2.700 E =  26.192 }
4f:    O + HO2 -> OH + O2      { a = 2.000E+13 n = 0.000 E =   0.000 }
5f:    O + H2O2 -> OH + HO2    { a = 9.630E+06 n = 2.000 E =  16.736 }
6f:    O + CH -> H + CO        { a = 5.700E+13 n = 0.000 E =   0.000 }
7f:    O + CH2 -> H + HCO      { a = 8.000E+13 n = 0.000 E =   0.000 }
8f:    O + CH2GSG-CH2 -> H2 + CO       { a = 1.500E+13 n = 0.000 E =   0.000 }
9f:    O + CH2GSG-CH2 -> H + HCO       { a = 1.500E+13 n = 0.000 E =   0.000 }
10f:   O + CH3 -> H + CH2O     { a = 5.060E+13 n = 0.000 E =   0.000 }
11f:   O + CH4 -> OH + CH3     { a = 1.020E+09 n = 1.500 E =  35.982 }
12f:   O + CO + M3 -> CO2 + M3 { ai = 1.800E+10 ni = 0.000 Ei =   9.979
                  a = 6.020E+14 n = 0.000 E =  12.552
      fcc = 1.0 fctc = 0.0
}
13f:   O + HCO -> OH + CO      { a = 3.000E+13 n = 0.000 E =   0.000 }
14f:   O + HCO -> H + CO2      { a = 3.000E+13 n = 0.000 E =   0.000 }
15f:   O + CH2O -> OH + HCO    { a = 3.900E+13 n = 0.000 E =  14.811 }
16f:   O + CH2OH -> OH + CH2O  { a = 1.000E+13 n = 0.000 E =   0.000 }
17f:   O + CH3O -> OH + CH2O   { a = 1.000E+13 n = 0.000 E =   0.000 }
18f:   O + CH3OH -> OH + CH2OH { a = 3.880E+05 n = 2.500 E =  12.970 }
19f:   O + CH3OH -> OH + CH3O  { a = 1.300E+05 n = 2.500 E =  20.920 }
20f:   O + C2H -> CH + CO      { a = 5.000E+13 n = 0.000 E =   0.000 }
21f:   O + C2H2 -> H + HCCO    { a = 1.350E+07 n = 2.000 E =   7.950 }
22f:   O + C2H2 -> OH + C2H    { a = 4.600E+19 n = -1.410 E = 121.127 }
23f:   O + C2H2 -> CO + CH2    { a = 6.940E+06 n = 2.000 E =   7.950 }
24f:   O + C2H3 -> H + CH2CO   { a = 3.000E+13 n = 0.000 E =   0.000 }
25f:   O + C2H4 -> CH3 + HCO   { a = 1.250E+07 n = 1.830 E =   0.920 }
26f:   O + C2H5 -> CH3 + CH2O  { a = 2.240E+13 n = 0.000 E =   0.000 }
27f:   O + C2H6 -> OH + C2H5   { a = 8.980E+07 n = 1.920 E =  23.807 }
28f:   O + HCCO -> H + 2 CO    { a = 1.000E+14 n = 0.000 E =   0.000 }
.
.
.
```

2. Thermodynamic property data file (thermo.dat)

```
THERMO
   300.000  1000.000  5000.000
! GRI-Mech Version 3.0 Thermodynamics released 7/30/99
! NASA Polynomial format for CHEMKIN-II
! see README file for disclaimer
O               L 1/90O   1            G   200.000  3500.000  1000.000    1
 2.56942078E+00-8.59741137E-05 4.19484589E-08-1.00177799E-11 1.22833691E-15    2
 2.92175791E+04 4.78433864E+00 3.16826710E+00-3.27931884E-03 6.64306396E-06    3
-6.12806624E-09 2.11265971E-12 2.91222592E+04 2.05193346E+00                   4
O2              TPIS89O   2            G   200.000  3500.000  1000.000    1
 3.28253784E+00 1.48308754E-03-7.57966669E-07 2.09470555E-10-2.16717794E-14    2
-1.08845772E+03 5.45323129E+00 3.78245636E+00-2.99673416E-03 9.84730201E-06    3
-9.68129509E-09 3.24372837E-12-1.06394356E+03 3.65767573E+00                   4
H               L 7/88H   1            G   200.000  3500.000  1000.000    1
 2.50000001E+00-2.30842973E-11 1.61561948E-14-4.73515235E-18 4.98197357E-22    2
 2.54736599E+04-4.46682914E-01 2.50000000E+00 7.05332819E-13-1.99591964E-15    3
 2.30081632E-18-9.27732332E-22 2.54736599E+04-4.46682853E-01                   4
H2              TPIS78H   2            G   200.000  3500.000  1000.000    1
 3.33727920E+00-4.94024731E-05 4.99456778E-07-1.79566394E-10 2.00255376E-14    2
-9.50158922E+02-3.20502331E+00 2.34433112E+00 7.98052075E-03-1.94781510E-05    3
 2.01572094E-08-7.37611761E-12-9.17935173E+02 6.83010238E-01                   4
OH              RUS 78O   1H   1         G   200.000  3500.000  1000.000    1
 3.09288767E+00 5.48429716E-04 1.26505228E-07-8.79461556E-11 1.17412376E-14    2
 3.85865700E+03 4.47669610E+00 3.99201543E+00-2.40131752E-03 4.61793841E-06    3
-3.88113333E-09 1.36411470E-12 3.61508056E+03-1.03925458E-01                   4
H2O             L 8/89H   2O   1         G   200.000  3500.000  1000.000    1
 3.03399249E+00 2.17691804E-03-1.64072518E-07-9.70419870E-11 1.68200992E-14    2
-3.00042971E+04 4.96677010E+00 4.19864056E+00-2.03643410E-03 6.52040211E-06    3
-5.48797062E-09 1.77197817E-12-3.02937267E+04-8.49032208E-01                   4
.
.
.
```

3. Transport property data file (trans.dat)

```
Name/ Geometry/ ε/κB    /σ       /μ        /α       /Zrot
AR              0   136.500    3.330    0.000    0.000    0.000
C               0    71.400    3.298    0.000    0.000    0.000 ! *
C2              1    97.530    3.621    0.000    1.760    4.000
C2O             1   232.400    3.828    0.000    0.000    1.000 ! *
CN2             1   232.400    3.828    0.000    0.000    1.000 ! OIS
C2H             1   209.000    4.100    0.000    0.000    2.500
C2H2            1   209.000    4.100    0.000    0.000    2.500
C2H2OH          2   224.700    4.162    0.000    0.000    1.000 ! *
C2H3            2   209.000    4.100    0.000    0.000    1.000 ! *
C2H4            2   280.800    3.971    0.000    0.000    1.500
C2H5            2   252.300    4.302    0.000    0.000    1.500
C2H6            2   252.300    4.302    0.000    0.000    1.500
C2N             1   232.400    3.828    0.000    0.000    1.000 ! OIS
```

```
C2N2          1   349.000    4.361    0.000    0.000    1.000 ! OIS
C3H2          2   209.000    4.100    0.000    0.000    1.000 ! *
C3H4          1   252.000    4.760    0.000    0.000    1.000
C3H6          2   266.800    4.982    0.000    0.000    1.000
C3H7          2   266.800    4.982    0.000    0.000    1.000
C4H6          2   357.000    5.180    0.000    0.000    1.000
I*C3H7         2   266.800    4.982    0.000    0.000    1.000
N*C3H7           2   266.800    4.982    0.000    0.000    1.000
C3H8          2   266.800    4.982    0.000    0.000    1.000
C4H           1   357.000    5.180    0.000    0.000    1.000
.
.
.
```

4. initial profile data file (abc) (example CH4_p01_0phi1_0000tu0300)

```
title = "unstretched freely propagating premixed flame"
mechanism = "ch4.pre"
author = ""
date = "Tue Mar 12 16:13:10 2019"

fuel = "CH4"
pressure = 1 [bar]
fuel-air-equivalence-ratio = 1
Tmax = 2200.88 [K]

T10mm = 2199.71 [K]

unburnt
begin
    Temperature = 300 [K]
    Massfraction-N2 = 0.724808
    Massfraction-O2 = 0.220038
    Massfraction-CH4 = 0.0551538
    Molefraction-N2 = 0.714925
    Molefraction-O2 = 0.190043
    Molefraction-H2 = 1.05457e-05
    Molefraction-CH4 = 0.0950216
    MassfractionBC-N2 = 0.724808
    MassfractionBC-O2 = 0.220038
    MassfractionBC-CH4 = 0.0551538
end

burningVelocity = 38.2149 [cm/sec]
FlameThickness = 0.000404549 [m]
numOfSpecies = 53
gridPoints = 527

body
y [m]
    0.000000e+00   8.404026e-05   1.680106e-04   2.518039e-04   3.352772e-04
    4.182350e-04   5.003833e-04   5.812745e-04   6.602733e-04   7.365560e-04
    8.091673e-04   8.771572e-04   9.397371e-04   9.964229e-04   1.047075e-03
.
```

.

5. **FlameMaster input file (FlameMaster.input)**

```
#############
# Numerics #
#############

#### Newton solver ####

UseNumericalJac is TRUE
UseSecondOrdJac is TRUE
UseModifiedNewton = TRUE
#timedepflag = True
deltatstart = 0.001
DampFlag = TRUE
LambdaMin = 1.0e-2

MaxIter = 5000
TolRes = 1.0e-15
TolDy = 1e-4

#### grid ####

DeltaNewGrid = 25
OneSolutionOneGrid = TRUE
initialgridpoints = 89
maxgridpoints = 525
q = -0.25
R = 60

########################
# Sensitivity Analysis #
########################

#ReactionFluxAnal is TRUE
#SensAnal is TRUE
#SensObj is M

#######
# I/O #
#######

WriteEverySolution = TRUE
PrintMolarFractions is TRUE

#OutputPath is ./Output
#StartProfilesFile is ./CH4_p01_0phi1_0000tu0298

##############
# Chemistry #
##############

#MechanismFile is CH4.72.pre
globalReaction is CH4 + 2 O2 == CO2 + 2 H2O;
#globalReaction is C2H2 + 2.5 O2 == 2 CO2 + H2O;
```

```
#globalReaction is C4H6 + 5.5 O2 == 4 CO2 + 3 H2O;
#globalReaction is MMETHAC-C5H8O2 + 6 O2 == 5 CO2 +  4 H2O;

fuel is CH4
oxidizer is O2

#########
# Flame #
#########

Flame is UnstretchedPremixed
ExactBackward is TRUE

#phi = 0.6
#phi = 1.3
phi = 0.6
#phi = 1.2
 #phi = 1.3

pressure = 1.0e5
#pressure = 1.3e5
#pressure = 2.0e5

ComputeWithRadiation is TRUE
Thermodiffusion is TRUE

########################
# Boundary conditions #
########################

#ConstMassFlux is TRUE
#MassFlowRate = 0.1238

Unburnt Side {
      dirichlet {
            t =300
        X->O2 =  0.205752

      X->MMETHAC-C5H8O2 = 0.020211

      }
}

#TimeDepFlag is TRUE
#TempProfileFile is ./temp5
#RelaxTemp is TRUE

#ContInc = 25
#ContSide is left
#ContType is Temperature
#ContBound = 600.0

#ContBound = 0.1
#ContInc = 0.0005
  ---------------------------------------------------------------------------
```

Commands to make runs

1. *CreateBinFile -i thermo.dat -m trans.dat -o ch4.bin*
   Creates ch4.bin file
2. *ScanMan -i ch4.mech -t ch4.bin -3 Ssr >& log*
   Creates ch4.pre file
3. *FlameMaster -i FlameMaster.input -r ch4.pre -s CH4_p01_0phi1_0000tu0300*
   At the end of run outputs result data file
4. *LT outputfilename*
   Creates 'outputfile.kg' file which can be opened in MS word excel

When convergence is not achieved, run transient calculation

In the FlameMaster.input file uncomment (*i.e.* delete #)

timedepflag = True
deltatstart = 0.001 (can set to lower value if still does not converge)

This may require running several times. The unconverged result is stored in ouputfile with name ending _t.

FlameMaster -i FlameMaster.input -r ch4.pre -s outputfile_t