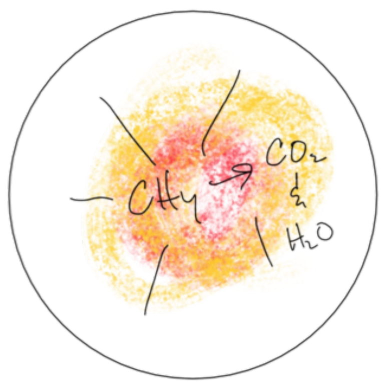
Instructor Notes



Combustion Inside Closed Container

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

3 mol $\longrightarrow$ 3 mol

$r_{CH_4} = -k P_{CH_4}^a P_{O_2}^b$ or as an approximation

$r_{CH_4} = -k$

Mole Balance

total : $\frac{dn}{dt} = 0$ for stoichiometric mixture other mixture (fuel lean)
since 3 moles $\to$ 3 moles
• also assuming the water stays in the vapor phase

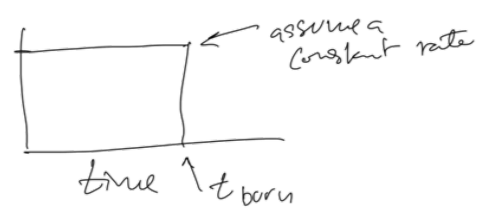
Energy Balance — could include heat loses to surroundings $q \sim \underset{\text{conv.}}{hA(T-T_s)}$ or $\underset{\text{radiation}}{\sigma \varepsilon A F(T^4 - T_s^4)}$

$\frac{dnU}{dt} = gen = +k\,\Delta H_{rxn}$ [=] $\frac{\text{mol } CH_4}{\text{sec}} \cdot \frac{J}{\text{mol } CH_4}$ [=] $\frac{J}{\text{sec}}$

$n\frac{dU}{dt} + U\cancel{\frac{dn}{dt}}^{\,0} = nC_v\frac{dT}{dt} \to \Delta H_{rxn}\int_0^t k(time)\,dt = nC_v(T_f - T_i)$

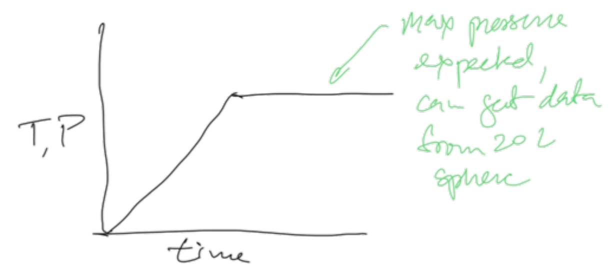
Ideal Gas : $PV = nRT$
• Can solve above conditions for n(constant) & T(changing) with V constant to get P as a f(time), including P_{max} and impulse

Example : Give $k(time)$ =



$T_i + \frac{\Delta H_{rxn} \cdot kt}{nC_v} = T$ ← temperature of gases in volume
(k: estimated constant burn rate; t: time up to t_{burn})

$P = \frac{nR}{V}\left[T_i + \frac{\Delta H_{rxn} \cdot kt}{nC_v}\right]$



Add Vent

What if the pressure expected is greater than the rating for the vessel?
↳ venting, burst disk, fast acting

S-curve : $\frac{1}{1+e^{-at+5}}$ ← Mimics the opening dynamics of the burst disk (a: rate of increase)

opening time, 67% open = $\frac{5.708}{a}$

$0.67 = \frac{1}{1+e^{-at+5}}$ $\quad 0.67\,e^{-at+5} = 1 - 0.67 = 0.33$

$e^{-at+5} = 0.33/0.67 =$

$-at+5 = \ln\left(\frac{0.33}{0.67}\right) = -0.708$

$t_{open} = 5.708/a \;\propto$ mass of vent (proportional)

or

So, vent area is a function of time : $\quad a = \frac{5.708}{t_{open}}$ (t_{open} → 67% open)

$A = A_{fo} \cdot \frac{1}{1+e^{-at+5}}$ (A_{fo}: fully open area) $\quad t = 0$ when P equals the set pressure of the relief

$\frac{dn}{dt} = \cancel{\dot{n}_{in}}^{\,0} - \dot{n}_{out} + \cancel{gen}^{\,0} \to \frac{dn}{dt} = -\dot{n}_{out}$

$\frac{dnU}{dt} = n\frac{dU}{dt} + U\frac{dn}{dt} = \cancel{\dot{n}_{in}H_{in}}^{\,0} - \dot{n}_{out}\bar{H} + \Delta H_{rxn} rV$

assume constant properties for simplicity

$H = U + PV$
for Ideal Gas
$H = U + RT$

$nC_v\frac{dT}{dt} = +\bar{U}\dot{n}_{out} - \dot{n}_{out}\bar{H} + \Delta H_{rxn} rV$

$= (\bar{U} - \bar{H})\dot{n}_{out} + \Delta H_{rxn} rV$

$nC_v\frac{dT}{dt} = -RT\dot{n}_{out} + \Delta H_{rxn} rV$

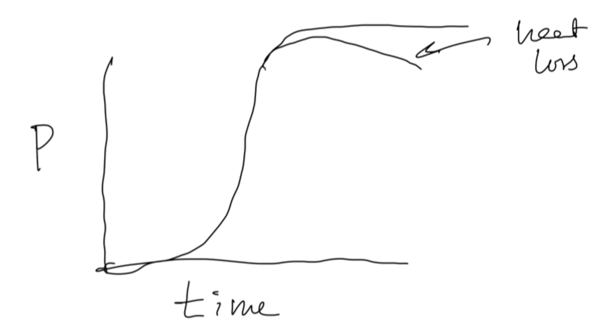
$\dot{n}_{out}$ = gaseous flow equation with the Area equal to 0 if $P < P_{burst\,disk}$

$A_{fo} \cdot \frac{1}{1+e^{-at+5}}$ if $P > P_{burst\,disk}$
where $t = 0$ when $P = P_{burst\,disk}$

See Python Files

In-class Discussion Notes

Combustion of Fuel inside Closed container



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

3 moles $\quad$ 3 moles

total mole b. $\frac{dn}{dt} = 0$ no vent, not produced moles

total Energy b. : $\frac{dn\bar{U}}{dt} = \cancel{in}^{\,0} - \cancel{out}^{\,0} + gen$

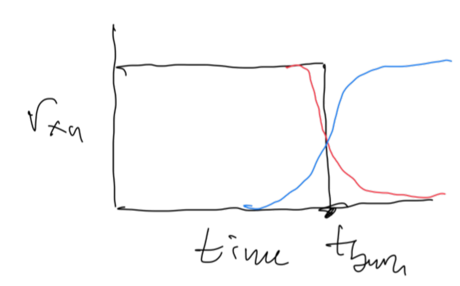
gen : $r_{CH_4} = -kn$ (k constant) $\quad k = Ae^{-E/RT}$

$\frac{\text{mol}}{\text{sec} \cdot m^3}$

$\frac{dn\bar{U}}{dt} = +kn \cdot \Delta H_{rxn} \cdot V$ [=] $\frac{\text{mol}}{\text{sec} \cdot m^3} \cdot m^3 \cdot \frac{J}{\text{mol}}$ $\quad k = \frac{1}{\text{sec} \cdot m^3}$

$\Delta H_{rxn} = \sum H^\circ_{prod} - \sum H^\circ_{react}$

$\frac{dn\bar{U}}{dt} = n\frac{d\bar{U}}{dt} + \bar{U}\cancel{\frac{dn}{dt}}^{\,0}$



$n\frac{d\bar{U}}{dt} = kn\,\Delta H_{rxn} \cdot V$

$\bar{U} = C_v(T - T^\phi)$

$\frac{d\bar{U}}{dt} = C_v\frac{dT}{dt}$

$1 - \frac{1}{1 + \exp(-at+b)}$

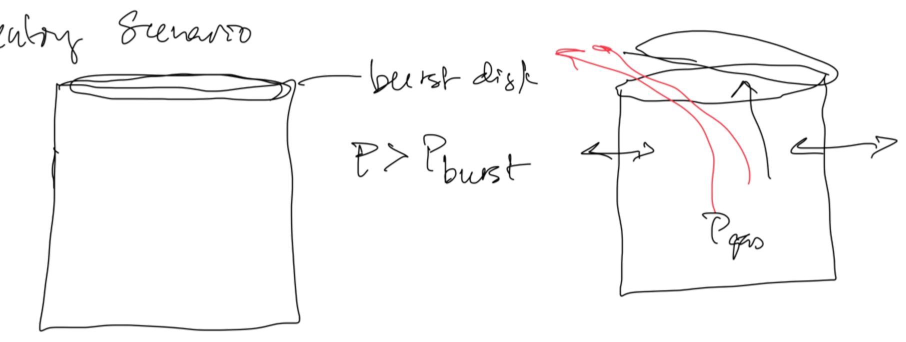
$\boxed{nC_v}\frac{dT}{dt} = kn\,\Delta H_{rxn} \cdot V$

$\frac{dT}{dt} = \frac{kn\,\Delta H_{rxn} V}{nC_v} \cdot$ sigmoid

$P_{(t)} = \frac{nRT(t)}{V}$ ← $T(t)$

Add Vent

Venting Scenario



$\frac{dn}{dt} = \cancel{in}^{\,0} - out + \cancel{gen}^{\,0} = -\dot{n}_{out}$

$\dot{m}$ — gases flowing through an orifice

$= PA\,Ma\sqrt{\frac{\gamma}{RTM_w}}\left(1 + Ma^2\right)\left(f(\gamma)\right)$

Ideal Gas $P = nRT/V$

Energy Balance $\frac{dn\bar{U}}{dt} = \cancel{\dot{n}_{in}H_{in}}^{\,0} - \dot{n}_{out}\bar{H} + gen$ (gen = $r_a V \cdot \Delta H_{rxn}$)

See Python code on the course website