CHEMICAL ENGINEERING DESIGN & SAFETY

CHE 4253

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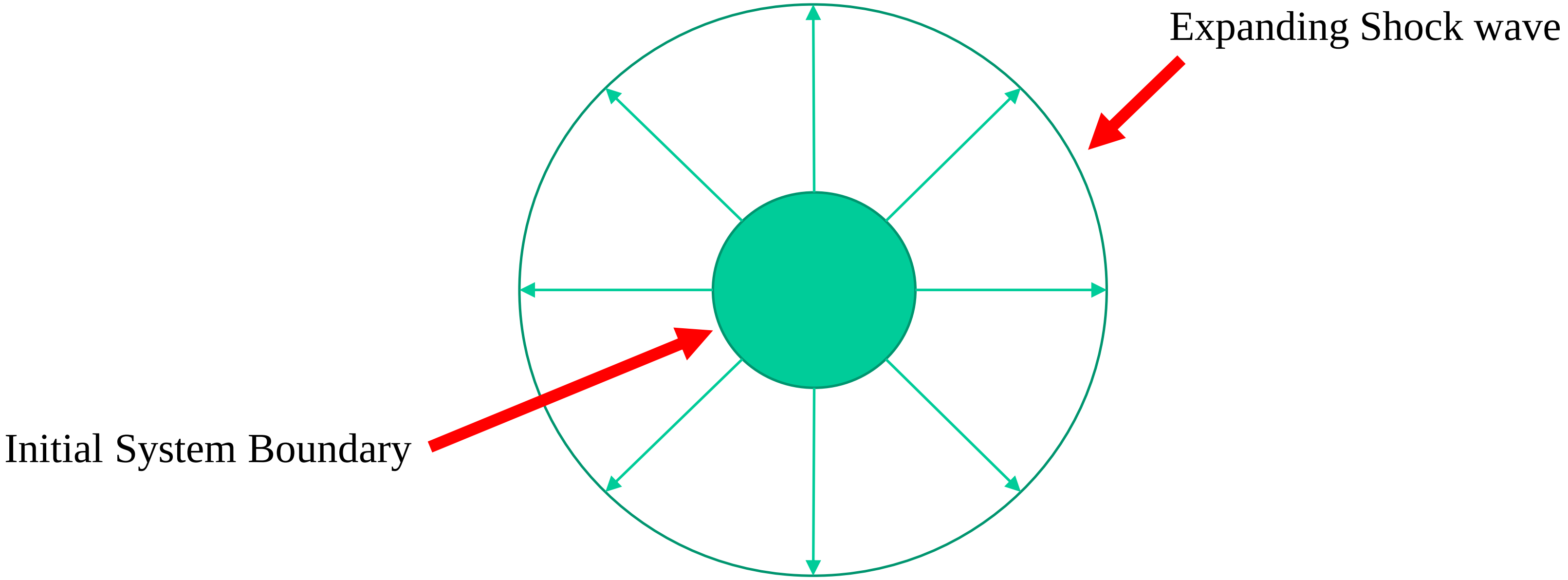
Explosions Explained

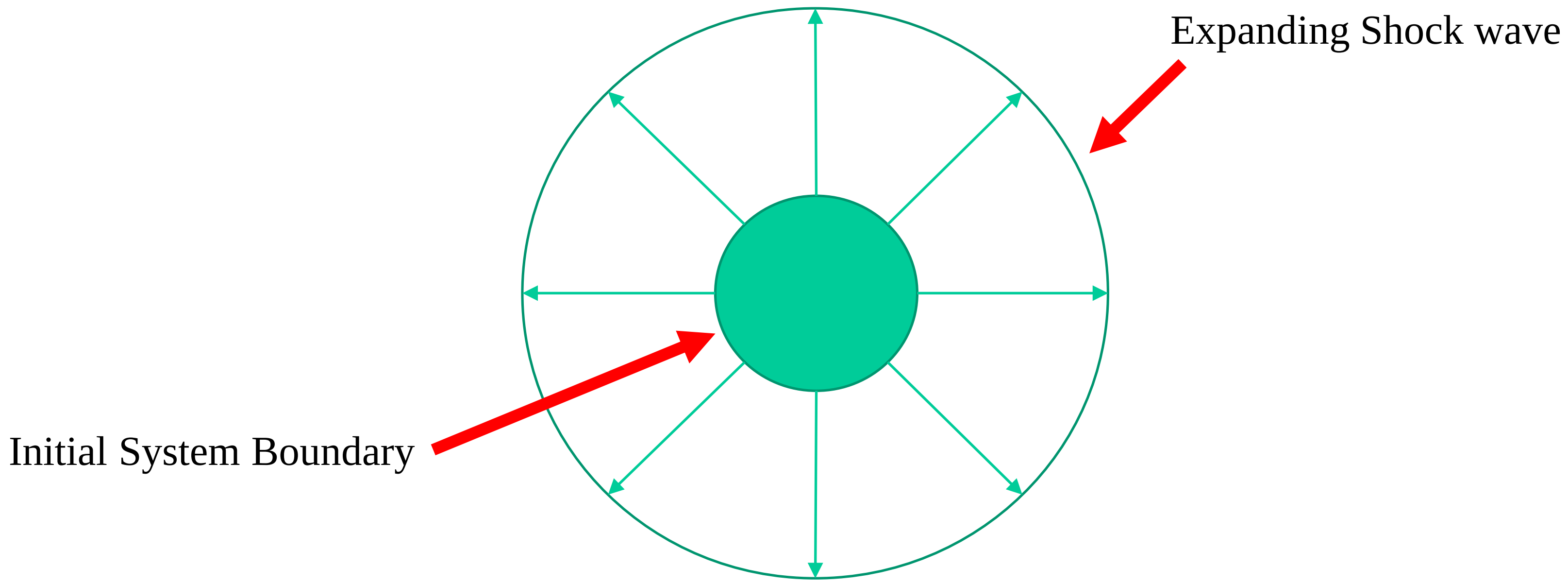
EXPLOSION

A rapid and uniform expansion



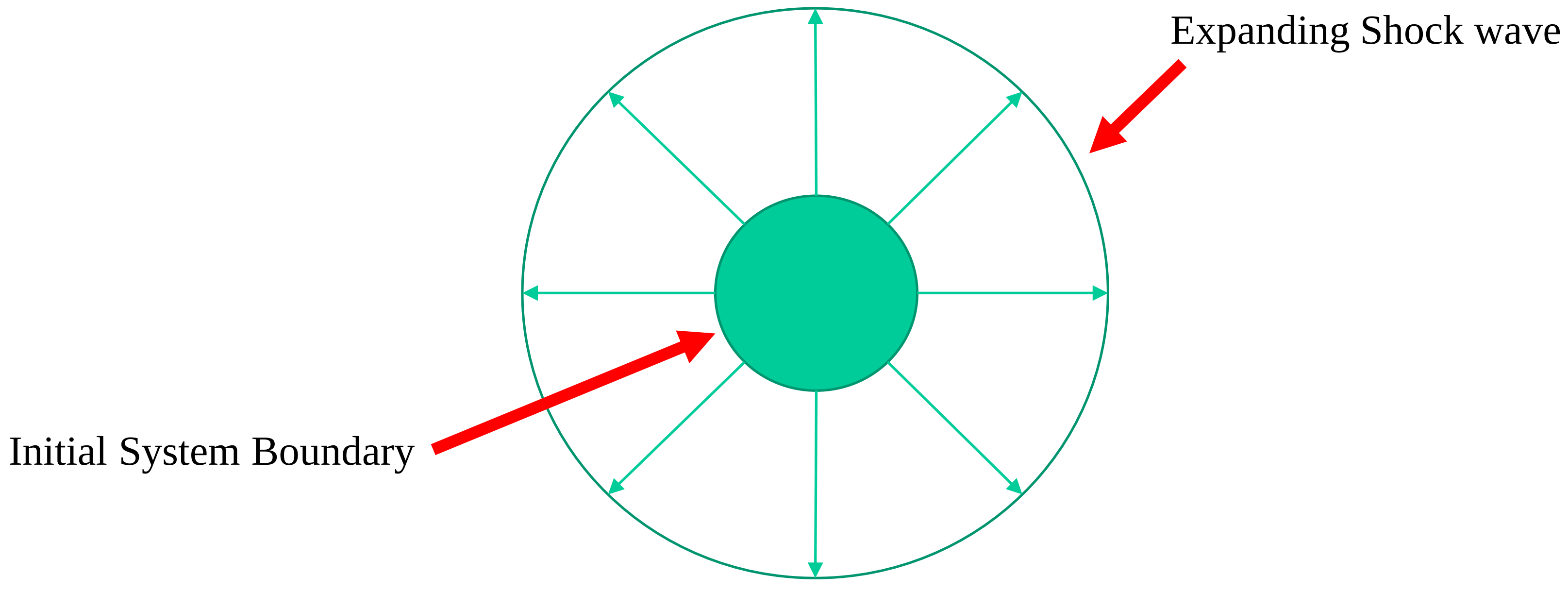
EXPLOSION

The expansion ends when the Pressure of the Final System is P=1atm.

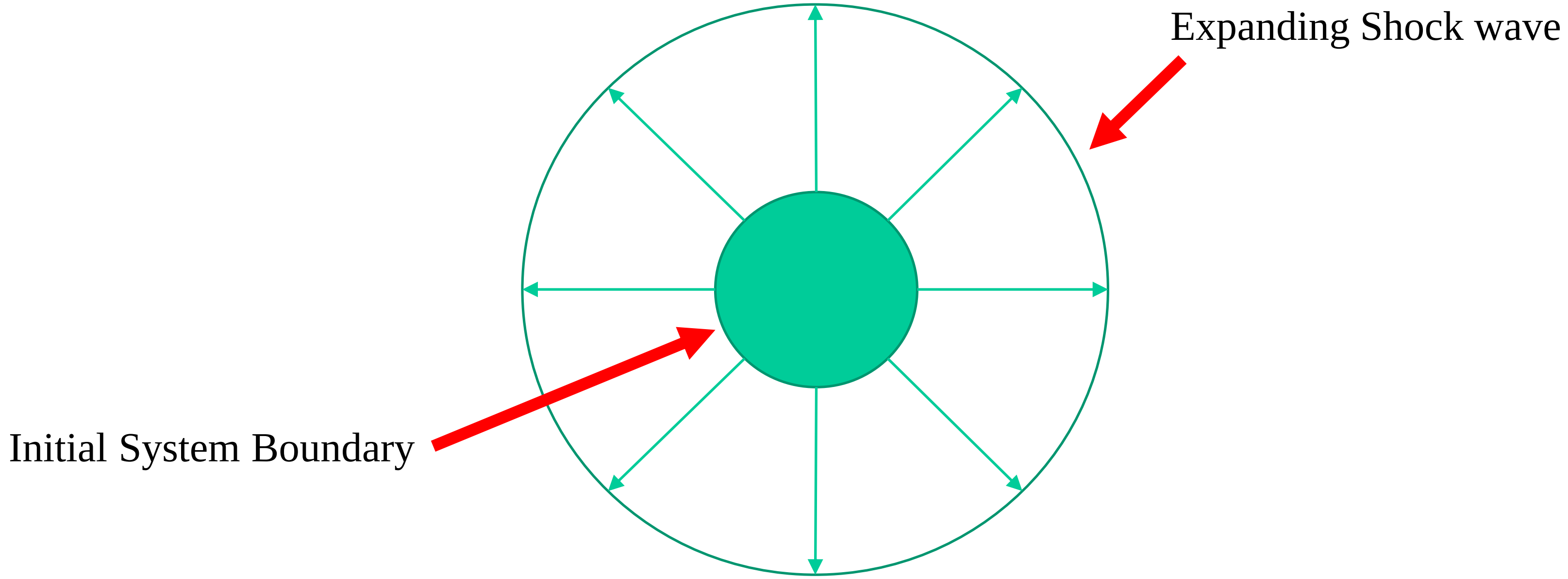


EXPLOSION

The limit for the expansion velocity is the speed of sound, achieved only when the initial pressure at detonation is sufficiently high.



EXPLOSION THERMODYNAMICS



EXPLOSION

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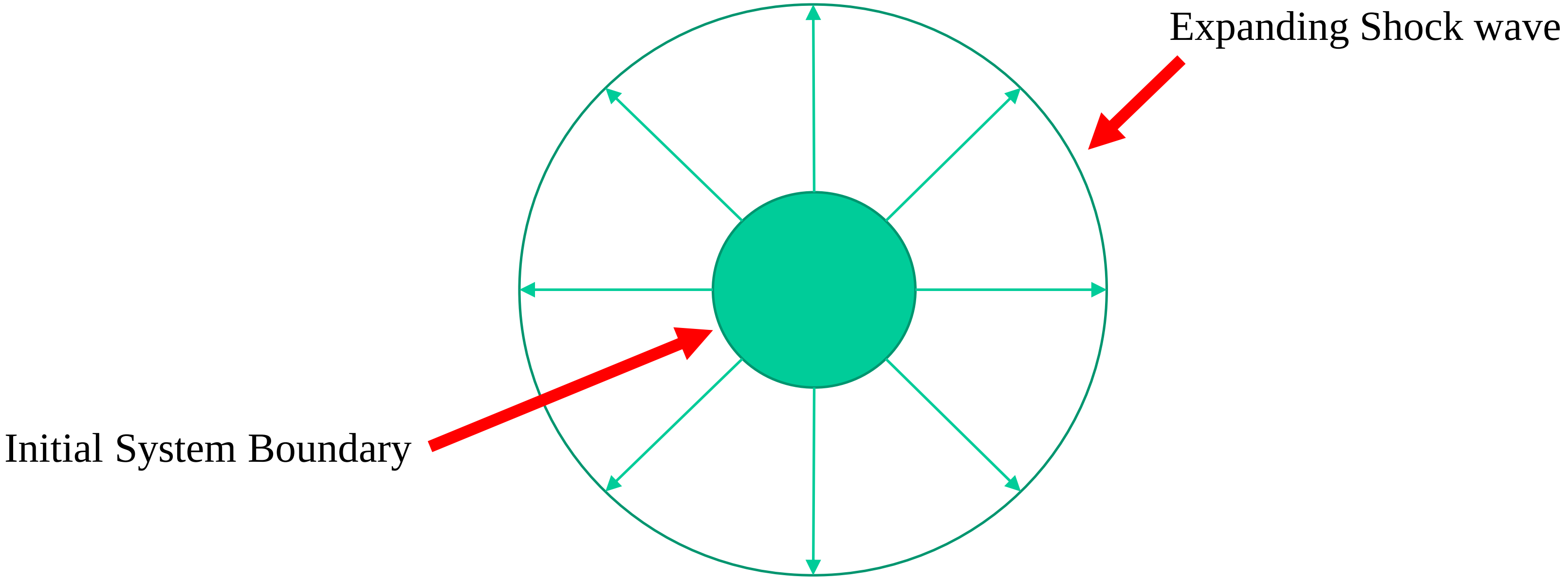


EXPLOSION THERMODYNAMICS

First Law

Energy added/subtracted associated to mass entering /leaving the system

Heat added

$$\frac{d}{dt}\left\{U + M\left(\frac{v^2}{2} + \psi\right)\right\} = \sum_{k=1}^{K} \dot{M}_k \left(\hat{U} + \frac{v^2}{2} + \psi\right)_k + \dot{Q} + \dot{W}_s - P\frac{dV}{dt} + \sum_{k=1}^{K} \dot{M}_k (P\hat{V})_k$$

Rate of change of Total Energy (Internal + External) of the system.

Shaft work

Expansion Work

Work done by fluid entering/leaving the system

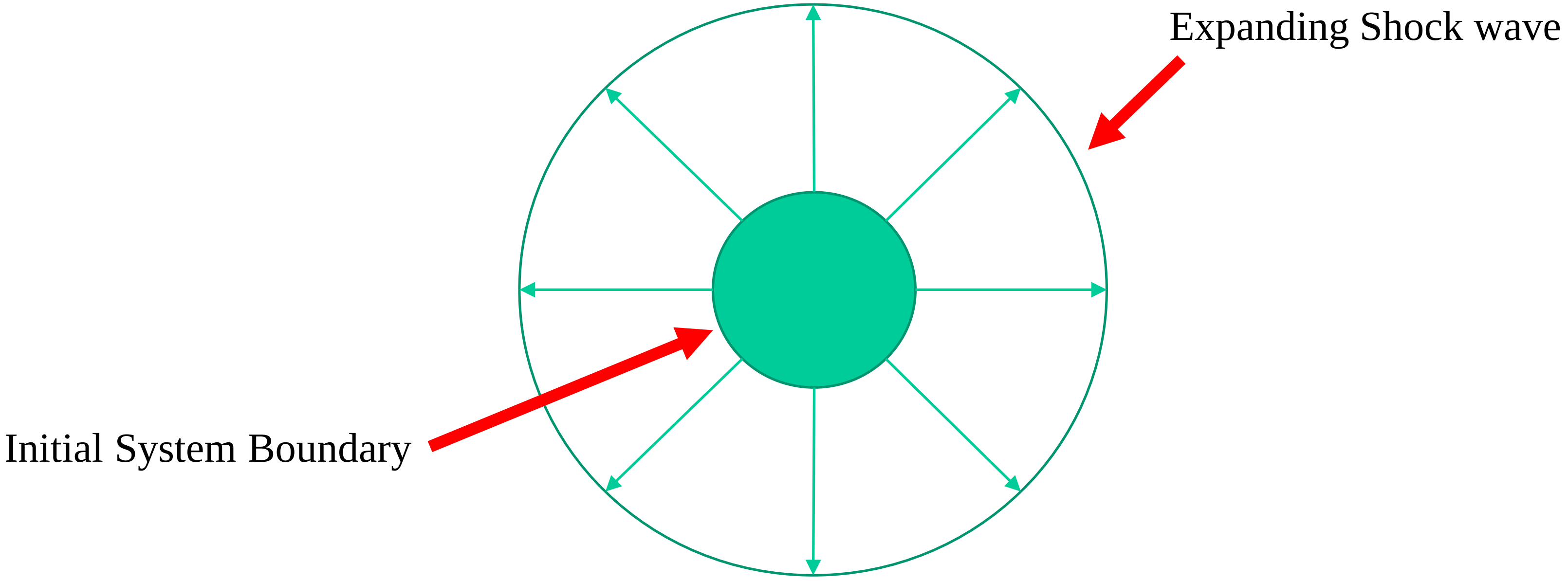
EXPLOSION THERMODYNAMICS

Second Law

$$\boxed{\frac{dS}{dt} = \sum_{k=1}^{K} \dot{M}_k \hat{S}_k + \frac{\dot{Q}}{T} + \dot{S}_{\text{gen}}}$$

EXPLOSION THERMODYNAMICS

Closed System: $M_{final}=M_{initial}$



EXPLOSION THERMODYNAMICS

First Law

$$\frac{dU}{dt} + M\frac{d}{dt}\left(\frac{v^2}{2} + \psi\right) = \dot{Q} + \dot{W} \quad = \dot{Q} - P\frac{dV}{dt}$$

Second Law

$$\frac{dS}{dt} = \frac{\dot{Q}}{T} + \dot{S}_{gen}$$

However, the system is adiabatic!!! ➔ Q=0

EXPLOSION THERMODYNAMICS

Closed and Adiabatic system

First Law

$$\frac{dU}{dt} + M\frac{d}{dt}\left(\frac{v^2}{2} + \psi\right) = -P\frac{dV}{dt}$$

Second Law $$\frac{dS}{dt} = \dot{S}_{gen}$$

Explosion is uniform, so the only entropy generation takes place at the boundary, **which can be neglected**!!!

EXPLOSION THERMODYNAMICS

Closed and Adiabatic system

First Law

$$\frac{dU}{dt} + M\frac{d}{dt}\left(\frac{v^2}{2} + \psi\right) = -P\frac{dV}{dt}$$

Second Law $$\frac{dS}{dt} = 0$$

The speed of the system as well as its potential energy does not change, **Then**

$$\frac{d}{dt}\left\{M\left(\frac{v^2}{2} + \psi\right)\right\} = 0$$

EXPLOSION THERMODYNAMICS

Closed and Adiabatic system

First Law

$$\frac{dU}{dt} = -P\frac{dV}{dt}$$

Second Law

$$\frac{dS}{dt} = \mathbf{0}$$

We now integrate from t_i=0 to t_f

EXPLOSION THERMODYNAMICS

Closed and Adiabatic system

First Law

$$\frac{dU}{dt} = -P\frac{dV}{dt}$$

$$\Rightarrow M\left[\hat{U}(P_f,T_f) - \hat{U}(P_i,T_i)\right] = W = -\int_{t=0}^{t_f} PdV$$

Second Law

$$\frac{dS}{dt} = 0$$

$$\Rightarrow \quad \hat{S}(P_f,T_f) - \hat{S}(P_i,T_i) = 0$$

SUMMARIZING

First Law

$$M\left[\hat{U}(P_f = P_{atm}, T_f) - \hat{U}(P_i, T_i)\right] = W$$

Second Law

$$\hat{S}(P_f = P_{atm}, T_f) - \hat{S}(P_i, T_i) = 0$$

EXPLOSION THERMODYNAMICS

OBJECTIVE: OBTAIN W!!!

This means that one has to compute

$$W = M\left[\hat{U}(P_f = P_{atm}, T_f) - \hat{U}(P_i, T_i)\right] =$$

$$= N\left[\underline{U}(P_f = P_{atm}, T_f) - \underline{U}(P_i, T_i)\right]$$

If the initial pressure and temperature is know, we can compute $\hat{U}(P_i, T_i)$. Now to compute $\hat{U}(P_f = P_{atm}, T_f)$, one needs the second Law

$$\hat{S}(P_f = P_{atm}, T_f) - \hat{S}(P_i, T_i) = 0$$

TANK EXPLOSION- No reaction

A 0.1 m^3 tank contains steam at 600 ^oC and 1 MPA and it bursts. OBTAIN W!!!

We need $\hat{U}(P_i,T_i)$ and M. At 1 Mpa and 600 ^oC (steam table) $\hat{V}(P_i,T_i)$=0.4011 m^3/kg. Then M= 0.1 m^3/0.4011 m^3/kg=0.249 kg. Also $\hat{U}(P_i,T_i)$ = 3296.8 kJ/kg.

Now we use $\hat{S}(P_f=P_{atm},T_f)=\hat{S}(P_i,T_i)$. $\hat{S}(P_i,T_i)$ =8.029 kJ/(kg K). Now using this entropy value at P=1 atm, to find T_f =248 ^oC $\hat{U}(P_f=P_{atm},T_f)$ = 2731 kJ/kg

$$W=M\left[\hat{U}(P_f=P_{atm},T_f)-\hat{U}(P_i,T_i)\right]$$ = -141 kJ

(31 g of TNT)

TANK EXPLOSION- No reaction

OBJECTIVE: OBTAIN W!!! Gases

To use $\hat{S}(P_f = P_{atm}, T_f) - \hat{S}(P_i, T_i) = 0$ we recall that for ideal gases

$$\hat{S}(P_f = P_{atm}, T_f) - \hat{S}(P_i, T_i) = Cp^* \ln\left(\frac{T_f}{T_i}\right) - R\ln\left(\frac{P_f = P_{atm}}{P_i}\right)$$

Then T_f can be obtained using P_f=1 atm making the equality zero. Thus

$$T_f = T_i \left(\frac{P_f = P_{atm}}{P_i}\right)^{R/Cp^*}$$

Then

$$W = N\left[\underline{U}(P_f = P_{atm}, T_f) - \underline{U}(P_i, T_i)\right] = NCv^*(T_f - T_i)$$

Where $N = \dfrac{P_i V_S}{RT_i}$.

TANK EXPLOSION- No reaction

OBJECTIVE: OBTAIN W!!! Gases

Then $W = N\left[\underline{U}(P_f = P_{atm}, T_f) - \underline{U}(P_i, T_i)\right] = NCv^*(T_f - T_i)$

$$W = N\left[\underline{U}(P_f = P_{atm}, T_f) - \underline{U}(P_i, T_i)\right] = \frac{P_i V_S}{R T_i} Cv^* \left[T_i \left(\frac{P_f = P_{atm}}{P_i} \right)^{R/Cp^*} - T_i \right]$$

$$W = \frac{P_i V_S}{R} Cv^* \left[\left(\frac{P_f = P_{atm}}{P_i} \right)^{R/Cp^*} - 1 \right]$$

TANK EXPLOSION- No reaction

A compressed air tank (V_S= 0.167 m^3) at 25 °C and 250 bar (high!!) explodes. OBTAIN W!!!

Data Cp of air is 29.3 J/(mol K). For ideal gases Cp-Cv=R

$$W = \frac{P_i V_S}{R} Cv^* \left[\left(\frac{P_f = P_{atm}}{P_i} \right)^{R/Cp^*} - 1 \right]$$ =8,853 kJ

This is equivalent to ~2 kg of TNT. Energy of TNT=4600 kJ/kg

This is a sizable explosion!!!
It could destroy everything within 4 m, produce substantial structural damage within 7 m, minor damage within 35 m, breaking glasses within 80 m and ear drum rupture within 5 m. These numbers are approximate, of course,

TANK EXPLOSION- No reaction

If the tank (15 kg) is accelerated with that energy, at 45 degrees, how far would it go?

We assume all the energy goes to the tank and no friction.

$E=m\,v^2/2 \rightarrow v_0=sqrt(2E/m)=$

$=sqrt(2*\ 8{,}853{,}000\ J/15)=1{,}086\ m/s$ (sound=343m/s; expect sonic boom!)

$v_x=v_0\cos(45)$, $v_y= v_0\sin(45) - gt$; $d= v_x 2t_{max}$

$v_0\sin(45) - gt_{max=0} \rightarrow d=\sin(45)\cos(45)\,v_0^2/g$ $\quad$ d= 120 km!!!!

TANK EXPLOSION- No reaction

If the tank (15 kg) is accelerated with that energy, at 45 degrees, how far would it go?

We assume all the energy goes to the tank and we consider friction.

v_0=1086 m/s; Drag force is f= $C_D \rho A v^2/2$

Force = $\vec{f} + \vec{g} = m\,\vec{a}$; $a_x = -k\,v^2 \cos(\theta)/m$ $a_y = -(k\,v^2 \sin(\theta)+g)$

Too complicated to solve analytically!!!

But we can solve a few meters and compare to the case without friction.

TANK EXPLOSION- No reaction

If the tank (15 kg) is accelerated with that energy, at 45 degrees, how far would it go? We assume all the energy goes to the tank and we consider friction.

v_0=1086 m/s; Drag force is $f=C_D \rho A v^2/2$ (C_D values are listed in https://en.wikipedia.org/wiki/Drag_coefficient). We use 0.3.

Force = $\vec{f} + \vec{g} = m\vec{a}$;

$a_x = -C_D A v^2 \cos(\theta)/m$

$a_y = -(C_D A v^2 \sin(\theta) + g)$

$$\frac{dv_x}{dt} = -k(v_x^2 + v_x^2)\cos(\theta)$$

$$\frac{dv_y}{dt} = -k(v_x^2 + v_x^2)\sin(\theta) - g$$

$$\frac{dx}{dt} = v_x$$

$$\frac{dy}{dt} = v_y$$

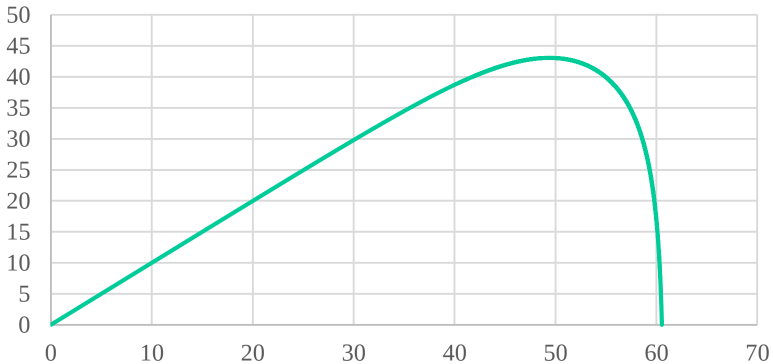
$$\tan(\theta) = \frac{v_y}{v_x}$$

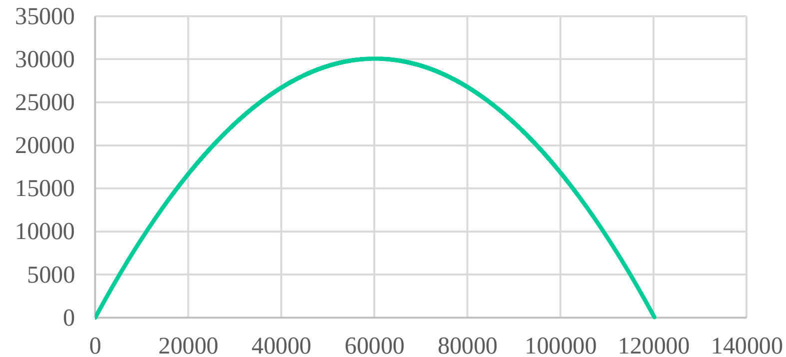
This can be solved numerically

TANK EXPLOSION- No reaction

If the tank (15 kg) is accelerated with that energy, at 45 degrees, how far would it go? We assume all the energy goes to the tank and we consider friction.

v_0=1086 m/s;   Drag force is $f=C_D \rho A v^2/2$





60 meters instead of 120 Km. !!!!!!

TANK EXPLOSION- No reaction

If the tank (15 kg) is accelerated with that energy, at 45 degrees, how far would it go? We assume all the energy goes to the tank and we consider hitting a concrete wall first.

v_0=1086 m/s; Momentum conservation

$mv_0+M\cancel{v_M}= mv_0=(m+M)v_{sys.} \rightarrow v_{sys}= v_0 m/(m+M)$

But v_{sys}~0. Actually M is the mass of the wall and the earth attached to it.

Thus, the energy absorbed by the wall is 8,853 kJ. To calculate the damage we need mechanical engineers.

TANK EXPLOSION- reactions

The initial temperature and pressure are needed.

Assume propane in air. The reaction is:

$C_3H_8 + 5\ O_2 + 18.8\ N_2 \rightarrow 3\ CO_2 + 4H_2O + 18.8\ N_2$

Initially the # of moles is N_b=24.8 and the temperature and pressure are T_b P_b.
After the reaction: N_i=25.8, Thus

$$P_i = P_b\ N_i\ T_i/(N_b\ T_b)$$

TANK EXPLOSION- reactions

The initial temperature and pressure are needed.

C_3H_8+ 5 O_2+ 18.8 N_2 → 3 CO_2 +4H_2O+ 18.8 N_2

We now need the temperature after the explosion, but before the expansion starts.

First Law says: $\frac{dU}{dt} = 0$. Then $\hat{U}(P_b, T_b) = \hat{U}(P_i, T_i)$ and assuming ideal gases.

$$\sum\left(3C_{V,CO2} + 4C_{V,H2O} + 18.83C_{V,N2}\right)\left(T_i - T_{ref}\right) =$$

$$= \sum\left(C_{V,C3H8} + 5C_{V,O2} + 18.83C_{V,N2}\right)\left(T_b - T_{ref}\right)$$

TANK EXPLOSION- reactions

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$C_3H_8 + 5\ O_2 + 18.8\ N_2 \rightarrow 3\ CO_2 + 4H_2O + 18.8\ N_2$

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$$= \sum \left(C_{V,C3H8} + 5C_{V,O2} + 18.83C_{V,N2}\right)\left(T_b - T_{ref}\right)$$

and one can obtain T_i

What if there are solids or liquids or the ideal gas assumption cannot be made? Solids and Liquids:

$$\hat{U}(P_b,T_b) \approx \hat{H}(P_b,T) = \hat{H}(P_{ref},T_{ref}) + \int_{T_{ref}}^{T_b} C_p(T)dT$$

Non ideal gases: Need $\hat{U}(P_b,T_b)$ and $\hat{U}(P_b N_i T_i/(N_b T_b),T_i)$ need to be obtained using the equation of state.