ME140 Fall 2006
Prof Fernandez-Pello
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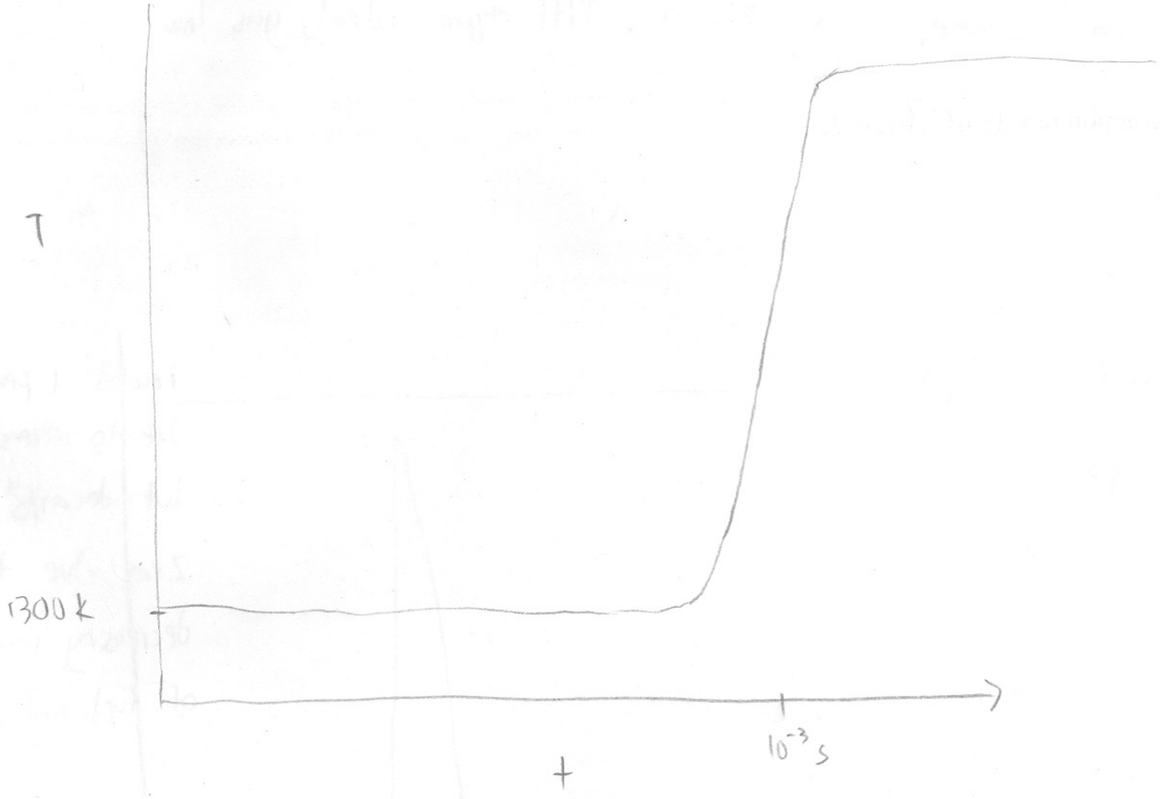
Midterm #1
10/05/06

1) (25 points) Consider a constant-volume homogeneous well-mixed combustor containing a stoichiometric mixture of a hydrocarbon fuel and air. The combustor is adiabatic and there is no mass transfer in or out of the combustor. The reaction rate can be described according to a single-step, global reaction:

$$\frac{dC_F}{dt} = -AC_F C_{O_2} \exp\left(-\frac{E}{RT}\right)$$

where t is time [s], C_F is the fuel concentration [mole/m^3], C_{O_2} is the O_2 concentration [mole/m^3], A is a pre-exponential factor [m^3/(mole-s)] of the one-step reaction, E is the activation energy [J/mole] of the one-step reaction, R is the universal gas constant [J/(mole-K)], and T is the temperature inside the combustor [K]. Assume complete combustion and that the only species involved are fuel, N_2, O_2, CO_2, and H_2O. Assume that the initial pressure (P) is 1 atm and that the initial temperature is 1300 K. The fuel is completely consumed within 10^{-3} seconds. With t as the x-axis, sketch approximate plots of the following:

1a) $T(t)$:



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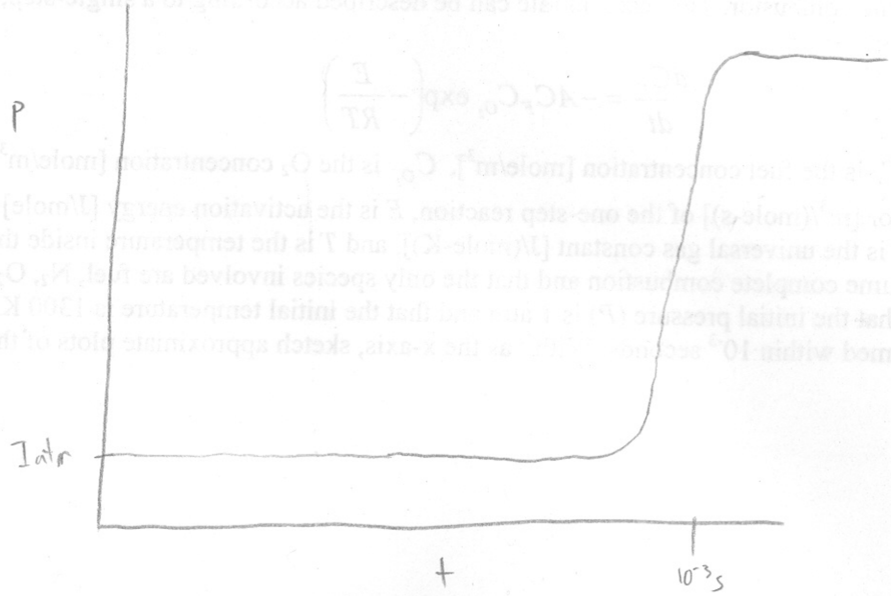
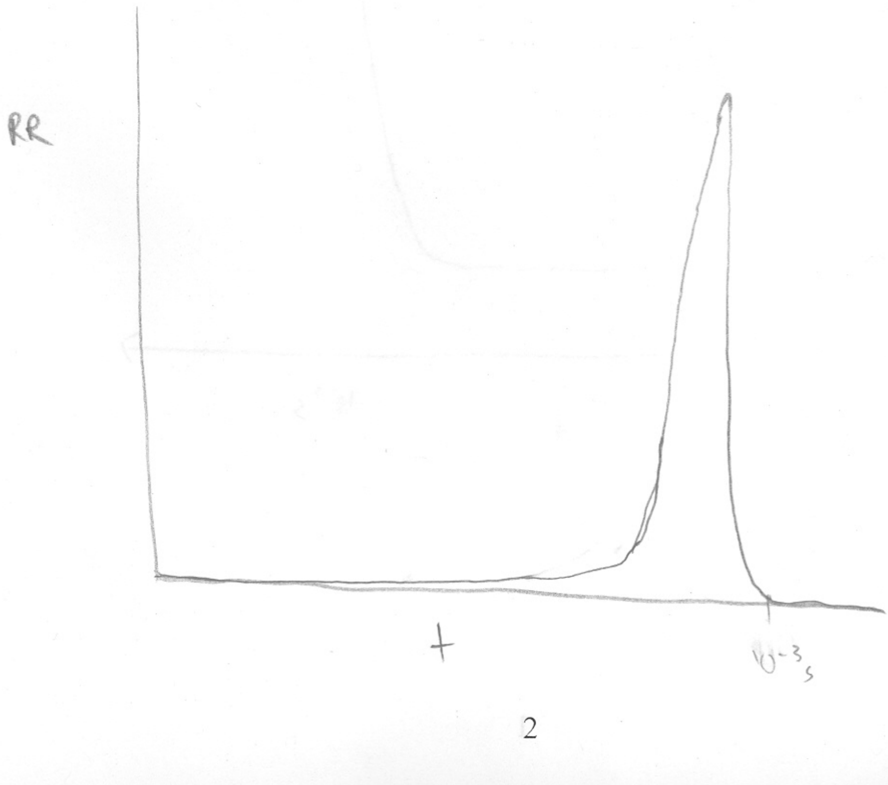
1b) $P(t)$:



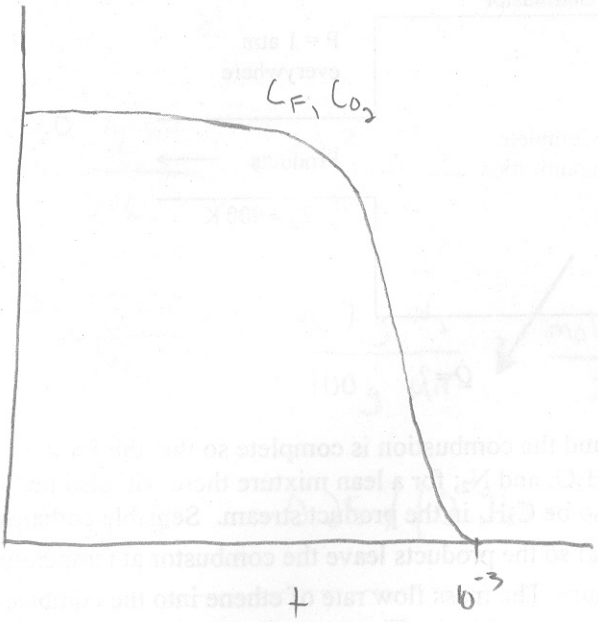
constant volume, so $P(t) \propto T(t)$ from ideal gas law

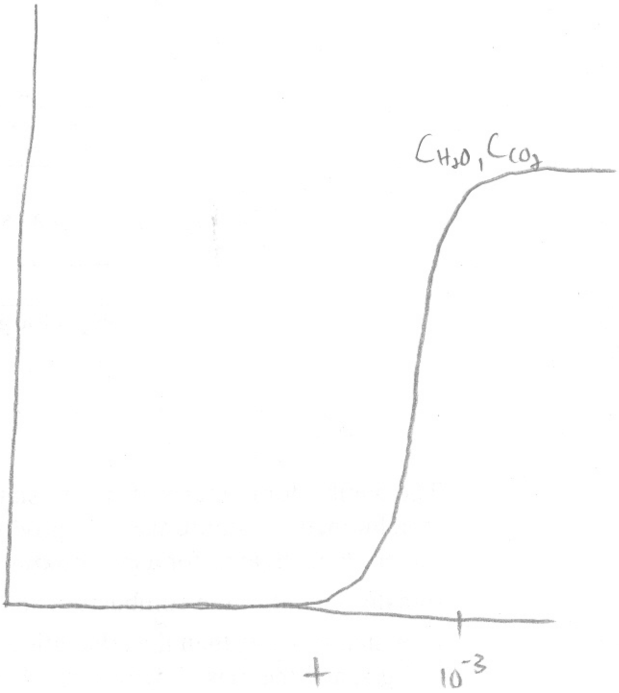
1c) Reaction rate $\left(-dC_F(t)/dt\right)$:

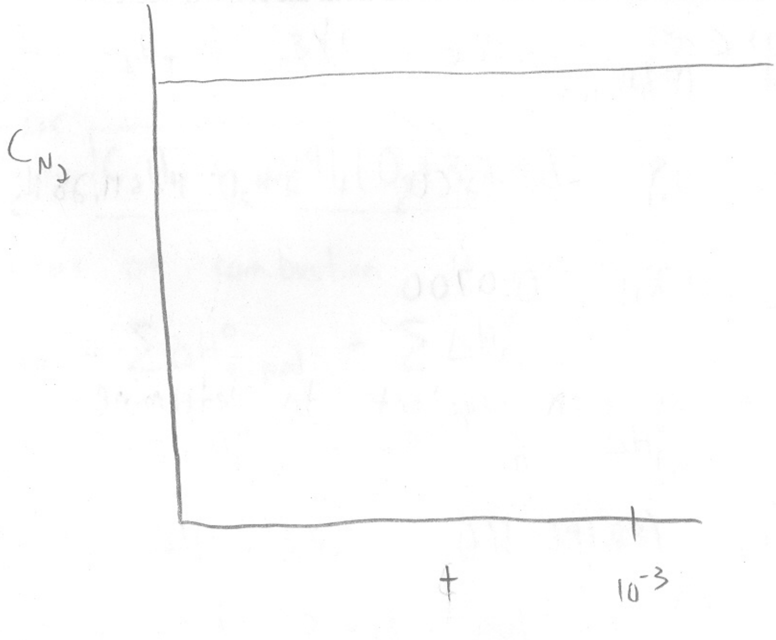


reaches a peak due to increasing T but decays to zero due to decreasing concentrations of fuel and oxygen

1d) $C_F(t)$, $C_{O_2}(t)$, $C_{N_2}(t)$, $C_{H_2O}(t)$, $C_{CO_2}(t)$:







(N_2 does not react)

ME140 Fall 2006
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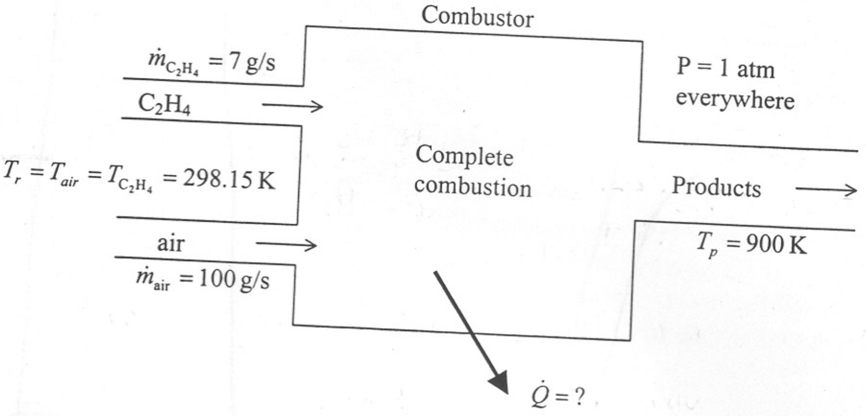
2) (75 points) Consider the combustor, shown schematically below, in which ethene (C_2H_4) and air are mixed and burned.



The combustor operates at steady-state conditions and the combustion is complete so that ~~the~~ for a stoichiometric mixture the only products are CO_2, H_2O, and N_2; for a lean mixture there will also be O_2 in the product stream; for a rich mixture there will also be C_2H_4 in the product stream. Sensible enthalpy is transferred out of the combustor at a rate of $\dot{Q}$ (kJ/s) so the products leave the combustor at temperature T_p which is lower than the adiabatic flame temperature. The mass flow rate of ethene into the combustor is 7 g/s, and the mass flowrate of air into the combustor is 100 g/s. The reactants enter the combustor at a temperature of $T_r = 298.15$ K and a pressure of $P_r = 1$ atm, and the products leave the combustor at a temperature of $T_p = 900$ K and a pressure of $P_p = 1$ atm. What is the rate of heat transfer $\dot{Q}$ out of the combustor?

Note: Air is 23.3% oxygen and 76.7% nitrogen **by mass** (21.1% oxygen and 79.9% nitrogen **by volume**). The molecular weights of ethene, oxygen, and nitrogen are 28 g/mol, 32 g/mol, and 28 g/mol, respectively. If you need it, the heat of formation of ethene can be found from the JANAF tables at 298.15 K.

First, balance rxn to find $(F/A)_{stoic}$:

$$C_2H_4 + 3(O_2 + 3.76\,N_2) \rightarrow 2\,CO_2 + 2\,H_2O + 11.28\,N_2$$

$$\therefore (F/A)_{stoic} = 1/[(3)(4.76)] = 0.0700$$

Next, find molar flowrates of each reactant to determine $(F/A)_{act}$.

→

$$\dot{n}_{C_2H_4} = \frac{7\,g}{s} \times \frac{mol}{28\,g} = 0.25\ \frac{mole\ C_2H_4}{sec}$$

$$\dot{n}_{O_2} = \frac{100\ g\ air}{sec} \times \frac{23.3\ g\ O_2}{100\ g\ air} \times \frac{mole\ O_2}{32\ g\ O_2} = 0.728\ \frac{mole\ O_2}{sec}$$

$$\dot{n}_{N_2} = \frac{100\ g\ air}{sec} \times \frac{76.7\ g\ N_2}{100\ g\ air} \times \frac{mole\ N_2}{28\ g\ O_2} = 2.739\ \frac{mole\ N_2}{sec}$$

$$(F/A)_{act} = 0.25/(0.728 + 2.739) = 0.0721$$

$$\boxed{\phi = \frac{(F/A)_{act}}{(F/A)_{stoic}} = \frac{0.0721}{0.0700} = 1.03 \quad \text{(slightly rich)}}$$

The actual reaction is:

$$1.03\,C_2H_4 + 3(O_2 + 3.76N_2) \rightarrow 2CO_2 + 2H_2O + 11.28\,N_2 + 0.03\,C_2H_4$$

or

$$\boxed{C_2H_4 + 2.91(O_2 + 3.76N_2) \rightarrow 1.94\,CO_2 + 1.94\,H_2O + 10.95\,N_2 + 0.029\,C_2H_4}$$

The heat of combustion is calculated as:

$$Q_P = \sum \Delta H^0_{f,prod} - \sum \Delta H^0_{f,reac}$$

$$= 2\Delta H^0_{f,CO_2} + 2\Delta H^0_{f,H_2O} - \Delta H^0_{f,C_2H_4}$$

$$= (2)(-393.52) + (2)(-241.83) - 52.467$$

$$= -1323.2\ kJ/mol$$

$$\boxed{\Delta H_c = 1323.2\ kJ/mol}$$

- The rate of heat release due to combustion can be calculated by noting that 1 mole of C_2H_4 is consumed for every 2.91 moles of O_2:

$$\boxed{\dot{Q}_{HRR} = \frac{0.728 \text{ moles } O_2}{\text{sec}} \times \frac{1 \text{ mole } C_2H_4}{2.91 \text{ moles } O_2} \times \frac{1323.2 \text{ kJ}}{\text{mole } C_2H_4} = 331 \text{ kW}}$$

- The rate at which sensible enthalpy flows into the combustor is zero because the reactants are at 298.15 K
- The rate at which sensible enthalpy flows out of the combustor can be determined as:

$$\dot{Q}_{out,flow} = \sum \dot{n}_i h_i(900\text{K})$$

where $h_i(900\text{K})$ is determined from the JANAF tables.
Therefore, we need $\dot{n}_i$ for each product:

$$\dot{n}_{CO_2} = 1.94\ \dot{n}_{C_2H_4,in} = (1.94)(0.25) = 0.485 \text{ moles/sec}$$

$$\dot{n}_{H_2O} = 1.94\ \dot{n}_{C_2H_4,in} = (1.94)(0.25) = 0.485 \text{ moles/sec}$$

$$\dot{n}_{N_2} = 10.95\ \dot{n}_{C_2H_4,in} = (10.95)(0.25) = 2.738 \text{ moles/sec}$$

$$\dot{n}_{O_2} = 0 \qquad = 0 \text{ moles/sec}$$

$$\dot{n}_{C_2H_4} = 0.029\ \dot{n}_{C_2H_4,in} = (0.029)(0.25) = 0.0073 \text{ moles/sec}$$

$$\dot{Q}_{out,flow} = (0.485)(28.03) + (0.485)(21.94) + (2.738)(18.22) + 0 + (0.0073)(41.51)$$

$$\boxed{\dot{Q}_{out,flow} = 74.4 \text{ kW}}$$

An overall energy balance (sensible enthalpy) on the system gives:

$$\cancelto{0}{IN} - \underset{\dot{Q}+\dot{Q}_{flow,out}}{\underset{\uparrow}{OUT}} + \underset{\dot{Q}_{HRR}}{\underset{\uparrow}{GEN}} = \cancelto{0}{STOR}$$

$$\therefore \quad -\dot{Q} - \dot{Q}_{flow,out} + Q_{HRR} = 0$$

$$\dot{Q} = \dot{Q}_{HRR} - \dot{Q}_{flow,out}$$

$$\dot{Q} = 331 \text{ kW} - 74.4 \text{ kW}$$

$$\boxed{\dot{Q} = 256.6 \text{ kW}}$$

∼ 257 kW is transferred <u>out</u> of the combustor

(see other solution method)

Alternatively, total (chemical plus sensible) enthalpy is conserved during combustion, except for heat losses:

$$\therefore \sum \dot{n}_{i,in} h_{T,i} - \sum \dot{n}_{j,out} h_{T,j} = \dot{Q}_{out}$$

here $h_{T,i} = \underset{\substack{\uparrow \\ \text{Chemical enthalpy} \\ \text{(enthalpy of formation)}}}{h_i^o} + h_{s,i}$ ↖ sensible enthalpy

$$\dot{Q}_{out} = \dot{n}_{C_2H_4,in} h_{T_{C_2H_4}}(298K) + \dot{n}_{O_2,in} h_{T\,O_2}(298K) + \dot{n}_{N_2,in} h_{T\,N_2}(298K)$$

$$- \left[\dot{n}_{C_2H_4,out} h_{T\,C_2H_4}(900K) + \dot{n}_{CO_2,out} h_{T_{CO_2}}(900K) + \dot{n}_{H_2O,out} h_{T\,H_2O}(900K) + \dot{n}_{C_2H_4,out} h_{T_{C_2H_4}}(900K)\right]$$

recall:

$\dot{n}_{C_2H_4,in}$ = 0.25 moles/sec

$\dot{n}_{O_2,in}$ = 0.728 moles/sec

$\dot{n}_{N_2,in}$ = 2.739 moles/sec

$\dot{n}_{C_2H_4,out}$ = 0.0073 moles/sec

$\dot{n}_{O_2,out}$ = 0

$\dot{n}_{N_2,out}$ = 2.739 moles/sec

$\dot{n}_{CO_2,out}$ = 0.485 moles/sec

$\dot{n}_{H_2O,out}$ = 0.485 moles/sec

From JANAF tables:

$h_{T,C_2H_4}(298K) = 52.5$ kJ/mol

$h_{T,O_2}(298K) = 0$ kJ/mol

$h_{T,N_2}(298K) = 0$ kJ/mol

$h_{T,C_2H_4}(900K) = 52.5 + 41.51 = 94.01$ kJ/mol

$h_{T,O_2}(900K) =$ N/A

$h_{T,N_2}(900K) = 0 + 18.22 = 18.22$ kJ/mol

$h_{T,CO_2}(900K) = -393.5 + 28.03 = -365.47$ kJ/mol

$h_{T,H_2O}(900K) = -241.83 + 21.94 = -219.89$

Substituting values:

$$\dot{Q}_{out} = (0.25)(52.5) + (0.728)(0) + (2.739)(0)$$

$$- \left[(0.0073)(94.01) + (0.485)(-365.47) + (0.485)(-219.89) + (2.734)(18.22) \right]$$

$$\dot{Q}_{out} = 13.13 + 0 + 0 - 0.69 + 177.3 + 106.6 - 49.9$$

$$\dot{Q}_{out} = 246.4 \text{ kJ/s}$$

$$\boxed{\dot{Q}_{out} = 246.4 \text{ kW}}$$

* Solutions differ by ~ 4%. They should match exactly, so there's probably an algebra error.