Lecture 26

Turbulence - Chemistry

ChE 641 | Lecture 26

Chemistry-Turbulence Interactions

1. Idea of time scales (from Smoot & Smith, p. 269-273

2. Magnussen-Hjertager approach from {Fluent Manual, Magnussen & Hjertager, 16th Symp., 1976, Smith & Fletcher, CST, 1988

3. Mixture fraction approach

4. Assumed-shape PDF

5. Smith & Fletcher paper

THE PROBLEM

Species continuity equ:

$$\frac{\partial}{\partial t}(Y_i \rho) + \nabla \cdot (\rho u Y_i - \rho \mathcal{D}_{Y_i} \nabla Y_i) = R_{Y_i}$$

Introduce time-mean (Reynolds) averaging

$$Y_i = \overline{Y_i} + Y_i' \qquad \overline{Y}_i = \frac{1}{\Delta t}\int_0^{\Delta t} Y_i \, dt \quad \text{(short time)}$$

For now, assume density fluctuations are small, ~~$\overline{Y_i' u'} \cong 0$~~

$$\frac{\partial}{\partial t}(\bar{\rho} \tilde{Y}_i) + \nabla \cdot (\bar{\rho} \tilde{u} \tilde{Y}_i - \bar{\rho} \bar{\mathcal{D}}_{Y_i} \nabla \tilde{Y}_i) = \bar{R}_{Y_i}$$

HOWEVER, $\overline{R}_{Y_i} \neq R_{\bar{Y}_i}$

$$\overline{R}_{Y_i} = \frac{1}{\Delta t}\int_0^{\Delta t} R_{Y_i} \, dt$$

$$= \frac{1}{\Delta t}\int_0^{\Delta t} \sum_{rxns} \nu_i A_i e^{-E_i/RT} Y_{i_1} Y_{i_2} \, dt$$

(1) Very sensitive to fluctuations in T

(2) cannot ignore $\overline{Y_i' T'}$ correlations

(3) bad to assume $\overline{R}_{Y_i} = \sum \nu_i A_i e^{-E_i/R\bar{T}} \overline{Y}_{i_1} \overline{Y}_{i_2}$

(although some people have done this)

(4) fluctuations in T affect energy equation as well

$\Rightarrow$ Need for some slick model!!

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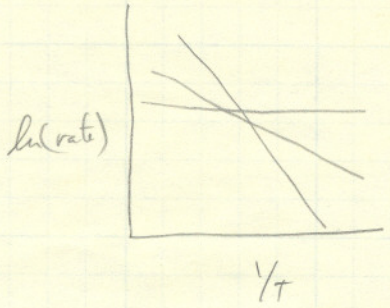
Concept of time scales

A. 1st think of reaction rate (like of a solid)



→ the lowest rate controls

B. Rate of mixing vs. rate of reaction → lowest rate controls

τ_r = reaction time scale (time to react ~ 90%)

τ_m = mixing time scale (time to mix on a molecular level)

Case 1

$\tau_m \ll \tau_r$ $\qquad \bar{R}_i = f(\bar{C}_i, \bar{C}_j, \bar{\rho}, \bar{T}) = A e^{-\frac{E}{RT}} \bar{C}_i^{\alpha} \bar{C}_j^{\beta}$

Case 2

$\tau_m \gg \tau_r$

- Calculate mixing rate only
- If its mixed, its burned
- equilibrium kinetics after mixing
- not valid for premixed systems

Case 3

$\tau_m \cong \tau_r$ - Difficult to handle

What usually happens in combustion?

Case 3 (or case 2 for diffusion flames)

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Magnussen - Hjertager 16th Symp., 1976

Proposal: Calculate (a) the mixing rate
(b) the reaction rate based on mean values

Take the lower of (a) & (b)

Fuel + Oxidizer → Products

A. Mixing-limited rate of fuel consumption:

(1) $R_f = A \bar{C}_f \left(\frac{\varepsilon}{k}\right)$

A: empirical constant; $\frac{\varepsilon}{k}$: mixing rate

B. Mixing-limited rate of oxidizer consumption

(2) $R_f = A \frac{\bar{C}_{ox}}{r_f} \left(\frac{\varepsilon}{k}\right)$, r_f = stoichiometric oxygen requirement

C. For premixed flames, you need the rate of mixing of hot products

(3) $R_f = A \cdot B \cdot \frac{\bar{C}_p}{1+r_f} \frac{\varepsilon}{k}$

D. Arrhenius reaction rate

(4) $R_f = k_0 e^{-E/(R\bar{T})} C_f^a C_o^b$

⇒ Actual Rate = Minimum of $\{(1), (2), (3), (4)\}$

→ You either get reactants or products (no intermediates, like CO)
→ one reaction may not be totally controlling
→ multiple reactions? not!
→ fast! (computationally)

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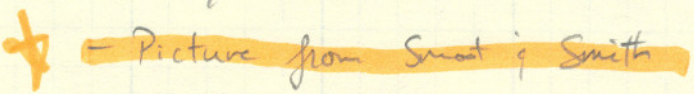
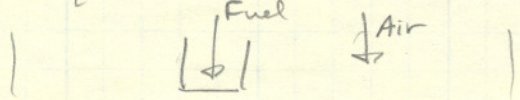
Mixing-limited reactions

People have found experimentally that species concentrations and temperatures in laminar diffusion flames are functions of the local equivalence ratio.



Equivalence Ratio is a function of Mixture Fraction



$$f = \frac{m_p}{m_p + m_s}$$

Any conserved scalar "s" can then be calculated

$$s = f\, s_p + (1-f)\, s_s$$

(s_p: value of s in pure primary)

Examples of conserved scalar:
- mass of element i (1-phase)
- density (non-reacting only)
- enthalpy (adiabatic only)

Idea: Calculate f, then get all of the species!!

Conservation equation for "$\tilde{f}$":

$$\frac{\partial}{\partial t}(\bar{\rho}\,\tilde{f}) + \vec{\nabla}\cdot\left(\bar{\rho}\,\tilde{f}\tilde{\vec{v}} - \mathcal{D}_{turb,f}\,\vec{\nabla}\tilde{f}\right) = 0$$

$$\mathcal{D}_{turb,f} = \frac{\nu_g^t}{\sigma_f}$$

Smoot & Smith 11.21

Also, define $\hat{g}_f = \overline{(\rho f - \rho\bar{f})^2}$ (density weighted)

$\bar{\rho}$

Transport eqn:

$$\frac{\partial}{\partial t}(\rho g_f) + \nabla\cdot(\rho\vec{v}\, g_f - \mathcal{D}_g \nabla g_f) = C_{g_1}\mu_t\left[\left(\frac{\partial\tilde{f}}{\partial x}\right)^2 + \left(\frac{\partial\tilde{f}}{\partial r}\right)^2\right] - \frac{C_{g_2}\bar{\rho}\tilde{\varepsilon}\,\hat{g}_f}{k^2}$$

generation; dissipation

Smoot & Smith 11.29

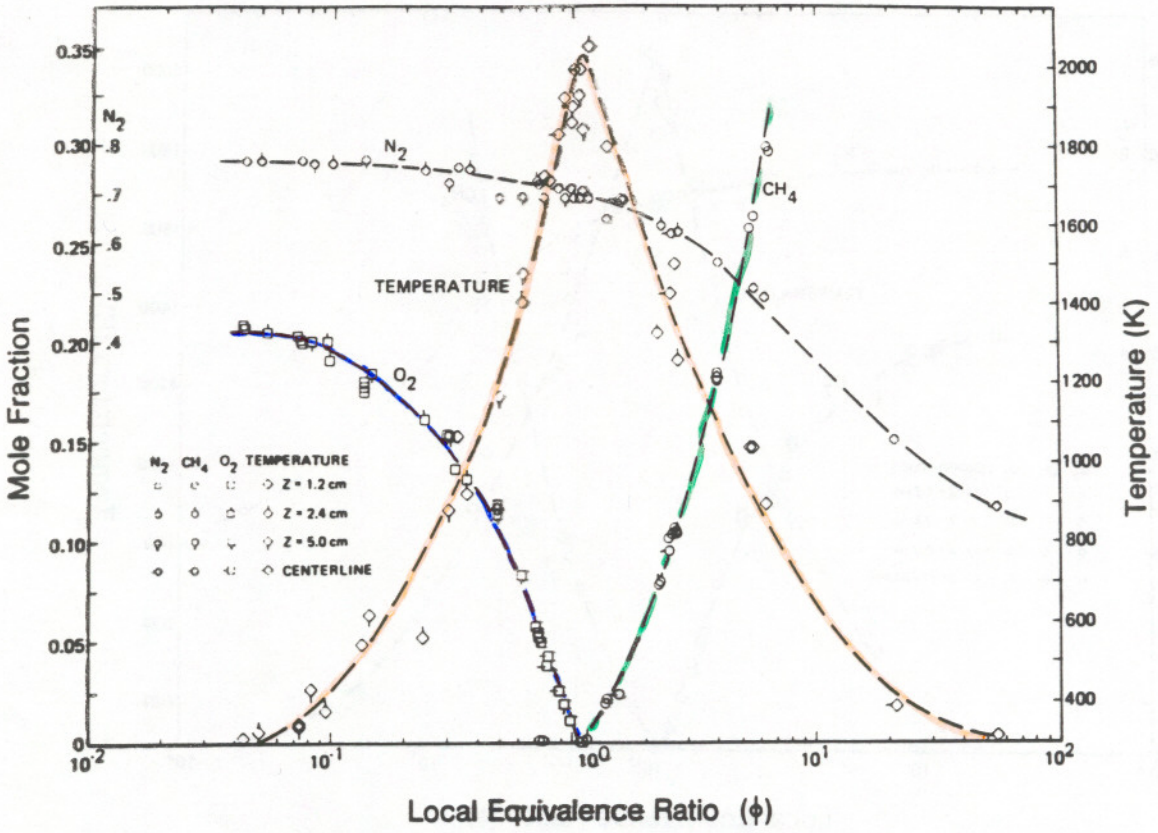


Figure 11.4. Measured temperature and reactant concentration as a function of the local equivalence ratio in a laminar methane diffusion flame. (Figure used with permission from Mitchell *et al.*, 1980.)

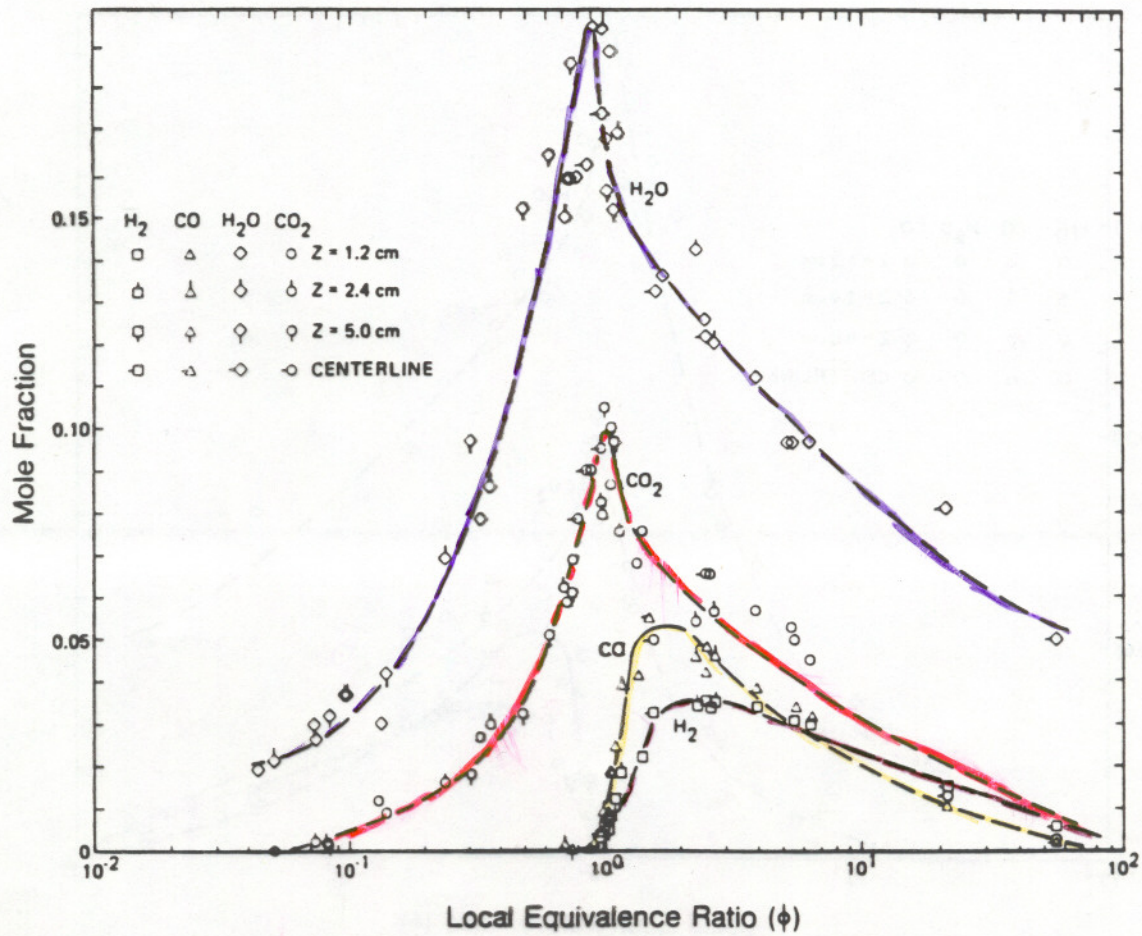


Figure 11.5. Measured major-product concentration as a function of the local-equivalence ratio in a laminar methane diffusion flame. (Figure used with permission from Mitchell *et al.*, 1980.)

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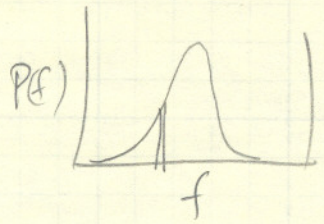
PDF's for

turbulent combustion

(PDF's)

$P(f)\,df$ = fraction of time you are at f



Properties of PDF's (identities)

$$\int_0^1 P(f)\,df = 1$$

$$\bar{f} = \int_0^1 f\,P(f)\,df$$

$$g_f = \int_0^1 (f-\bar{f})^2\,P(f)\,df$$

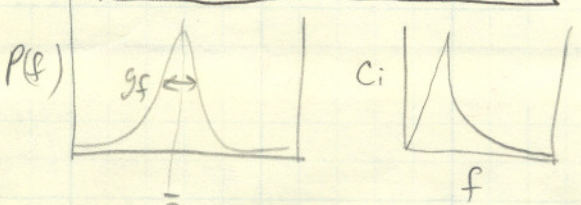
Idea: ① Assume gaussian shape, which is defined by $\bar{f}$ & g_f $\quad P(f) = \frac{1}{\sqrt{2\pi g_f}}\, e^{\frac{(f-\bar{f})^2}{2g_f}}$

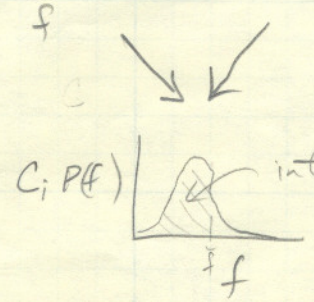
② Instantaneous properties (species) can be obtained for each instantaneous f [table of Y_i vs f] (use equilibrium based on elemental comp. and h)

③ Mean properties can be obtained using the PDF

$$\bar{\beta} = \int_0^1 \beta\,P(f)\,df$$

if $\beta = f(\text{elemental comp., enth})$ $= f(f)$





$\bar{C}_i$ ← wanted!

- (more important than rxn rate!)
- (species cont. eqns. not solved)

PDF's (cont.)

PDF

Advantages

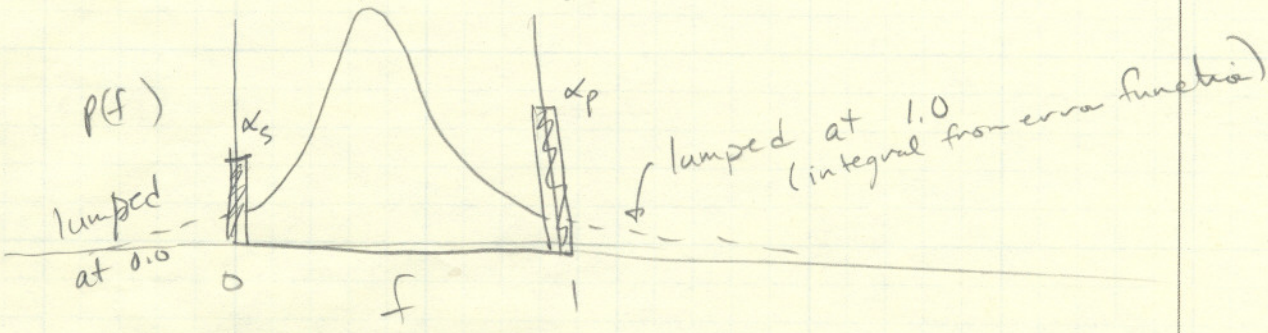
- no reaction rates required (use equilibrium & data)
- intermediate species predicted
- only <u>one</u> transport equation!

Disadvantages

- non-premixed flames only
- reactions may <u>not</u> be mixing-limited in some cases, which goes against assumptions

Other: you may have pockets of pure, unreacted primary or secondary

⇒ intermittency



readjust integrals so

$$\alpha_p + \alpha_s + \int_0^1 P(f)\,df = 1$$

$$\alpha_p f_p + \alpha_s f_s + \int_0^1 f\,P(f)\,df = \bar{f}$$

also g_f ⇒ must be correct (remember $f_s = 0$, $f_p = 1$)

⇒ Table 11.2 in Smoot & Smith

TABLE 11.2. Parameters for Clipped Gaussian Probability Density Function

$$P(f) = (2\pi G_f)^{-1/2} \exp(-Z_f^2/2)$$

$$\alpha = (2\pi)^{-1/2} \int_L^U \exp(-Z_f^2/2)\, dZ_f$$

Intermittency	U	L	Z_f
α_p	∞	$(1-F)/G_f^{1/2}$	$(f-F)/G_f^{1/2}$
α_s	$-F/G_f^{1/2}$	$-\infty$	$(f-F)/G_f^{1/2}$

where F and G_f come from

$$\bar{f} = \alpha_p + (2\pi G_f)^{-1/2} \int_{0+}^{1-} f \exp\left(\frac{-(f-F)^2}{2G_f}\right) df$$

$$g_f = \alpha_p - \bar{f}^2 + (2\pi G_f)^{-1/2} \int_{0+}^{1-} f^2 \exp\left(\frac{-(f-F)^2}{2G_f}\right) df$$

Example

CH_4/air at 300 k

Primary = CH_4 @ 300 k, $H_p = -17.889$ $\frac{kcal}{gmole}$

Secondary = Air @ 300 k, $H_s = 0$

$$CH_4 + 2O_2 \rightarrow 2H_2O + CO_2$$

Say we have 1 kmole/s of CH_4

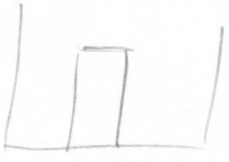
Need 2 kmoles/s of O_2

⇒ See computer disk

Fluent ⇒ uses a β-function instead of a Gaussian (no exponential involved)

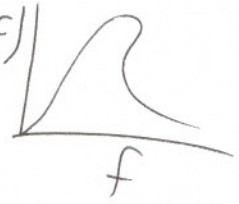
$$PDF = \frac{f^a(1-f)^b}{B}$$

⇒ Top hat can be used



⇒ stores completely integrated PDF stuff in a table

f	$g(f)$	$\bar{T}$	$\bar{Y}_{O_2}$	etc.
⋮	⋮	⋮	⋮	

1. 

from $\bar{f}, \sigma_f$

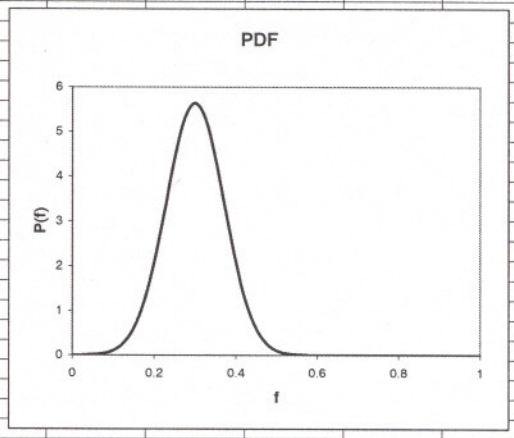
2. γ_k at different values of f
h " " " " "

f	γ_k's	h	T_{eq}	γ_i
			=	=
			=	=
			=	=
			=	=
			=	=

3. $\int T(f) P(f) \, df$

$\bar{T}$

Mean f	Variance				
0.3	5.00E-03				
f	P(f)	Integral of P(f)df	Integral of f P df	Integral of (f-fbar) P df	
0	0.00069627				
0.025	0.00293139	4.53456E-05	9.16058E-07	3.55437E-06	
0.05	0.01089142	0.000172785	7.7232E-06	1.128E-05	
0.075	0.0357116	0.000582538	4.02868E-05	3.11077E-05	
0.1	0.10333494	0.001738082	0.000162648	7.42662E-05	
0.125	0.26387501	0.004590124	0.000541473	0.000152682	
0.15	0.59465151	0.010731581	0.001527276	0.00026826	
0.175	1.18260574	0.022215716	0.003701922	0.000398223	
0.2	2.0755377	0.040726793	0.007775794	0.00049042	
0.225	3.21465568	0.066127417	0.014230063	0.000485473	
0.25	4.39391335	0.095107113	0.022772198	0.00036334	
0.275	5.3000712	0.121174807	0.031949974	0.000178717	
0.3	5.64189642	0.136774595	0.039376106	4.14068E-05	
0.325	5.3000712	0.136774595	0.042688651	4.14068E-05	
0.35	4.39391335	0.121174807	0.04075491	0.000178717	
0.375	3.21465568	0.095107113	0.034292069	0.00036334	
0.4	2.0755377	0.066127417	0.025446387	0.000485473	
0.425	1.18260574	0.040726793	0.016660281	0.00049042	
0.45	0.59465151	0.022215716	0.009627508	0.000398223	
0.475	0.26387501	0.010731581	0.004911673	0.00026826	
0.5	0.10333494	0.004590124	0.002212601	0.000152682	
0.525	0.0357116	0.001738082	0.000880201	7.42662E-05	
0.55	0.01089142	0.000582538	0.000309236	3.11077E-05	
0.575	0.00293139	0.000172785	9.59479E-05	1.128E-05	
0.6	0.00069627	4.53456E-05	2.62913E-05	3.55437E-06	
0.625	0.00014595	1.05276E-05	6.36219E-06	9.75992E-07	
0.65	2.6997E-05	2.16178E-06	1.35955E-06	2.34033E-07	
0.675	4.4072E-06	3.92554E-07	2.56537E-07	4.90863E-08	
0.7	6.3491E-07	6.30259E-08	4.27409E-08	9.01679E-09	
0.725	8.072E-08	8.9454E-09	6.287E-09	1.45207E-09	
0.75	9.0565E-09	1.12221E-09	8.1643E-10	2.05175E-10	
0.775	8.9672E-10	1.24416E-10	9.35919E-11	2.54534E-11	
0.8	7.8354E-11	1.21884E-11	9.4705E-12	2.77388E-12	
0.825	6.042E-12	1.05495E-12	8.45852E-13	2.65674E-13	
0.85	4.1117E-13	8.0665E-14	6.66772E-14	2.23714E-14	
0.875	2.4692E-14	5.44823E-15	4.63871E-15	1.65677E-15	
0.9	1.3087E-15	3.25013E-16	2.84796E-16	1.07938E-16	
0.925	6.1206E-17	1.71232E-17	1.543E-17	6.18779E-18	
0.95	2.5263E-18	7.96659E-19	7.37699E-19	3.12201E-19	
0.975	9.202E-20	3.27289E-20	3.11212E-20	1.38661E-20	
1	2.958E-21	1.18723E-21	1.15847E-21	5.42201E-22	
	Integral	1.000	0.300	0.005	This is a consistency check!



A. Calculate Value of f at Stoichiometric Conditions

CH4-Air	Molar flow rat	Mass Flow	Stoich. f	Enthalpy (kcal/r	Enthalpy (kcal/100 g)
CH4	1	16	0.055045872	-17.889	-111.80625
O2	2	64		0	0
N2	7.52380952	210.7		0	0

B. Calculate Elemental Compositions as a Function of f

f	C	H	O	N	Enthalpy
0	**0**	**0**	**0.233009709**	**0.766990291**	**0**
0.02	0.015	0.00375	0.232135922	0.588944293	-2.236125
0.04	0.03	0.0075	0.231262136	0.589614478	-4.47225
0.06	0.045	0.01125	0.23038835	0.590284664	-6.708375
0.08	0.06	0.015	0.229514563	0.59095485	-8.9445
0.1	0.075	0.01875	0.228640777	0.591625035	-11.180625
0.2	0.15	0.0375	0.224271845	0.594975964	-22.36125
0.4	0.3	0.075	0.215533981	0.601677821	-44.7225
0.6	0.45	0.1125	0.206796117	0.608379678	-67.08375
0.8	0.6	0.15	0.198058252	0.615081535	-89.445
1	**0.75**	**0.25**	**0**	**0**	**-111.80625**

C. Calculate Equilibrium Temperature and Compositions from Elemental Compositions and Mixture Enthalpies Using EDWRDS

	Mole Fractions				
T (equil)	CO2	CH4	O2	MW	ER
300	**0**	**0**	**0.21**	**29**	**0**
1173	0.0354	0	0.1318	28.4	0.3494
1860	0.0696	0	0.0545	27.95	0.7134
2215	0.0764	0	0.0004	27.01	1.093
1913	0.0413	0	0	24.9	1.488
1626	0.0299	0	0	23.07	1.902
933	0.0300	0.028	0	17.75	
782	0.0150	0.22	0	14.96	
666	0.0030	0.535	0	15.81	
528	0.0003	0.825	0	16.68	
300	**0**	**1**	0	**16**	**inf**

D. Plot f vs. T

f	T
0	300
0.02	1173
0.04	1860
0.06	2215
0.08	1913
0.1	1626
0.2	933
0.4	782
0.6	666
0.8	528
1	300