

# Introduction to EES - 2

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**2.60/2.62/10.390 Fundamentals of Advanced Energy Conversion**

Spring 2020

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Credits: Adapted from the presentations created by Xiaoyu Wu and Aniket Patankar for 2.60

# Examples for Today

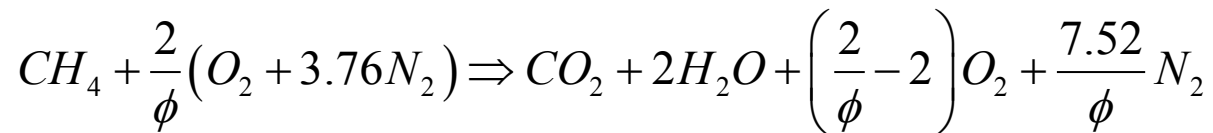
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1. Adiabatic Flame Temperature
2. Throttling, Joule-Thomson effect
3. Chemical Equilibrium

# Example 1: Adiabatic Flame Temperature

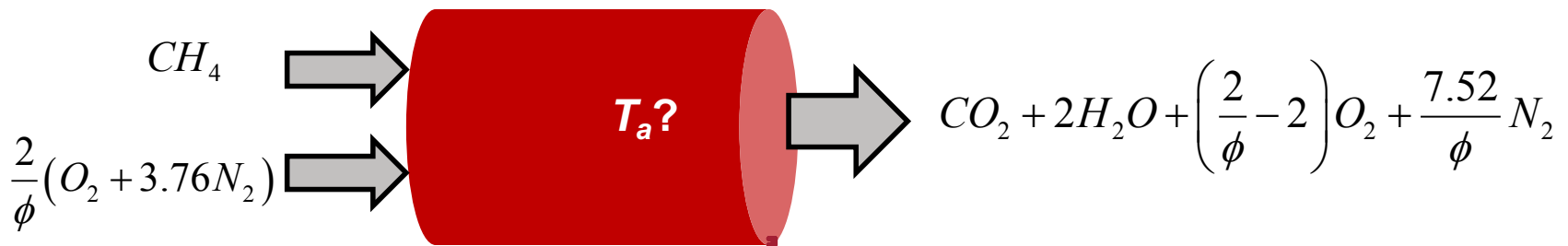
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- What's the adiabatic temperature  $T_a$  of lean burning when the equivalence ratio  $\phi$  changes ( $\phi < 1$ )



$$T_0 = 298 \text{ K}$$

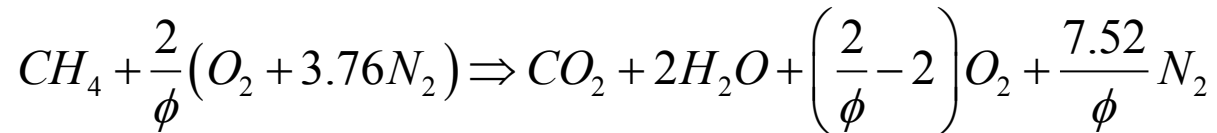
$$P_0 = 1 \text{ bar}$$



# Equations

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Assume: Only forward reaction occurs; constant pressure



Adiabatic condition:

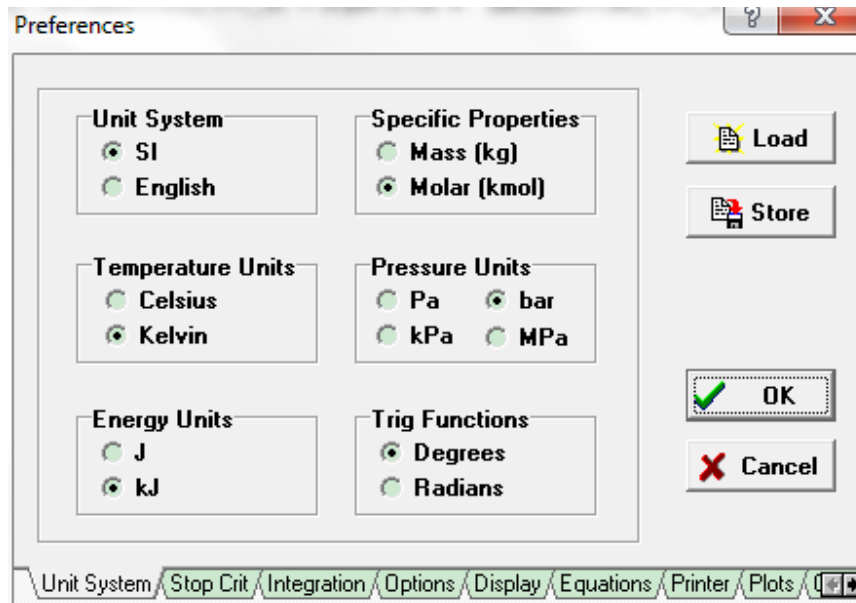
$$H_{reactants}(T_0, P_0) = H_{products}(T_a, P_0)$$

# Before writing code – Set the Units right!

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**Options → Unit Systems:** Set the unit system.

Recommended – T in Kelvin, Specific properties per unit mole



# Property Functions

## Options → Function Information

- Thermophysical properties
- Ideal gases/Real gas
- Then *Paste*

Function Information

Math and string functions

Thermophysical properties

Heat Transfer & Fluid Flow

Mechanical Design

Component Library

User-Defined

EES library routines

External routines

Real fluids

Ideal gases

AirH2O

NASA

Brines

Incompressible

? Function Info

? Fluid Info

Cp [J/kg-K]

Cv [J/kg-K]

Density [kg/m3]

Dipole [debye]

ek\_LJ [K]

Enthalpy [J/kg]

Enthalpy\_formation [J/kg]

Enthalpy\_fusion [J/kg]

Entropy [J/kg-K]

FluidType\$

C6H14

C8H18

CH3OH

CH4

CO

CO2

H2

H2O

He

N2

Independent Properties

Temperature [K]

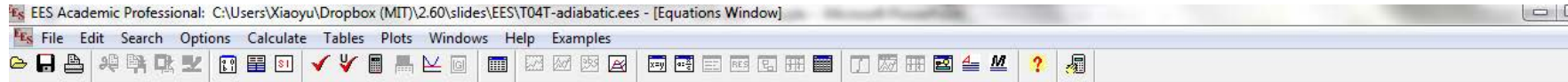
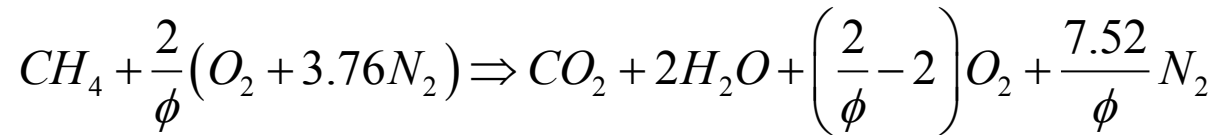
Ex: h=Enthalpy(CH4,T=T)

Paste

Done

# Equations

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"1) enthalpy of reactants"

$T_o = 298$

$h_R = \text{ENTHALPY}(CH_4, T=T_o) + 2/\phi * \text{ENTHALPY}(O_2, T=T_o) + 2/\phi * 3.76 * \text{ENTHALPY}(N_2, T=T_o)$

"2) enthalpy of products"

$h_P = 1 * \text{ENTHALPY}(CO_2, T=T_a) + 2 * \text{ENTHALPY}(H_2O, T=T_a) + (2/\phi - 2) * \text{ENTHALPY}(O_2, T=T_a) + 2/\phi * 3.76 * \text{ENTHALPY}(N_2, T=T_a)$

"3) energy balance"

$h_R = h_P$

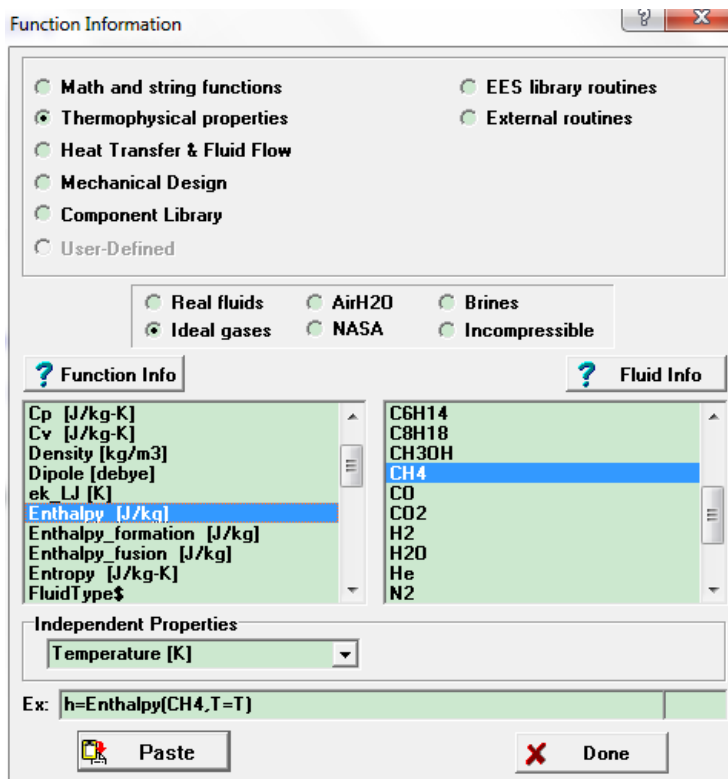
Why pressure isn't required?

ENTHALPY *per unit mole* in above formulation.

# Ideal gas vs Real fluids

Differences:

- Number of parameters required
- Name of fluid
- Reference values



Function Information

Math and string functions     EES library routines  
 Thermophysical properties     External routines  
 Heat Transfer & Fluid Flow  
 Mechanical Design  
 Component Library  
 User-Defined

Real fluids     AirH2O     Brines  
 Ideal gases     NASA     Incompressible

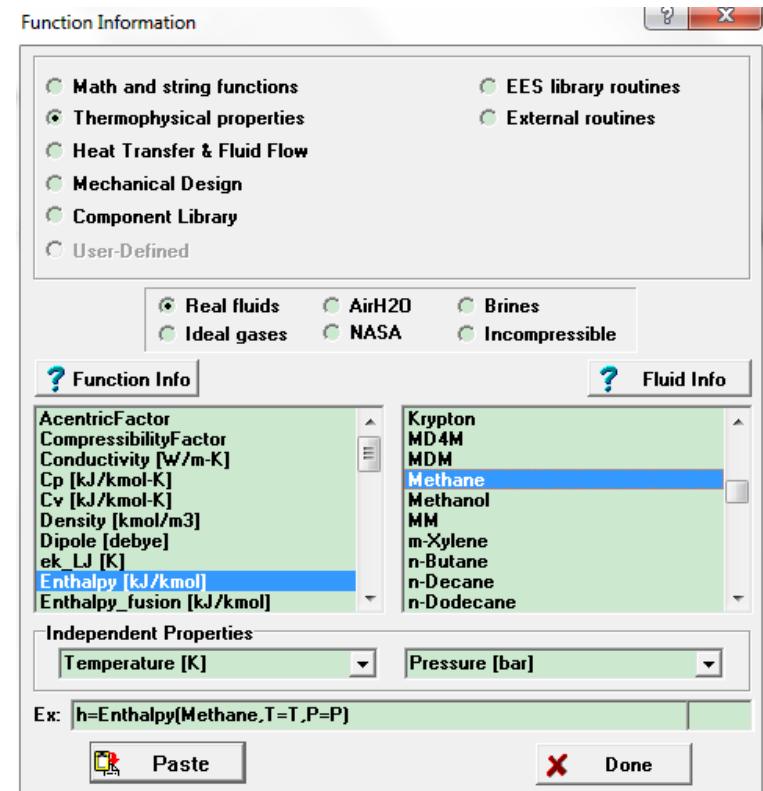
? Function Info    ? Fluid Info

Cp [J/kg-K]	C6H14
Cv [J/kg-K]	C8H18
Density [kg/m3]	CH3OH
Dipole [debye]	<b>CH4</b>
ek_LJ [K]	CO
<b>Enthalpy [J/kg]</b>	CO2
Enthalpy_formation [J/kg]	H2
Enthalpy_fusion [J/kg]	H2O
Entropy [J/kg-K]	He
FluidType\$	N2

Independent Properties  
Temperature [K]

Ex: `h=Enthalpy(CH4,T=T)`

Paste Done



Function Information

Math and string functions     EES library routines  
 Thermophysical properties     External routines  
 Heat Transfer & Fluid Flow  
 Mechanical Design  
 Component Library  
 User-Defined

Real fluids     AirH2O     Brines  
 Ideal gases     NASA     Incompressible

? Function Info    ? Fluid Info

AcentricFactor	Krypton
CompressibilityFactor	MD4M
Conductivity [W/m-K]	MDM
Cp [kJ/kmol-K]	<b>Methane</b>
Cv [kJ/kmol-K]	Methanol
Density [kmol/m3]	MM
Dipole [debye]	m-Xylene
ek_LJ [K]	n-Butane
<b>Enthalpy [kJ/kmol]</b>	n-Decane
Enthalpy_fusion [kJ/kmol]	n-Dodecane

Independent Properties  
Temperature [K]    Pressure [bar]

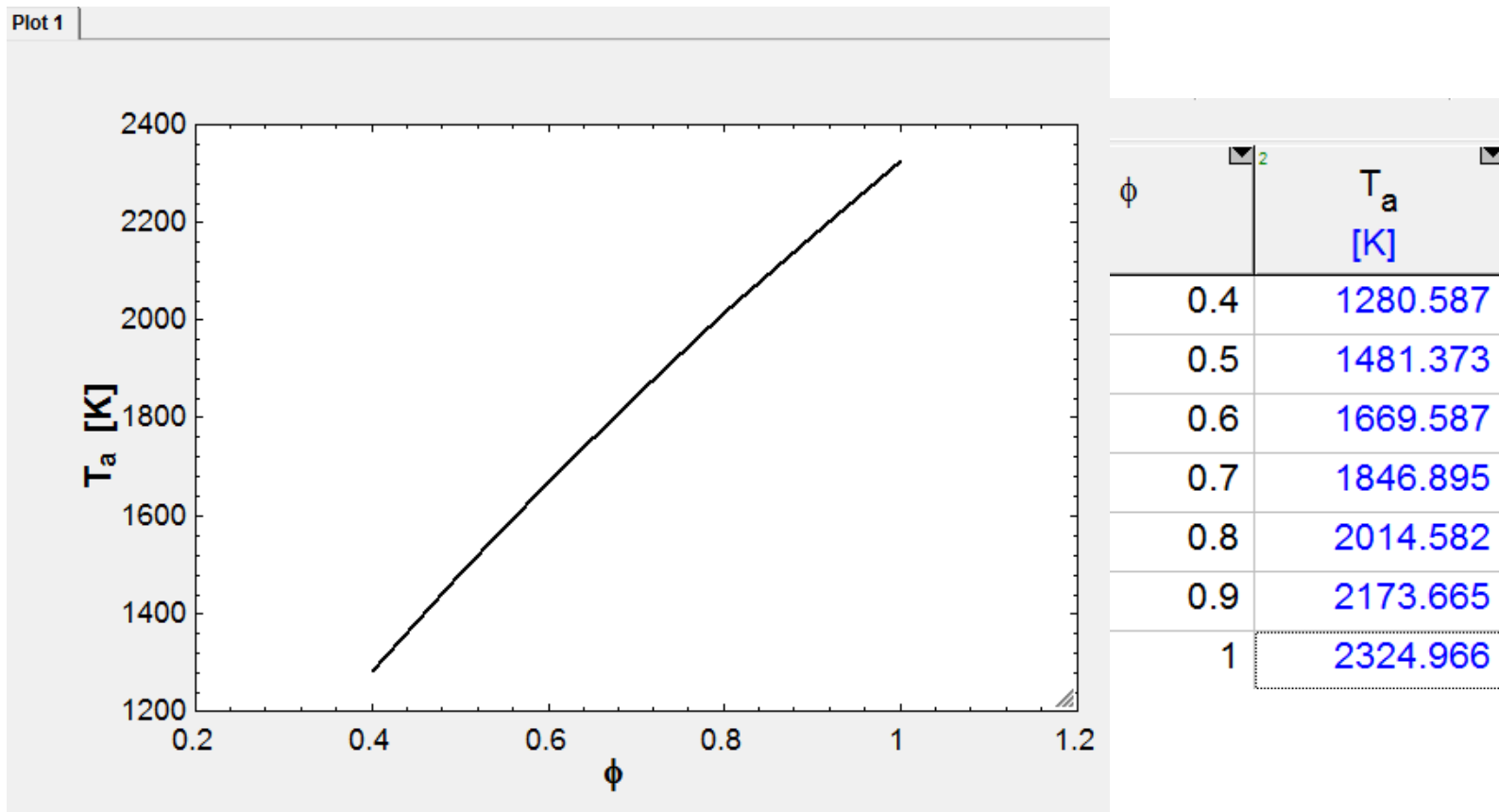
Ex: `h=Enthalpy(Methane,T=T,P=P)`

Paste Done

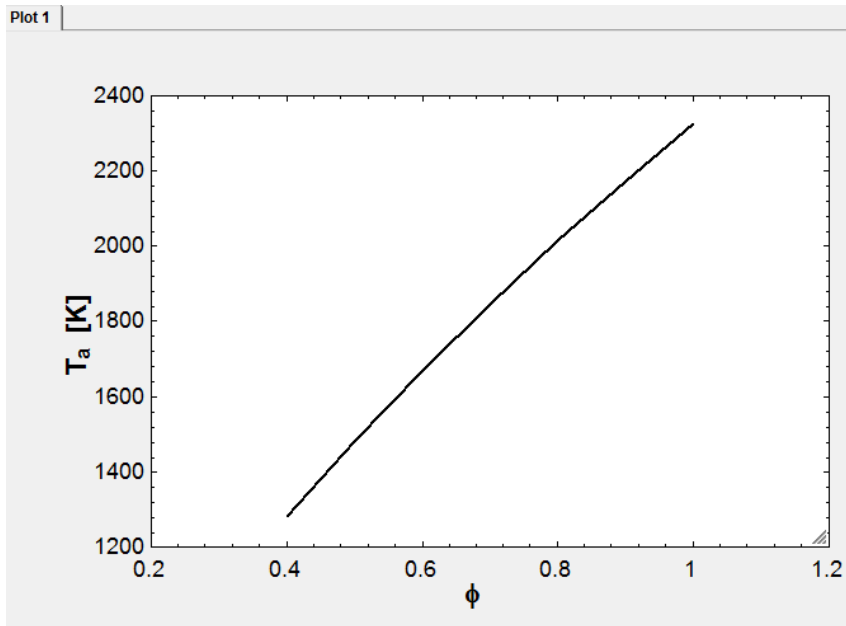


# Parametric Table and Plot

- Tables → New Parametric Table



# Throwback to the notes



Adiabatic flame temperature vs  
Equivalence ratio for Methane.  
Calculated using EES.

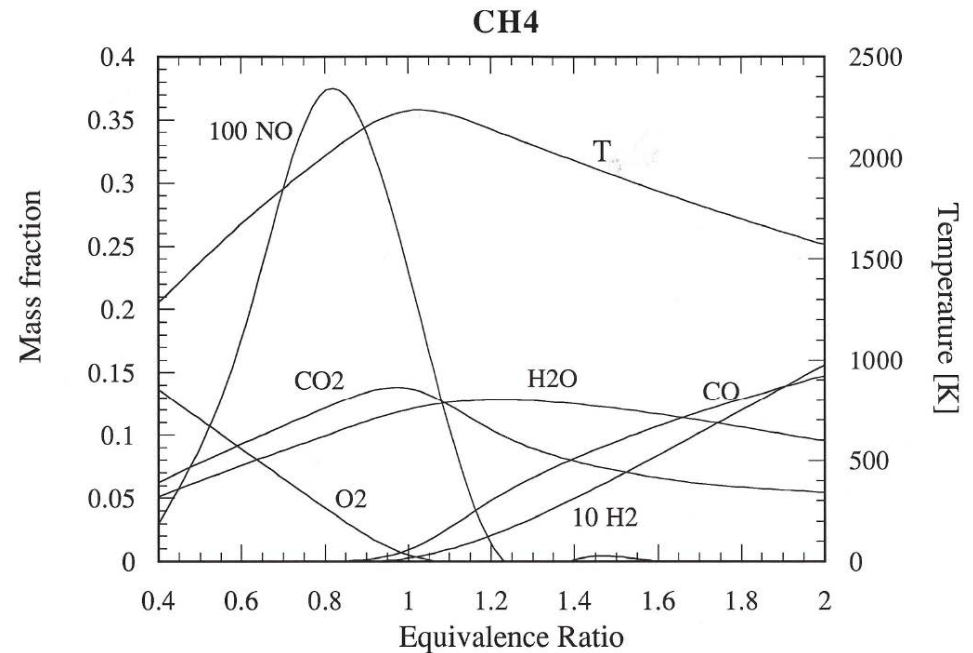


Figure from Chapter 3, 2.60 Spring  
2020

# Example 2 – Joule-Thomson Inversion

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Isoenthalpic expansion across a throttle valve can lead to an increase or decrease in temperature depending on conditions before throttling.

This effect is captured in terms of the Joule-Thomson coefficient defined below.

$$\mu_{JT} = \left( \frac{\partial T}{\partial P} \right)_H = \frac{V}{C_p} (\alpha T - 1)$$

(credits: Wikipedia.  $\alpha$  is the coefficient of thermal expansion)  
[https://en.wikipedia.org/wiki/Joule%E2%80%93Thomson\\_effect](https://en.wikipedia.org/wiki/Joule%E2%80%93Thomson_effect)

# The Joule-Thomson Inversion Curve

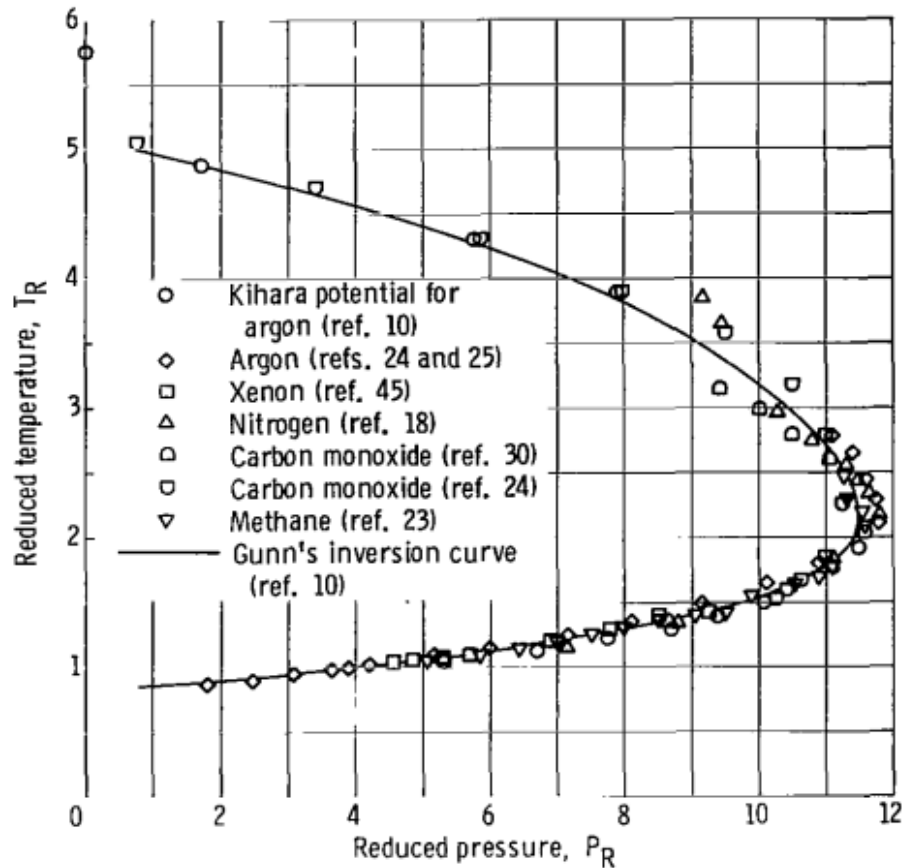


Figure courtesy of NASA.

Figure 1. - Generalized reduced inversion curve for several corresponding states fluids as determined by Gunn, Chueh, Prausnitz (ref. 10).

# Application to refrigeration and liquefaction: Linde-Hampson Cycle

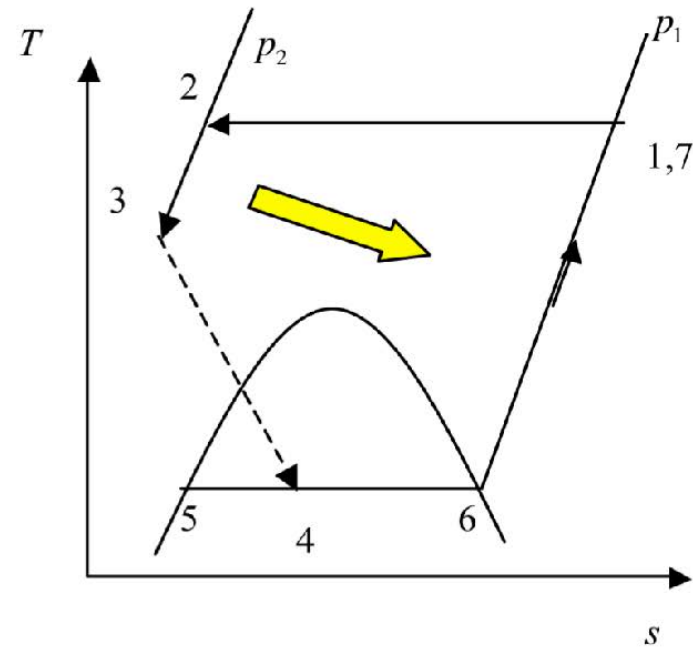
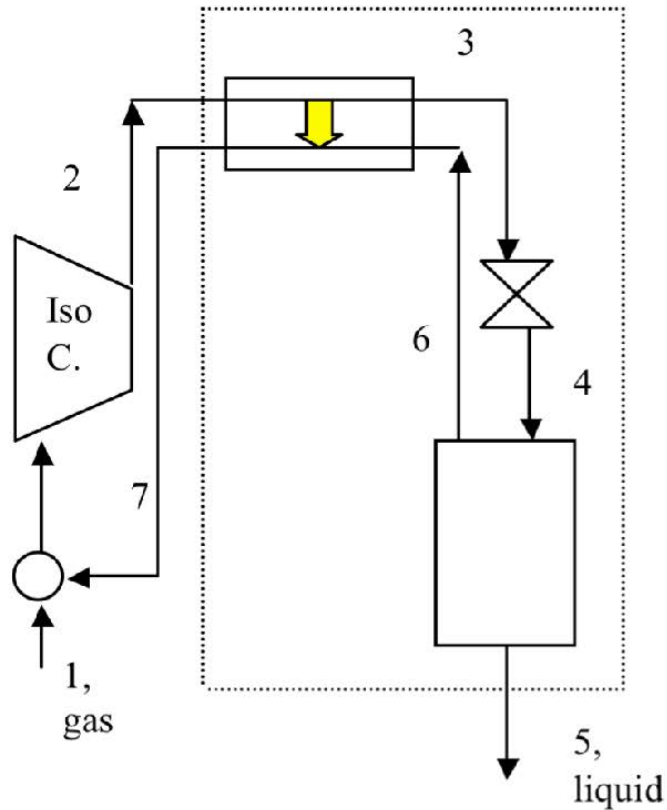


Figure from lecture 3, 2.60 Spring 2020

# EES for Joule-Thomson Inversion

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$P1 = 135.6$  [bar]

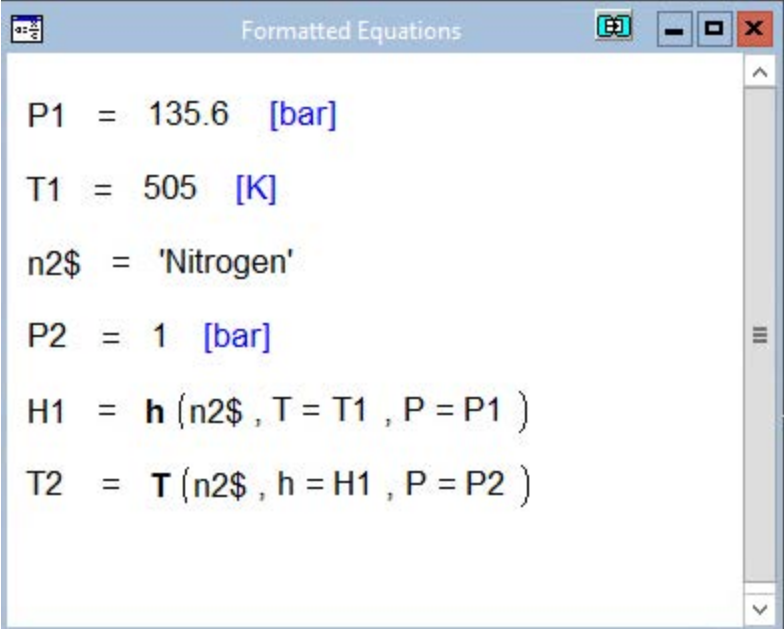
$T1 = 505$  [K]

$n2\$ = \text{'Nitrogen'}$

$P2 = 1$  [bar]

$H1 = \text{enthalpy}(n2\$, T=T1, P=P1)$

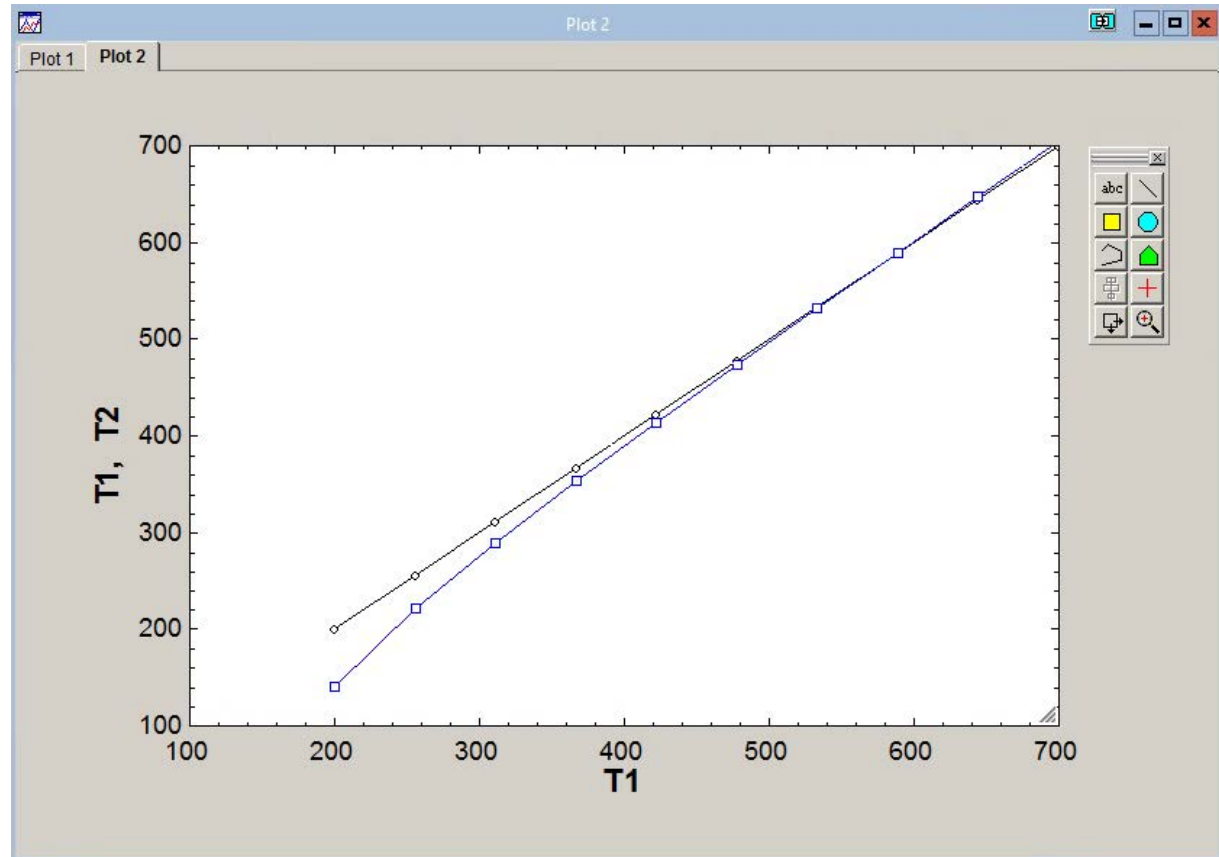
$T2 = \text{temperature}(n2\$, h=H1, P=P2)$



```
Formatted Equations
P1 = 135.6 [bar]
T1 = 505 [K]
n2$ = 'Nitrogen'
P2 = 1 [bar]
H1 = h (n2$, T = T1 , P = P1 )
T2 = T (n2$, h = H1 , P = P2 )
```

# Joule-Thomson Inversion of Nitrogen

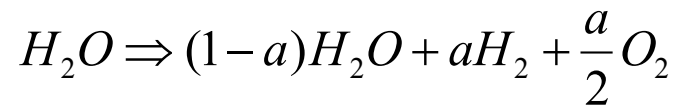
1..10	T1	T2
Run 1	200	140.6
Run 2	255.6	221.2
Run 3	311.1	289.5
Run 4	366.7	352.8
Run 5	422.2	413.8
Run 6	477.8	473.2
Run 7	533.3	531.8
Run 8	588.9	589.6
Run 9	644.4	647
Run 10	700	704



# Example 3: Water Dissociation at 3000 K

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- 1 mole of water dissociated at 3000 K, 1 atm



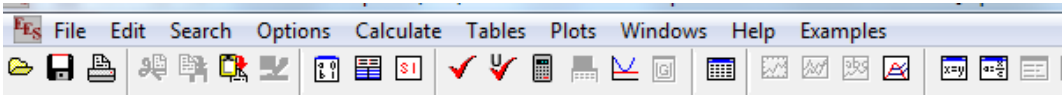
- The conditions for equilibrium is:

$$\sum_N \mu_i dn_i = 0$$

$$\mu_{H_2} \cdot n_{H_2} + \mu_{O_2} \cdot n_{O_2} = \mu_{H_2O} \cdot n_{H_2O}$$



# Equations



"Determine the equilibrium concentrations of different species for the dissociation of water  $\text{H}_2\text{O} \rightleftharpoons \text{H}_2 + 1/2 \text{O}_2$  at 3000 K."

"At 3000K, EES has already subtracted data at the reference state:"

T = 3000  
P = 101.5

• Conditions

h\_H2O = ENTHALPY(H2O,T=T)  
h\_H2 = ENTHALPY(H2,T=T)  
h\_O2 = ENTHALPY(O2,T=T)

s\_H2O = ENTROPY(H2O,T=T,P=P\*X\_H2O)  
s\_H2 = ENTROPY(H2,T=T,P=P\*X\_H2)  
s\_O2 = ENTROPY(O2,T=T,P=P\*X\_O2)

g\_H2O = h\_H2O - T\*s\_H2O  
g\_H2 = h\_H2 - T\*s\_H2  
g\_O2 = h\_O2 - T\*s\_O2

0 = n\_H2 \* g\_H2 + n\_O2 \* g\_O2 - (1-n\_H2O)\*g\_H2O

1 - n\_H2O = n\_H2  
1 - n\_H2O = 2\*n\_O2

X\_H2O = n\_H2O/(n\_H2 + n\_O2 + n\_H2O)  
X\_H2 = (n\_H2)/(n\_H2 + n\_O2 + n\_H2O)  
X\_O2 = (n\_O2)/(n\_H2 + n\_O2 + n\_H2O)

• Properties  
□ Entropies using Partial pressure

• Equilibrium

• Mass balance

• Units

$$X_{\text{H}_2\text{O}} = 0.7963$$

$$X_{\text{H}_2} = 0.1358$$

$$X_{\text{O}_2} = 0.0679$$

# Example 3: Code

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$T=3000$  [K]

$P = 101.5$  [kPa]

$h_{\text{H}_2\text{O}} = \text{enthalpy}(\text{H}_2\text{O}, T=T)$

$h_{\text{H}_2} = \text{enthalpy}(\text{H}_2, T=T)$

$h_{\text{O}_2} = \text{enthalpy}(\text{O}_2, T=T)$

$s_{\text{H}_2\text{O}} = \text{entropy}(\text{H}_2\text{O}, T=T, P=P \cdot X_{\text{H}_2\text{O}})$

$s_{\text{H}_2} = \text{entropy}(\text{H}_2, T=T, P=P \cdot X_{\text{H}_2})$

$s_{\text{O}_2} = \text{entropy}(\text{O}_2, T=T, P=P \cdot X_{\text{O}_2})$

$g_{\text{H}_2\text{O}} = h_{\text{H}_2\text{O}} - T \cdot s_{\text{H}_2\text{O}}$

$g_{\text{H}_2} = h_{\text{H}_2} - T \cdot s_{\text{H}_2}$

$g_{\text{O}_2} = h_{\text{O}_2} - T \cdot s_{\text{O}_2}$

$0 = n_{\text{H}_2} \cdot g_{\text{H}_2} + n_{\text{O}_2} \cdot g_{\text{O}_2} - (1 - n_{\text{H}_2\text{O}}) \cdot g_{\text{H}_2\text{O}}$

$1 - n_{\text{H}_2\text{O}} = n_{\text{H}_2}$

$1 - n_{\text{H}_2\text{O}} = 2 \cdot n_{\text{O}_2}$

$X_{\text{H}_2\text{O}} = n_{\text{H}_2\text{O}} / (n_{\text{H}_2} + n_{\text{O}_2} + n_{\text{H}_2\text{O}})$

$X_{\text{H}_2} = n_{\text{H}_2} / (n_{\text{H}_2} + n_{\text{O}_2} + n_{\text{H}_2\text{O}})$

$X_{\text{O}_2} = n_{\text{O}_2} / (n_{\text{H}_2} + n_{\text{O}_2} + n_{\text{H}_2\text{O}})$

# Another approach – Equilibrium Constant

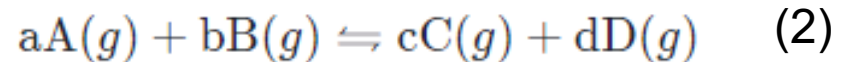
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1. Definition of equilibrium constant in terms of change in Gibbs Free energy.

$$K_p(T) = \exp\left(-\frac{\Delta G_{rxn}^o(T)}{\mathfrak{R}T}\right) \quad (1)$$

2. A sample reaction

3. Definition of equilibrium constant in terms of partial pressures of reactants and products

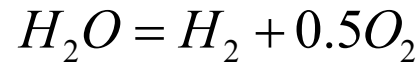


$$K_p = \frac{(P_C)^c (P_D)^d}{(P_A)^a (P_B)^b} \quad (3)$$

# Calculating Kp

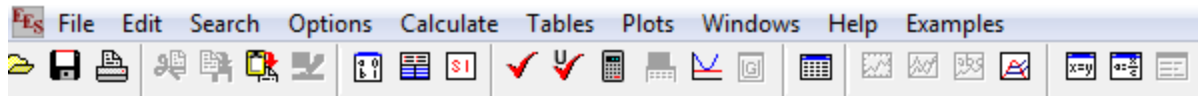
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- Standard Gibbs free energy of the reaction at  $T$ 
  - Evaluated the stoichiometric reaction
  - Standard  $G$  at  $T$  and  $P_0$



$$\Delta G_{rxn}^{\circ}(T) = v_{H_2} \cdot g_{H_2}^{\circ}(T) + v_{O_2} \cdot g_{O_2}^{\circ}(T) - v_{H_2O} \cdot g_{H_2O}^{\circ}(T)$$

# Equations



$$a = 0.1457$$

"Determine the equilibrium concentrations of different species for the dissociation of water  $H_2O \rightleftharpoons H_2 + 1/2 O_2$  at 3000 K."

"At 3000K, EES has already subtracted data at the reference state:"

T = 3000  
P = 101.5  
R = 8.314

h\_H2O = ENTHALPY(H2O,T=T)  
h\_H2 = ENTHALPY(H2,T=T)  
h\_O2 = ENTHALPY(O2,T=T)

s\_H2O\_0 = ENTROPY(H2O,T=T,P=P)  
s\_H2\_0 = ENTROPY(H2,T=T,P=P)  
s\_O2\_0 = ENTROPY(O2,T=T,P=P)

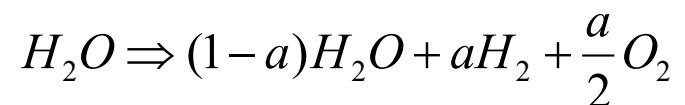
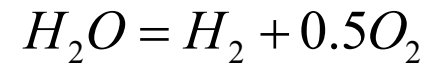
- Properties
  - Entropies using standard pressure

G\_p = 1\*h\_H2 + 0.5\*h\_O2 - T\*(1\*s\_H2\_0 + 0.5\*s\_O2\_0)  
G\_r = 1\*(h\_H2O - T\*s\_H2O\_0)  
DELTA\_G = G\_p - G\_r

- Standard Gibbs Free Energy

K\_P = exp(Delta\_G/R/T)  
a/(1+0.5\*a)\*(0.5\*a/(1+0.5\*a))^0.5/((1-a)/(1+0.5\*a)) = K\_P

- Equilibrium constant



# Example 3: Code (Approach II)

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$$T=3000 \text{ [K]}$$

$$P = 101.5 \text{ [kPa]}$$

$$R = 8.314$$

$$h_{\text{H2O}} = \text{enthalpy}(\text{H2O}, T=T)$$

$$h_{\text{H2}} = \text{enthalpy}(\text{H2}, T=T)$$

$$h_{\text{O2}} = \text{enthalpy}(\text{O2}, T=T)$$

$$s_{\text{H2O}_0} = \text{entropy}(\text{H2O}, T=T, P=P)$$

$$s_{\text{H2}_0} = \text{entropy}(\text{H2}, T=T, P=P)$$

$$s_{\text{O2}_0} = \text{entropy}(\text{O2}, T=T, P=P)$$

$$G_p = h_{\text{H2}} + 0.5 \cdot h_{\text{O2}} - T \cdot (s_{\text{H2}_0} + 0.5 \cdot s_{\text{O2}_0})$$

$$G_r = h_{\text{H2O}} - T \cdot s_{\text{H2O}_0}$$

$$\Delta G = G_p - G_r$$

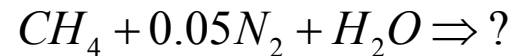
$$K_P = \exp(-\Delta G/R/T)$$

$$a/(1+0.5 \cdot a) \cdot (0.5 \cdot a/(1+0.5 \cdot a))^{0.5} / ((1-a)/(1+0.5 \cdot a)) = K_P$$

# Example 4: Methane reforming

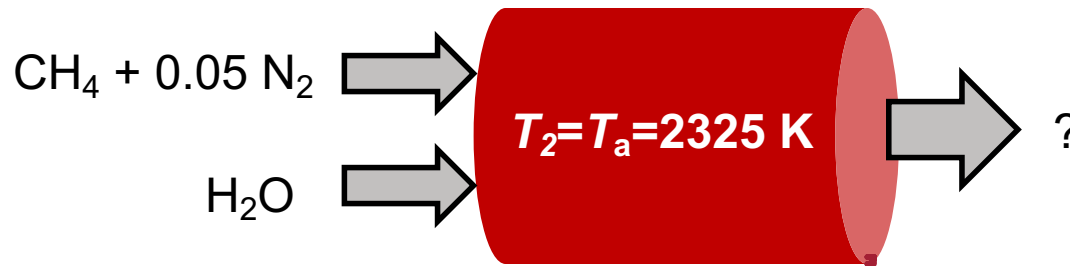
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- What's the equilibrium products of a methane reformer?
  - Natural gas contains 4 – 6%  $N_2$  when it is sold to the pipeline



**$P = 1$  bar**

**$T = 950 - 1350$  K**



# CHEM\_EQUIL libraries

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- CHEM\_EQUIL calculates the equilibrium composition for an ideal gas mixture containing elements C, H, O, N, and A (A = Argon).

- **INPUTS:**

- P: pressure [kPa]
- T: temperature [K] (600 K < T < 5000 K)
- AO: ratio of molecules of the inert species to atomic oxygen
- CO: ratio of atomic carbon to atomic oxygen
- HO: ratio of atomic hydrogen to atomic oxygen
- NO: ratio of atomic nitrogen to atomic oxygen

Note: AO can be set to zero. However, the minimum value for any of the other ratios is 1E-5.

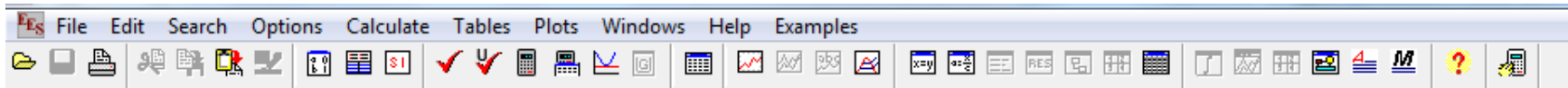
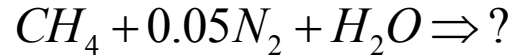
- Call function:

- CALL

```
CHEM_EQUIL(P,T,AO,CO,HO,NO:x_H2,x_O2,x_H2O,x_CO,x_CO2,x_OH,x_H,x_O,x_N2,x_N,x_NO,x_NO2,x_CH4,x_A)
```



# Equations



P=101.3 [kPa]

• Pressure

AIO=0 "ratio of inerts to oxygen atoms"  
C/O=1/1 "ratio of carbon to oxygen atoms"  
H/O=6/1 "ratio of hydrogen to oxygen atoms"  
N/O=0.05/1 "ratio of nitrogen to oxygen atoms"

• Atom ratios

CALL CHEM\_EQUIL(P,T,AIO,C/O,H/O,N/O:x\_H2,x\_O2,x\_H2O,x\_CO,x\_CO2,x\_OH,x\_H,x\_O,x\_N2,x\_N,x\_NO,x\_NO2,x\_CH4,x\_A)  
"CHEM\_EQUIL returns the equilibrium mole fractions for the above 14 species."

• Call function

\*\*You need to have CHEM\_EQUIL library installed (available on EES website).

# Example 4 - Code

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$P = 101.3$  [kPa]

{ $T = 950$ }

$AO = 0$

$CO = 1/1$

$HO = 6/1$

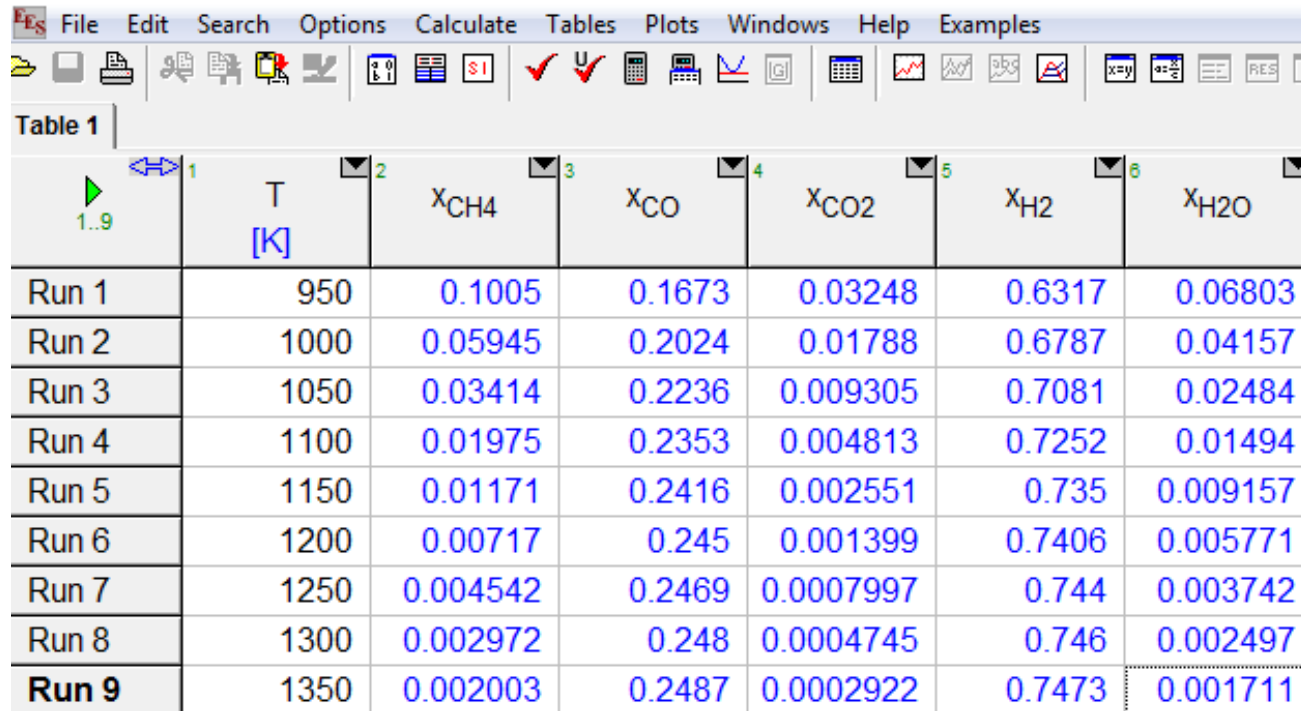
$NO = 0.05/1$

Call

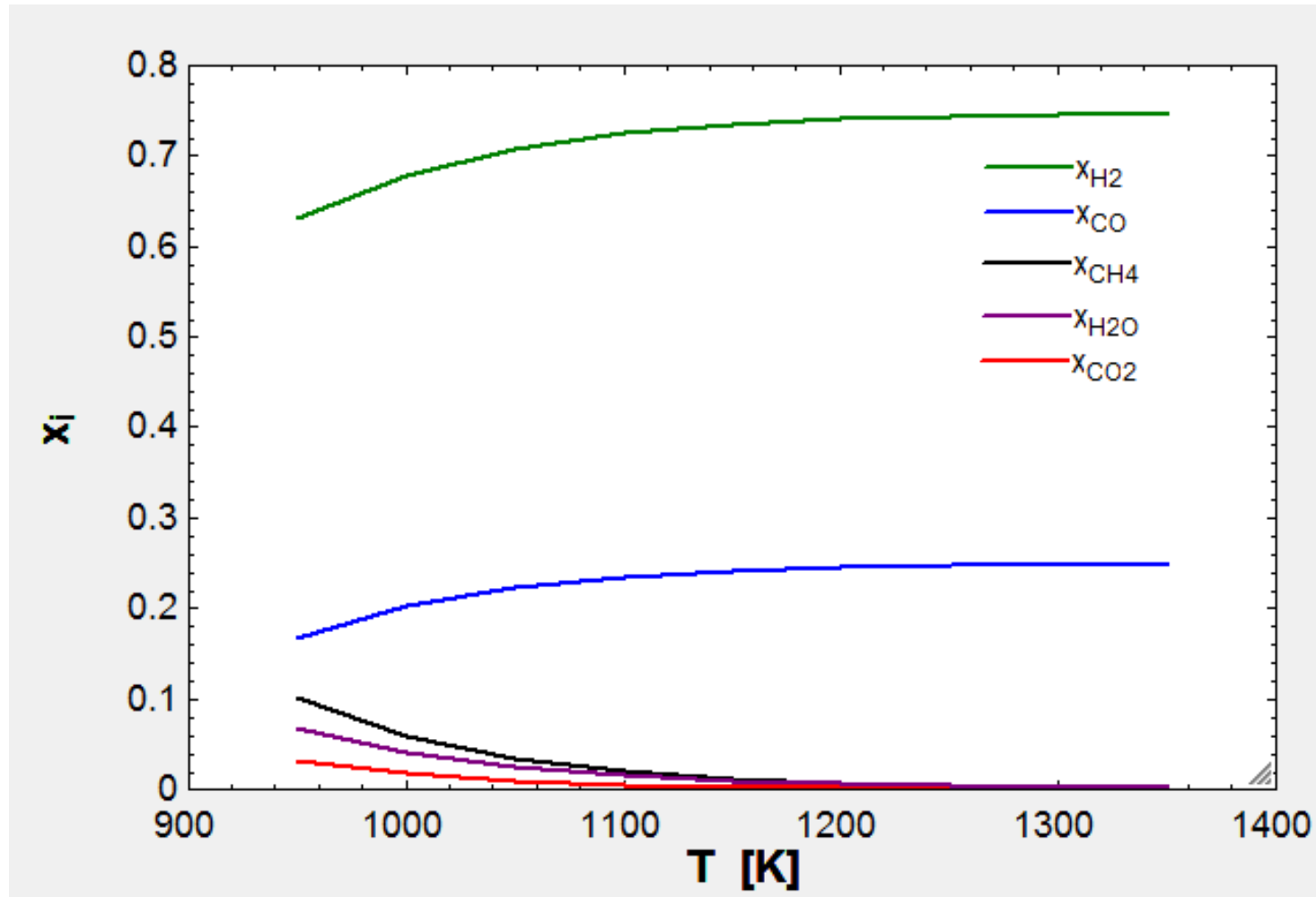
`chem_equil(P,T,AO,CO,HO,NO:x_H2,x_O2,x_H2O,x_CO,x_CO2,x_OH  
,x_H,x_O,x_N2,x_N,x_NO,x_NO2,x_CH4,x_A)`

# Parametric Table and Plot

- Tables → New Parametric Table
- Plot → New Plot Windows → X-Y Plot

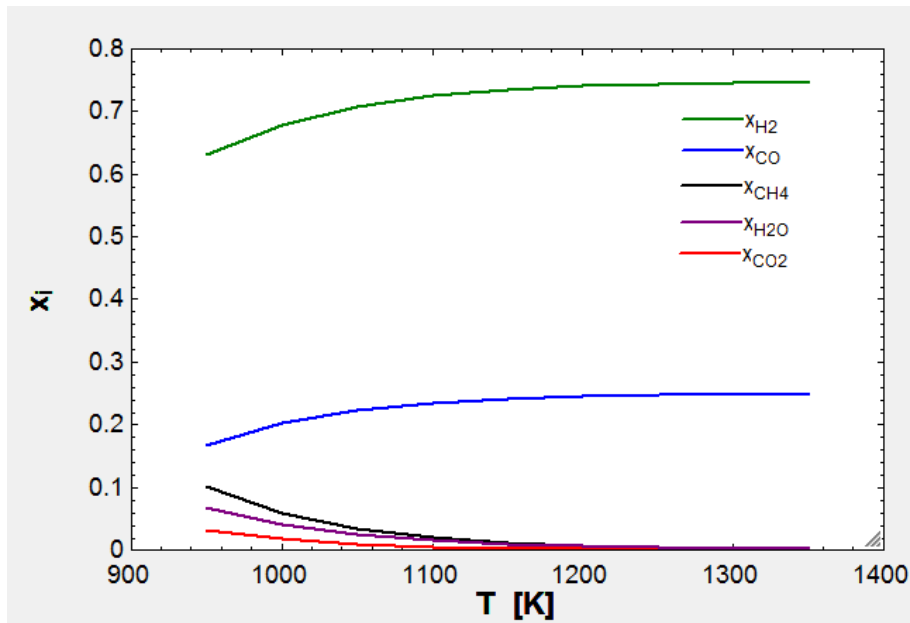


	1	2	3	4	5	6	7
	T [K]	X <sub>CH4</sub>	X <sub>CO</sub>	X <sub>CO2</sub>	X <sub>H2</sub>	X <sub>H2O</sub>	
Run 1	950	0.1005	0.1673	0.03248	0.6317	0.06803	
Run 2	1000	0.05945	0.2024	0.01788	0.6787	0.04157	
Run 3	1050	0.03414	0.2236	0.009305	0.7081	0.02484	
Run 4	1100	0.01975	0.2353	0.004813	0.7252	0.01494	
Run 5	1150	0.01171	0.2416	0.002551	0.735	0.009157	
Run 6	1200	0.00717	0.245	0.001399	0.7406	0.005771	
Run 7	1250	0.004542	0.2469	0.0007997	0.744	0.003742	
Run 8	1300	0.002972	0.248	0.0004745	0.746	0.002497	
<b>Run 9</b>	1350	0.002003	0.2487	0.0002922	0.7473	0.001711	



Plot of data from the previous slide. Steam reforming of Methane with  $N_2$  impurity.

# Throwback to the notes



Plot of data from the previous slide. Steam reforming of Methane with  $N_2$  impurity.

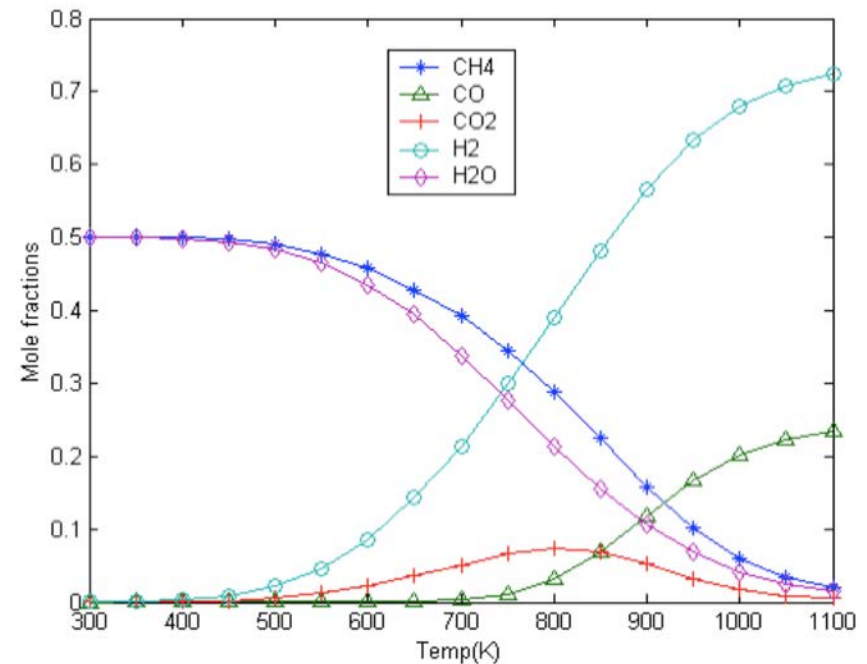


Figure from Lecture 6, 2.60 Spring 2020

# Examples for Today

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1. Adiabatic Flame Temperature
2. Throttling, Joule-Thomson effect
3. Chemical Equilibrium

# Summary

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## 1. Thermodynamics property libraries

- Ideal gas and Real fluids

## 2. Thermodynamic equilibrium

- Gibbs free energy
- Equilibrium constant
- Equilibrium Libraries

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2.60J Fundamentals of Advanced Energy Conversion  
Spring 2020

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