# Quantitative minimalism in combustion – Diffusion and/or kinetics

### [Reflections from the past of some meaning to the future]

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# What do I want to say?

- What is Quantitative minimalism?
- Early thinking and consequences
- Simple approaches to distinguishing differing theories for the same phenomenon -
  Case studies from my <u>personal file</u>*

    - AP burn rate

    - Erosive burning

    - Flame propagation in packed
      bed of biomass and coal

* Appropriate because of association of PJP in all these significantly

# Quantitative Minimalism

Meaning from dictionary: (usually of an artistic style) – "**using simple elements with little embellishment**"



Milk drop coronet, 1957

Bullet through apple, 1964

**Harold Edgerton** (MIT, USA) made it his career to record the unseen; some of his most famous photographs include the above – the pioneer in microsecond photography used world over by artists!

The essential thought is to practice minimalism quantitatively in combustion to capture the essence, for finally, it is all that counts and beautifully too.

# Early thinking and consequences

- My Ph. D thesis was on ignition-extinction problems in stagnation point diffusion flames (1965 – 1969)

    **– single step chemistry – clarifying ideas of equilibrium – S-curve ($T_{max}$ vs $D_1$) related questions, surface reaction aspects – singular perturbation analysis**

- The only substance carried over in literature is the equation for energy balance that involves F and a of my work with z, the mixture fraction and $\chi$, the scalar dissipation rate

$$\frac{\mathrm{d}^2 T}{\mathrm{d}Z^2} = -\frac{2B\nu'_F \rho\,(T_{st} - T_u)}{\chi Y_{F,1} Z_{st} W_{O_2}} Y_F Y_{O_2} \exp\left(-\frac{E}{RT}\right)$$

  used in turbulent flow calculations using flame-let approach.

- This was not anticipated by me at that time. It took almost a decade before these ideas became relevant.

- I was dissatisfied with my thesis on account of inadequacy of reality check.  This had serious impact on what to do in the next several years. These focused on full chemistry related aspects.

# ...So

- Detailed chemistry is inescapable for premixed flames.
- Hence a code development for one-d premixed flame propagation with full chemistry was produced (1979+).
- This became a far more robust tool than the Sandia code which was and is prevalent even now.
- PJP converted the chemistry segment from explicit to implicit scheme and made it far more robust than it was.
- Several students

   A. T. Bhashyam (code development and experimental comparison)
   K. N. Lakshmisha (flammability limit fundamental and actual aspects)
   G. Goyal (model calculations with $H_2$-NO system)
   D. P. Mishra (Stretch effects – single step and full chemistry)
   G. Sridhar (R/C engine simulation with $CO$-$H_2$-$CH_4$-$H_2O$-$N_2$ mixture)
   used this code effectively till 2002.

- Some fundamental aspects of flammability were decisively resolved in the studies by Lakshmisha

# Quantitative Minimalism (QM) in combustion

Confessions of past excesses and later corrections without any punishment…!

# QM in Combustion - 1

- AP combustion -

- Based on the observed pressure index that varied between 0.8 to 0.75 or so with increasing pressure, a number much lower than 1, it was "inferred" that one step in the chemistry (may not be rate limiting, but very important) must be of effective order 1 and the rest 2. This was the basis of a complex g-phase chemistry calculation based approach.

- This complex chemistry calculation was the basis of the thesis of H. K. Narahari and a symposium paper in 1984.

- The net effect of this may have looked "substantial" but of little significance in the long term!  Why do I say that?

# QM in Combustion - 2

- In 2000, P. A. Ramakrishna worked on the modeling of AP-sandwich that needed modeling of AP.

- A single step reaction in the gas phase with more detail on physics and chemistry at the "surface" (heat of reaction like in BDP and a pyrolysis law) were the ingredients.

- His "shocking" find was that the activation energy for pyrolysis was to be much lower than classical (used by all – Beckstead, Forman Williams, and others) because the calculations went unstable at larger activation energies – the question by one reviewer was " how could a lone set of researchers go against so many others?" – tough call, it was.

- This paper was published in JPP later; There was an earlier "encounter" with the distinguished small community propellant researchers at the 2002 symposium.

# QM in Combustion - 3

- A simple heat balance over the solid AP surface leads to

$$[\rho_p \, \dot{r} \, c_p \, / \, k]^2 = p^n \, k_r \, B_{AP} \, , \qquad \bar{B}_{AP} \;=\; \frac{c_{pg}(T_{f,AP} - T_{ss,AP})}{c_{pg}(T_{ss,AP} - T_0) - H_{AP}}$$

- This result is nearly same as the expression for the burning velocity for a premixed gas mixture – very simply obtained.

- The simple inference was that even with $n = 2$, one can get right variation of index because $T_{ss,AP}$ increases with pressure due to pyrolysis law, $\dot{r} = A_r \, exp \, (E_s/RT_{ss, AP})$

- The activation energy of pyrolysis, $E_s$ and an effective single step reaction are the takeaways from this work used even today – by Varun Shivakumar in modeling solid propellants for stable and unstable combustion…. This is quantitative mimimalism

# QM in Combustion - 4

Erosive burning in solid propellants – what is it? -
The burn rate sensitivity to lateral mass flux (apart from known p, initial T dependences)



Cylindrical portion of grain

Fin portion of grain.
Fin length = 550mm + taper

Nozzle
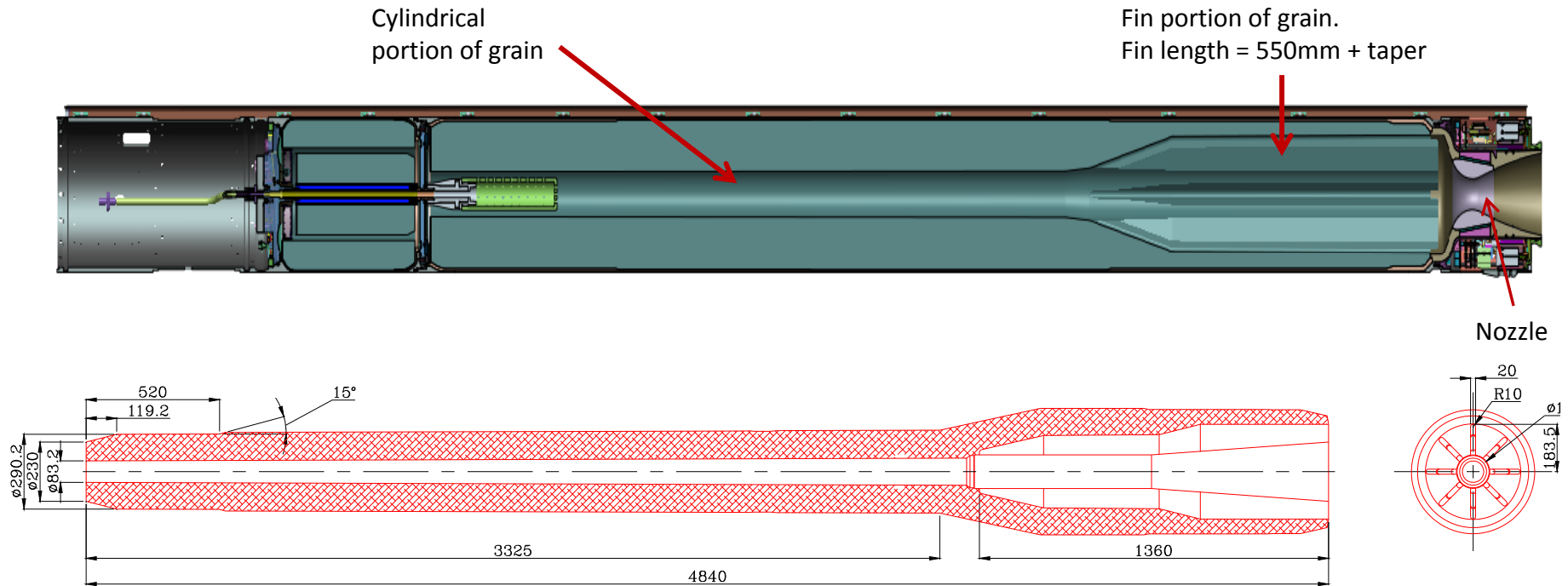
**Publications in**
**1978 (hsm),   1997 (hsm+pjp), 2014 (hsm,pjp, Javed, Debasis Chakraborty)**

# QM in Combustion - 5

- In 1978 paper, I had argued that beyond fluid flow effects, there was a role of kinetics on erosive burning.

- In a paper written two decades later, I and my colleague Paul argued for the universality of erosive burning behavior. The earlier work almost went close to the final one, but fell short of it conceptually.

- Two papers both accepted and published with differing view points! ...strange...why so?

- The 2014 paper is extension to complex geometries motivated by "user" related issues brought out (by DRDL)

# Later insights different…why?

- Large number of data were published only later than 1978 including a review paper by Kenneth Kuo.

- This appeared quite insipid as a large number of correlating parameters were chosen, plotted against each other creating more confusion than clarity.

- A review of all the work cited by him and some at a later time allowed the possibility of thinking along the lines of choosing dimensionless correlations – something "trivial" on hind-sight.

- Message: When you are in a frontier area, you might work with one kind of ideas one day that you yourself need to change later – if so, better done openly for one's own good.

Ishihara and Kubota [14]

| | | $\rho$ | $T_f$, K |
|---|---|---|---|
| High energy | 55.6NC + 40.4NG + 4.0DEP | 1600 | 2716 |
| Reference | 50.4NC + 36.6NG + 13.0DEP | 1600 | 2114 |
| Low energy | 47.5NC + 34.5NG + 18.0DEP | 1600 | 1778 |

High Energy
Reference
Low Energy

u (m/s)

$\eta$ as $r/r_0$ and $g_0 = G/\rho_p r_0$

G    mass flux through the port (kg/m² s)

High Energy
Reference
Low Energy

g
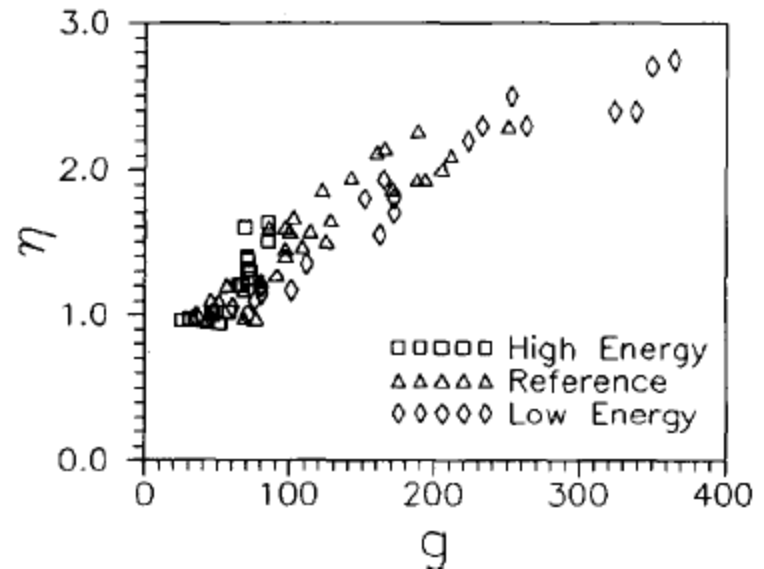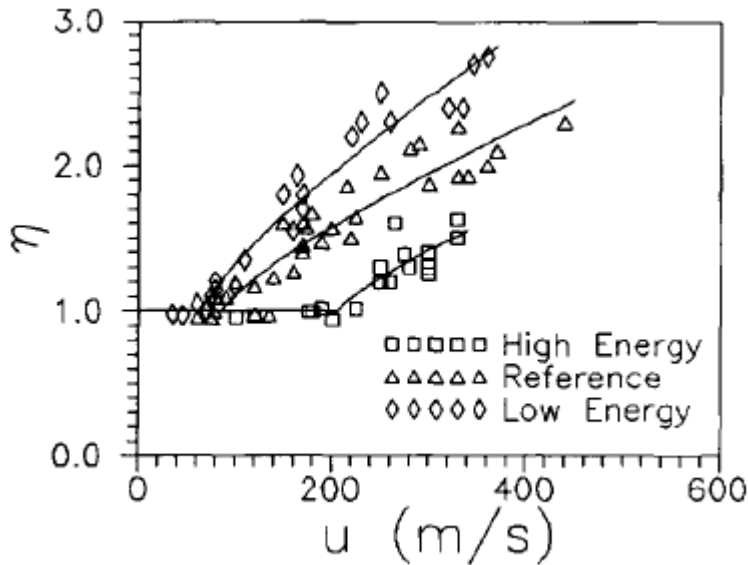
$Re_0$    Reynolds number based on propellant burn rate ($\rho_p r_0 d_0/\mu$)

$g_0$    ratio of port mass flux to nonerosive propellant mass burn rate ($G/\rho_p r_0$)

$g$    $g_0(Re_0/1000)^{-0.125}$

The idea is to pick the right dimensionless parameter responsible for erosive burning. Note that chemistry related parameters are absent in and the crucial role of mixing is turbulent, of course

Marklund and Lake [15]

| | | $\rho$ | $T_f$, K |
|---|---|---|---|
| Prop A | 65AP (24–30 $\mu$m) + 35polyester | 1620 | 1690 |
| Prop C | 75AP (24–30 $\mu$m) + 25polysulfide | 1700 | 2550 |
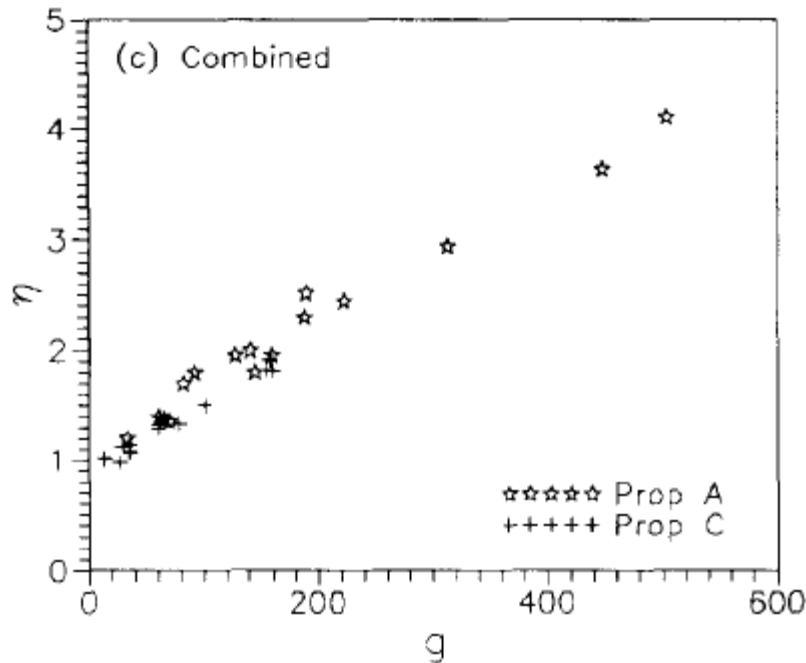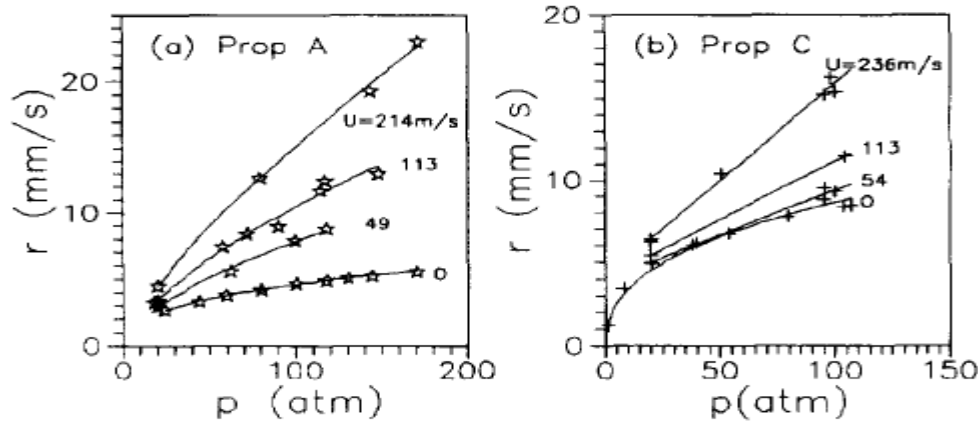
What you see are data on Composite propellants. It appears that as far as erosive burning is concerned, particle size does not matter, because the collapse on to the data on the transformed coordinate is impeccable…

Not unreasonable to expect fluid flow effects to be similar for AP particles and binder combustion process.

Could this not have been discovered in 1978?

Confession: I simply did not sharpen my thinking at that time!  This led to "excesses"

- These are essentially for cylindrical grains.

- It was doing not-too-well for partly symmetric grains like fin-o-cyl type.

$$\eta = 1 + 0.023(g^{0.8} - g_{th}^{0.8})\mathcal{H}(g - g_{th}), \quad (12)$$

where $g = g_0(\text{Re}_0/1000)^{-0.125}$ and $g_{th} = 35.0$.
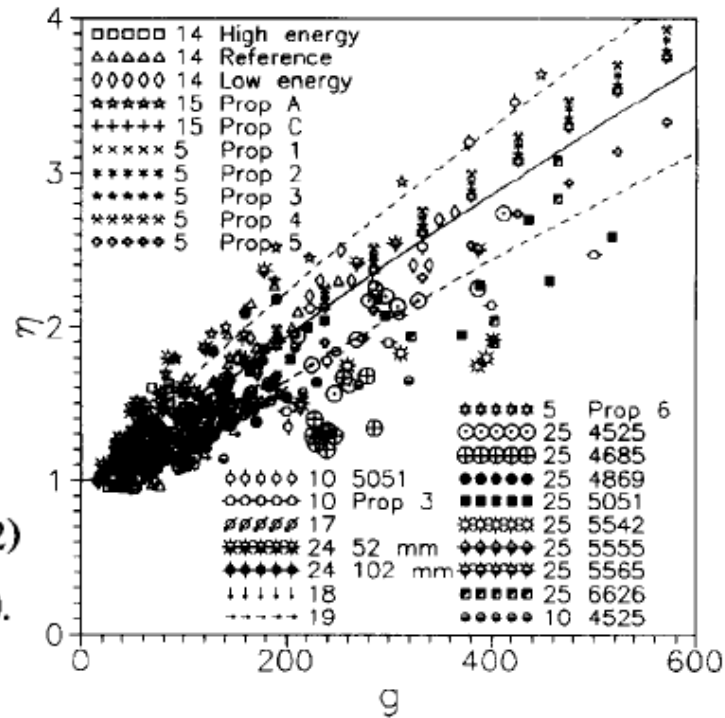


Fig. 9. Plot of $\eta$ vs $g$ for data of all authors for both double-base and composite propellants.

$\text{Re}_0$      Reynolds number based on propellant burn rate ($\rho_p r_0 d_0/\mu$)

- Work on 3-d simulation was performed using CFD by Debasis Chakraborty and Javed at DRDL.

- An analysis of these results showed that $d_0$ in $\text{Re}_0$ should be calculated using $d_0$ = Perimeter/$\pi$ instead of hydraulic diameter 4A/P

# Flame propagation in packed bed of biomass and coal

Technologies and the basis
- diffusion limited and reaction dominated segments
- conclusions from simple modeling

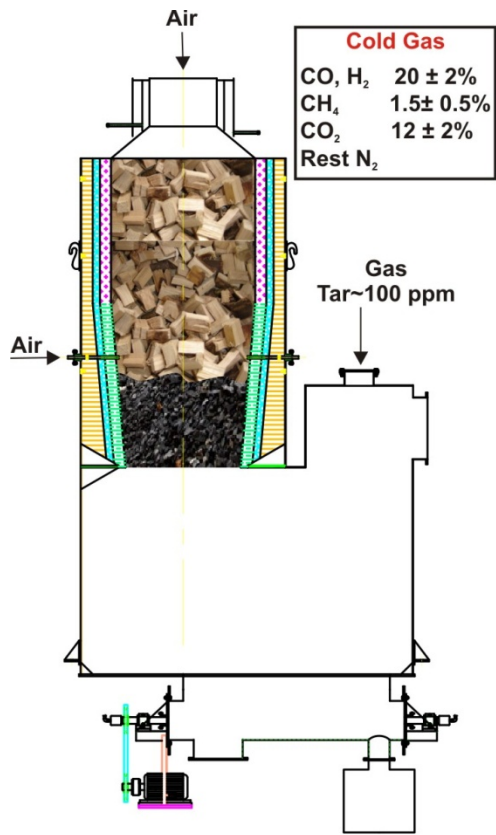1KgPH DINJAM PLANT


BMC GASIFIER PLANT(1700Kgph)

Cooking heat 0.8 kg/h

Electricity



Clean combustion of "producer gas"
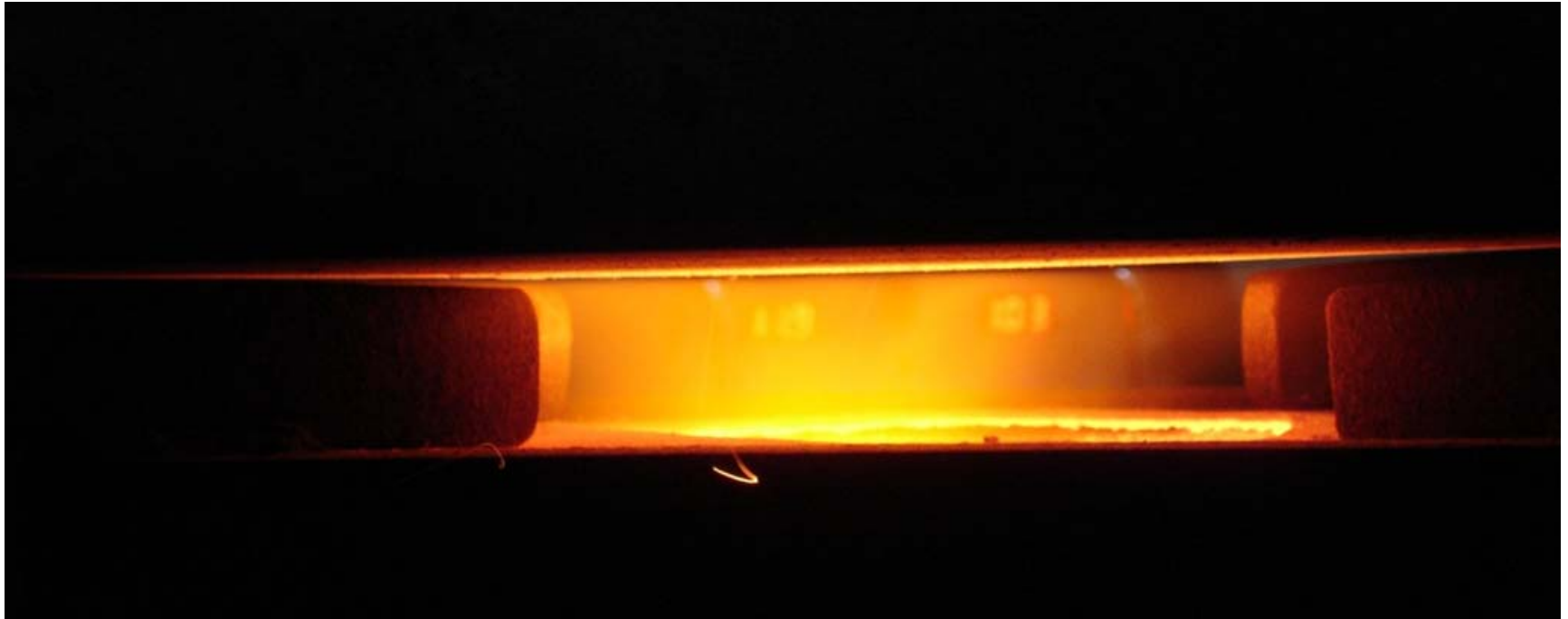
Clean combustion of biomass – 1250 °C
10 kg/h – 40 kWth system
Power for fan – 12 W

Cold Gas
CO, $H_2$    20 ± 2%
$CH_4$    1.5± 0.5%
$CO_2$    12 ± 2%
Rest $N_2$

Air

Gas
Tar~100 ppm

Air from top ~ 70%
Air from side ~ 30%
Char + Ash ~ 5%
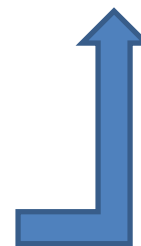Gas:Biomass ~ 2.7

**Gasifier operation for electricity generation**

Cold Gas
CO    14 - 17%
$H_2$    10 - 15%
$CH_4$    04 - 7%
$CO_2$    15 - 18%
Rest $N_2$

Air

Gas
Tar~3000 ppm
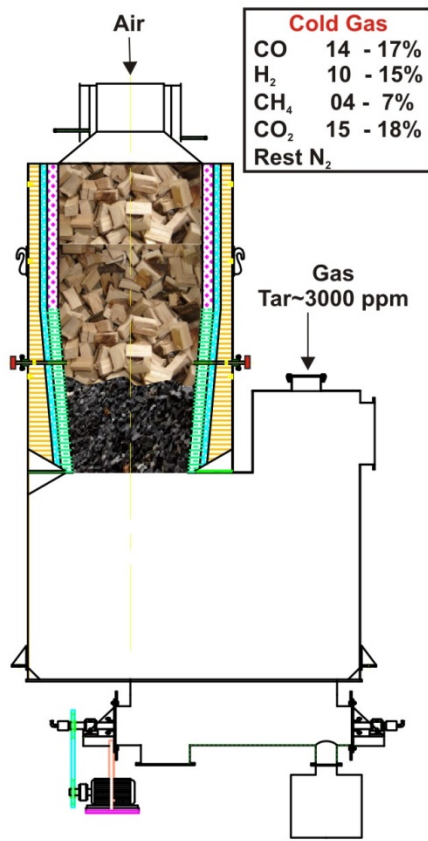
Air from top ~ 100%
Air from side ~ 0%
Char + Ash ~ 32%
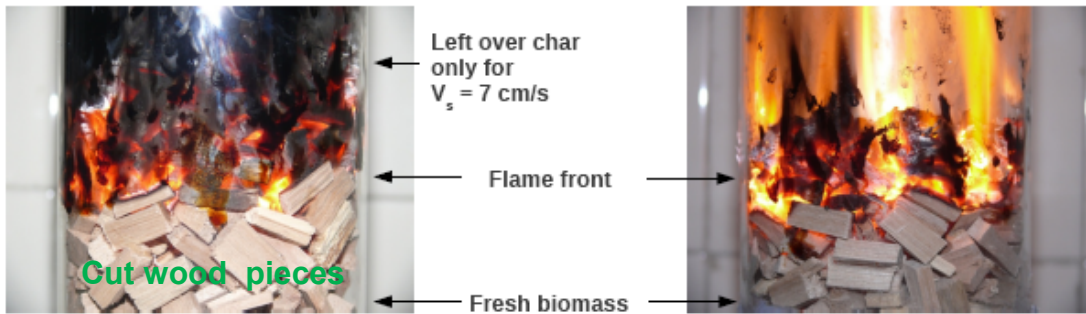Gas:Biomass ~ 2

**Gasifier operation for charcoal production**

Secondary Air
Fan
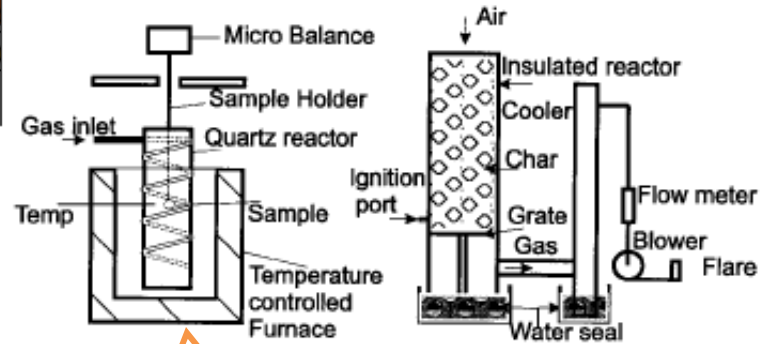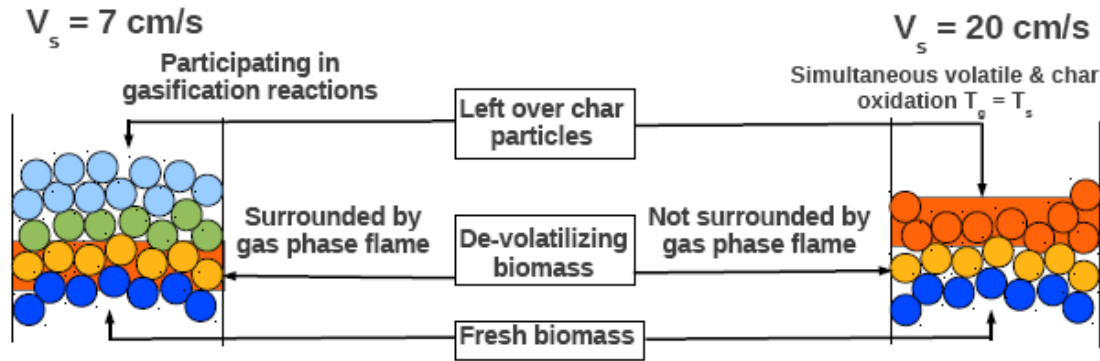Primary Air
Primary Control
Grate
Secondary Control
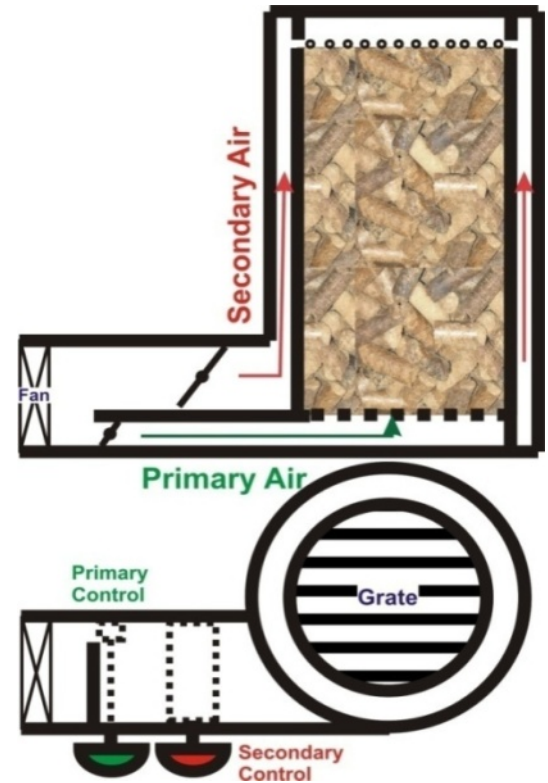
**Clean burning reverse-downdraft Gasifier stove (REDS)**

invert the gasifier

# Basic processes



- Dasappa and Varun have done studies on biomass idealized to spherical shape

- Wood combustion in air is diffusion limited  (like liquid droplets)
- Char combustion in air is also diffusion limited
- Both these are exothermic.
- The products of combustion – $H_2O$ and $CO_2$  react with char to produce $H_2$ and $CO$  - endothermic
- To study these reactions, one uses a temperature controlled furnace and a micro-balance

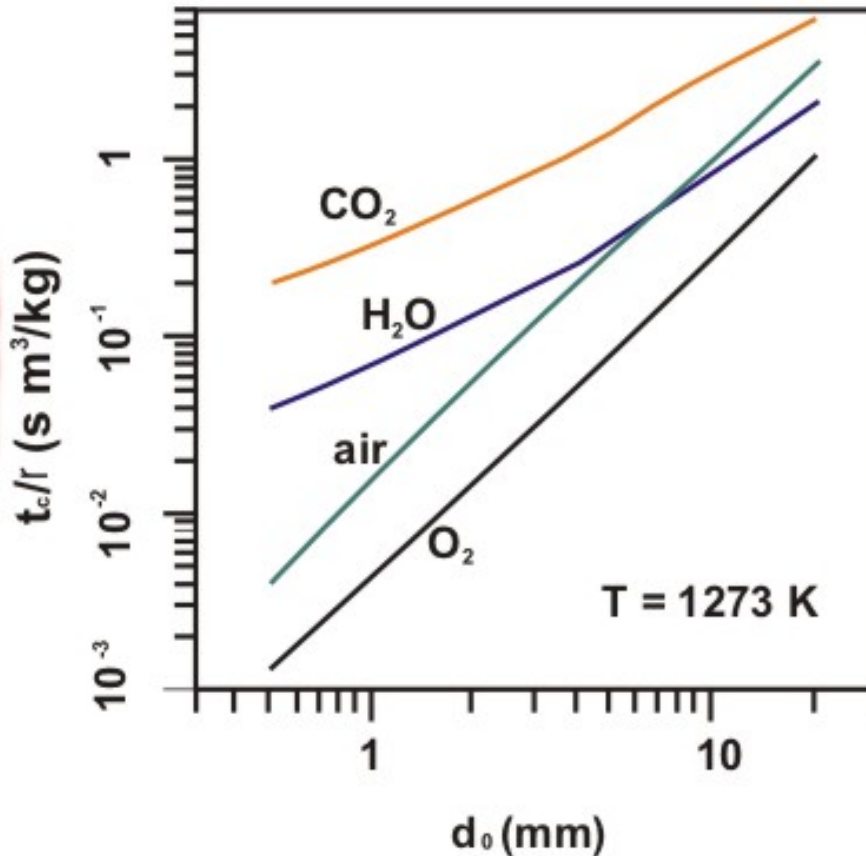# Combustion of alcohol, wood and char spheres in air and oxygen


Gas phase combustion


Gas phase combustion


Surface combustion


FLAMING ZONE
(A)

GLOWING ZONE
(B)
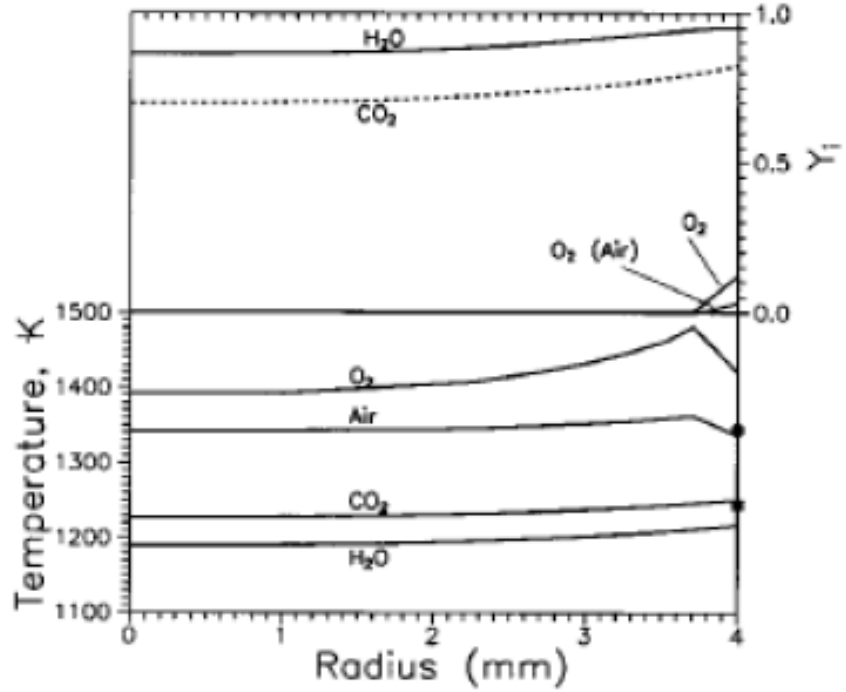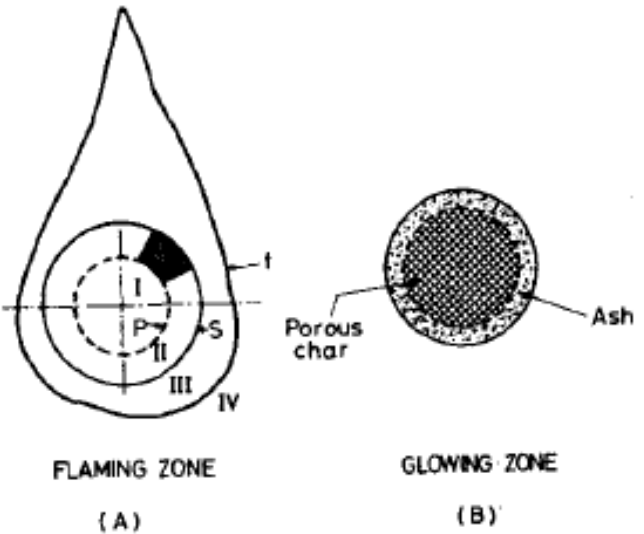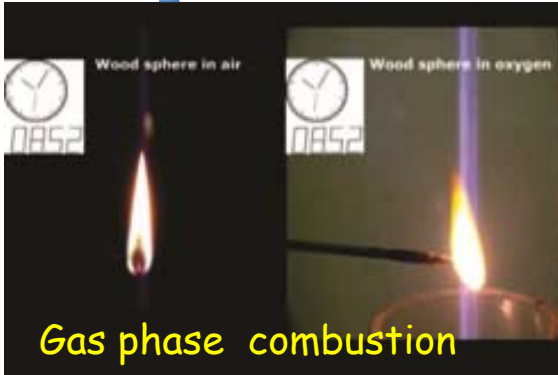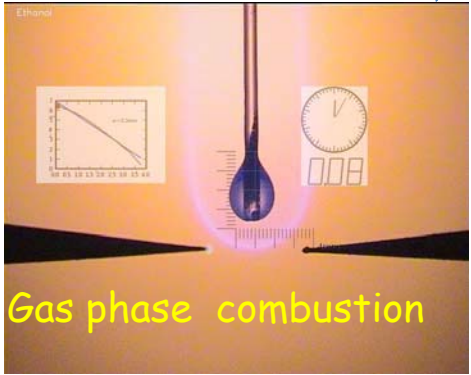
$$\frac{\dot{m} c_p}{4\pi k r_s} = \ln \eta_s$$

$$= \ln (1 + B)(1 + 0.17 \, Gr^{0.3} \, B^{-0.44})$$

# Comparison of Conversion time with diameter

Reactants : (a) $CO_2$ (b) $H_2O$ (c) air (d) $O_2$



| | | Kinetic and diffusion dependence |
|---|---|---|
| $t_b \sim d_0^{1.03}$ | $CO_2$ | Kinetic and diffusion dependence |
| $t_b \sim d_0^{1.2 -1.3}$ | $H_2O$ | Kinetic and diffusion dependence |
| $t_b \sim d_0^{1.9}$ | air | diffusion limited |
| $t_b \sim d_0^{2}$ | $O_2$ | diffusion limited |

**Conversion time for char reaction with**

1. $CO_2$ is 3-4 times that of $H_2O$

2. $H_2O$ is comparable to air at $d_p > 8$ mm

**Comment: There is so much of combustion physics in this, I wish char conversion is also taught in combustion courses; as far as I know only liquid drop combustion is taught.**

# Char conversion time vs ambient reactant mole fraction
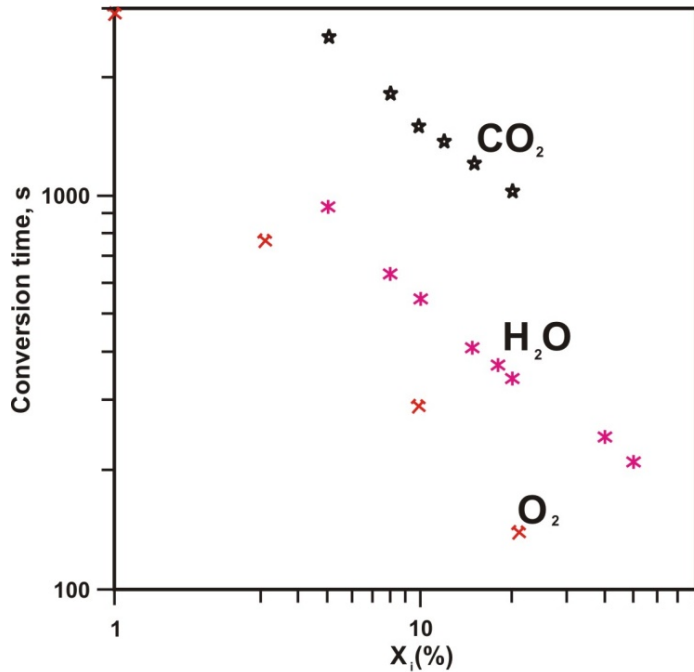
**Reactants :**

O₂, CO₂ and H₂O with N₂ as the dilutant

$$\left(\frac{t_c}{\rho}\right)_{CO_2} = a_0^{1.05} \exp\left[-1.715 + 35300\left(\frac{1}{T} - \frac{1}{1273}\right)\right] X_{CO_2}^{-0.65}$$

$$\left(\frac{t_c}{\rho}\right)_{H_2O} = a_0^{1/1050} \exp\left[-3.26 + 15470\left(\frac{1}{T} - \frac{1}{1273}\right)\right] X_{H_2O}^{-0.70}$$

$$\left(\frac{t_c}{\rho}\right)_{O_2} = 0.0022\, a_0^2\, X_{O_2}^{-1.0}$$

$X_i$ is the mole fraction of the reactant in the ambient

Validity : $d_0 > 4$ mm, T = 1000 to 1400 K

Accuracy $\pm 10\%$

# Experiments on packed bed – biomass and coal

- Experiments on packed bed have been made at several levels of detail by Dasappa on wood spheres and Varun Shivakumar on wood spheres and pellets. These are all with at initial temperatures of both pellets and air of 25 to 30 $^{o}C$.

- A new idea is being pursued to try high temperature operations essentially aimed at coal (both coal and air being at higher initial temperatures).

- Because of biogenic origin of coal, Seeking similarity between biomass and coal has many intrinsic values

- The idea is to improve the operation towards shorter conversion time – makes the operation more diffusion limited.

- Raise the temperature of operations to a little below the volatilization temperature ~ 180 to 200 $^{o}C$ for biomass or coal (20 % ash studied here). Steam injection is also allowed for, certainly in the case of coal.

| Item | Wood sphere | Wood Square | Coconut shell | Pellet cylinder | Pellet cylinder | Indian Coal Air | | | Indian Coal Air+steam | |
|---|---|---|---|---|---|---|---|---|---|---|
| $\rho_{biomass}$, kg/m³ | 615 | 615 | 850 | 1260 | 1260 | 1250 | | | 1250 | |
| Size, *mm* | 11.5 | 7 | 6-8 | 8 d,15 L | 8 d x 15 L | 3 - 8 | | | 3 - 8 | |
| Ash content, % | 1 | 1 | 1 | 1 | 9 | 21 | | | 21 | |
| Volatiles, % | 87 | 87 | 85 | 87 | 81 | 27 | | | 27 | |
| Sup. Vel, cm/s | | 19 | 19 | 20 | 20 | 5.7 | 19 | 28 | 44 | 68 |
| Air (mix) T (°C) | 28 | 175 | 155 | 28 | 28 | 145 | 150 | 155 | 170 | 170 |
| Fuel flux, kg/m²h | 120 | 435 | 470 | 120 | 100 | 126 | 728 | 960 | 799 | 604 |
| $\rho_{char}$, kg/m³ | 185 | 342 | 327 | 406 | 406 | 800 | 736 | 729 | 777 | 711 |
| $X_{H2O}$ | - | - | - | - | - | - | - | - | 0.29 | 0.31 |
| Char size, *mm* | 10 | 5 | 5 | 7 d,14L | 7 d x 14 L | 2 - 7 | 3-8 | 3-8 | 3-8 | 3-8 |



**Superficial velocity has a substantial effect.**

**Fuel flux – loading possible in the case of coal
Is limited by ash fusion.**

**Loose agglomerates**

Coal – $V_{sup}$ = 19 cm/s, $X_{H2O}$ = 0, Tgas = 150 C

**Loose agglomerates**

**Hard agglomerates**

Coal – $V_{sup}$ = 44 cm/s, $X_{H2O}$ = 0.29, Tgas = 170 C

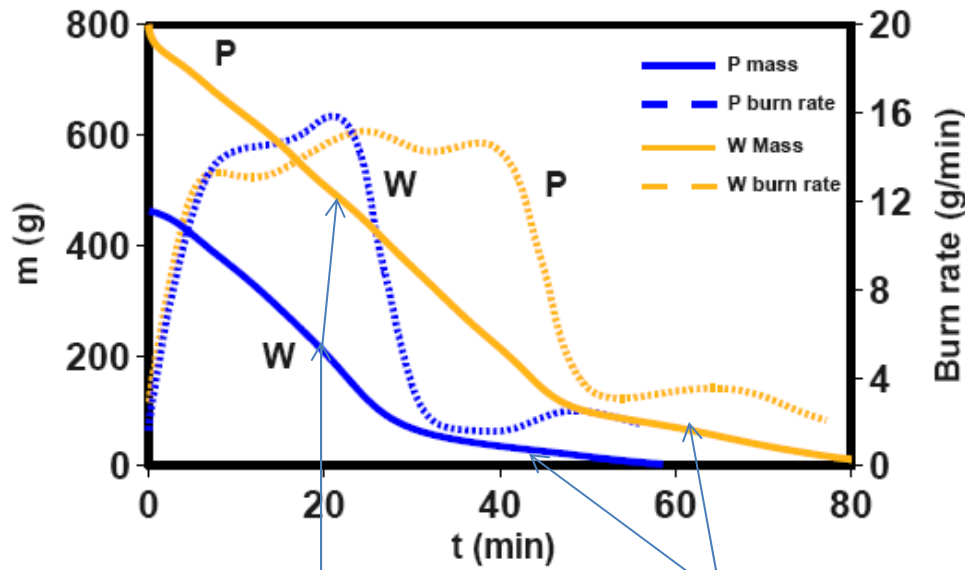$V_{sup}$ = 68 cm/s, $X_{H2O}$ = 0.31, Tgas = 170 C

# Experiments on coal packed bed

- A simple set up – a cylindrical container filled with wood chips or pellets or coal pieces (3 to 7 mm size)

- The carbon conversion is just complete – no ash fusion as well control of final temperatures calls for steam injection
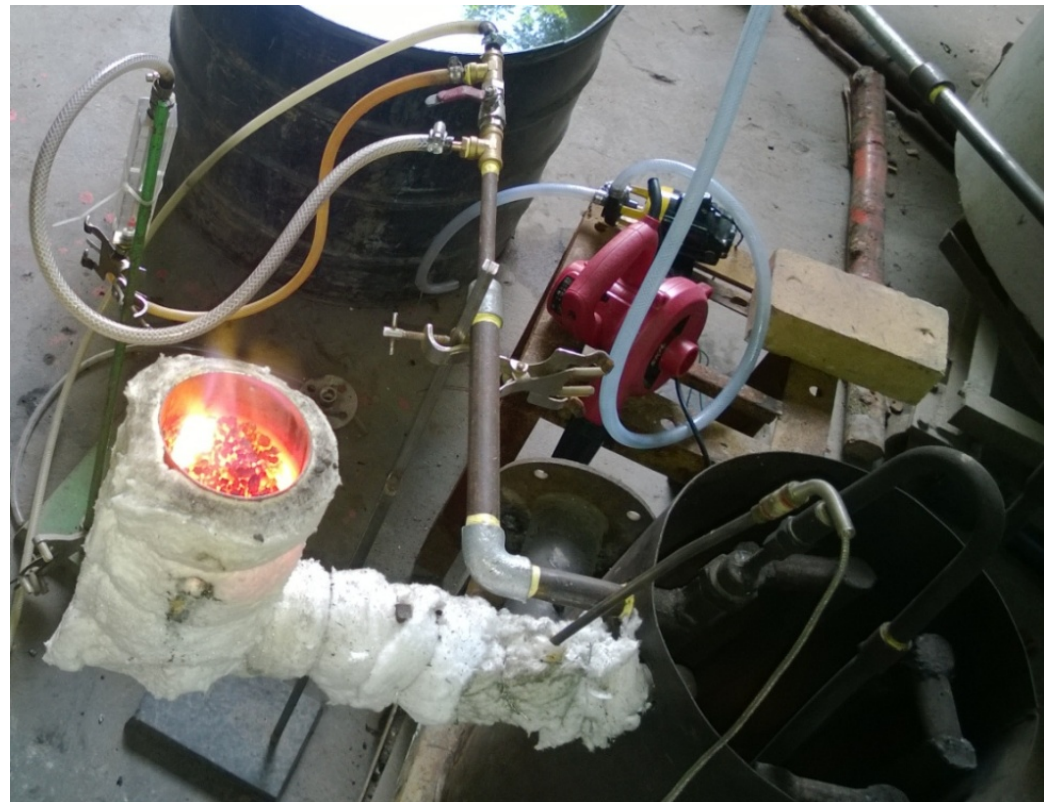
# The conversion behavior

wood/pellets@ambient conditions



Figure 4.2: Mass with time and burn rate for wood (W) and pellets (P) for 20 g/min air gasification air flow rate in flaming and char mode

Wood      Pellets

2.0 g/min      3.7 g/min

Char activity lower for wood than for pellets
only in a packed bed

Two segments:
Volatile rich combustion-gasification    (12.5 g/min)       Char gasification-combustion

$\rho_p$ = 650 kg/m³

Wood (W) $\rho_p$ = 550 kg/m³
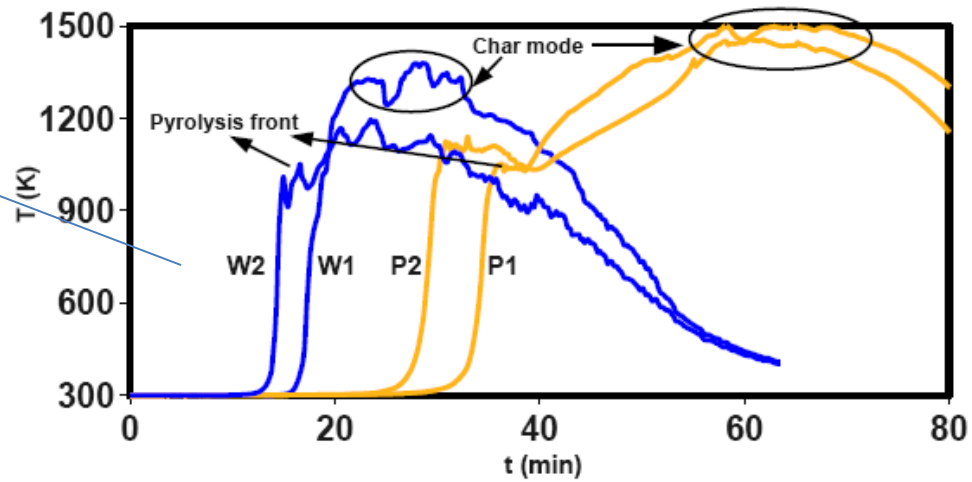
Pellets (P) $\rho_p$ = 1260 kg/m³

Sup vel: 5.7 cm/s



Figure 4.3: Bed temperature profiles at 20 g/min gasification air flow. Thermocouples W1, W2 and P1, P2 refer to wood and pellets positioned 10 mm and 30 mm above the grate
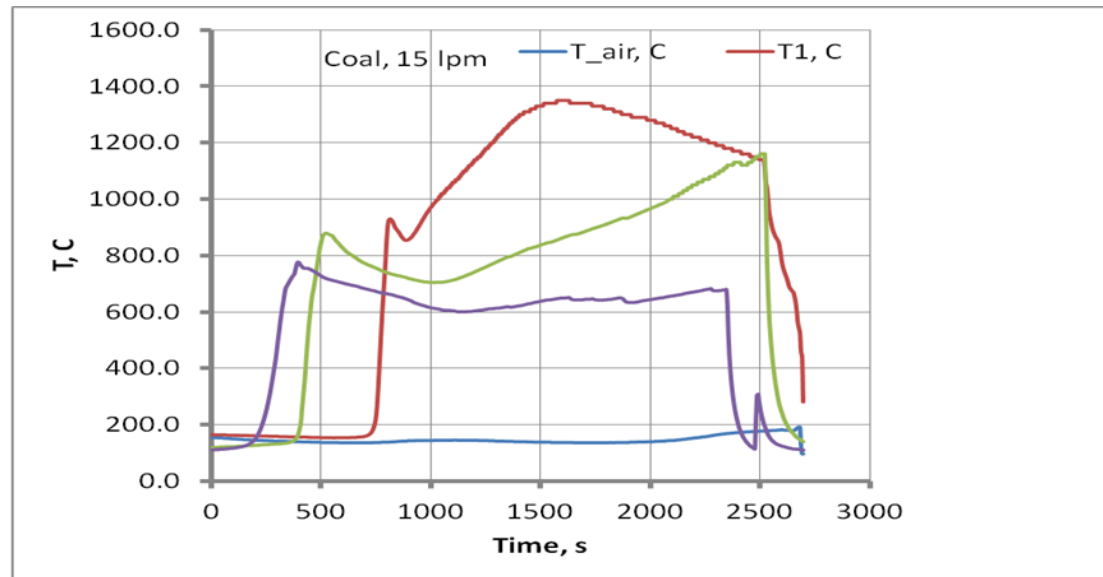
Coal –
$\rho_p$ = 1250 kg/m³

Ash = 21%

Sup vel: 5.7 cm/s

Fuel: 90 kg/m²h



In all cases, the ignition process is very fast. The time to reach peak temp is very high. Can we explain this?........

# Can we model the T vs. time - 1?

**For the ignition of the biomass the heat balance (also approximated) is**

$$mc_p \frac{dT_p}{dt} = A_s[f_{view}\epsilon\sigma(T_{pb}^4 - T_p^4)] - h(T_p - T_0)$$

$$\sim A_s[f_{view}\epsilon\sigma T_{pb}^3(T_{pb} - T_p)] - h(T_p - T_0)$$
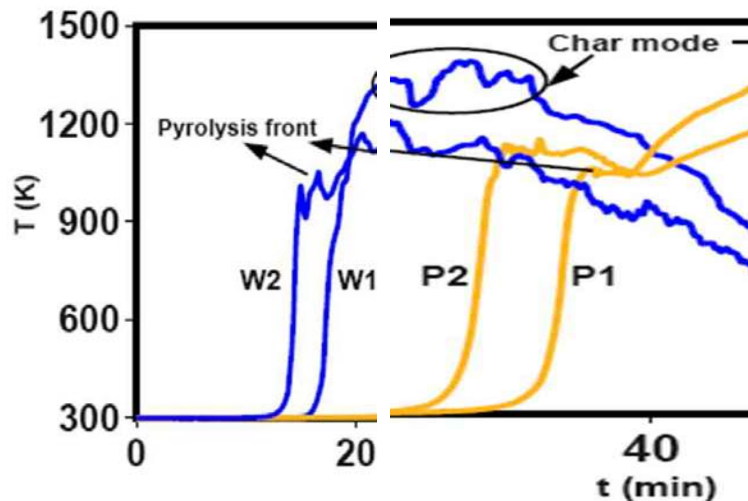
**The solution is obtained as with $T_p = T_0$ at $t = 0$**

$$T_p = (T_{pb} + A_0 T_0)/(1 + A_0) - (T_{pb} - T_0)e^{-(1+A_0)t'}$$

**The time for change from $T = T_0$ to $T_p = T_{p\ ign}$**

$$A_0 = h/(f_{view}\epsilon\sigma T_{pb}^3)$$

$$h = \frac{k_g}{d}(2 + \left[\frac{\rho_g V_s d}{\mu(1 + \phi)}\right]^{0.5})$$

$$t' = t(6f_{view}\epsilon\sigma T_{pb}^3)/(\rho_p c_p d)$$

$$t_{rise} = \frac{\rho_p c_p d}{6f_{view}\epsilon\sigma T_{pb}^3 + h} ln\left[\frac{T_{pb} - T_0}{T_{pb} - T_p - A_0(T_P - T_0)}\right]$$

# Can we model the T vs. time - 2?

For the conversion of hot char the heat balance (also approximated) is

$$mc_p \frac{dT_p}{dt} = A_s H(D\rho))_g Y_{O2}/\delta$$

$\delta$ is the gas phase mass transfer thickness including the ash layer effect.

This equation can be recast accounting for ash layer as

$$\frac{dT_p}{dt} = \frac{6H(D\rho)_g Y_{O2}}{\rho_p(d_0 - \dot{r}t)c_p(\delta_0 + \dot{r}t)}$$

The solution is obtained as
With $T_p = T_{p0}$ at $t = 0$

$$T_p = T_{p0} + \left[\frac{6H(D\rho)_g Y_{O2} t_b}{(1+A_1)\rho_p d_0^2 c_p}\right] ln \left[\frac{(A_1 + z)}{A_1(1 - z)}\right]$$

The time for change from
$T = T_0$ to $T_p = T_{p0}$

$$d_0 = \dot{r}t_b \qquad z = t/t_b \qquad A_1 = \delta_0/d_0$$

The solution for ignition has an exponential variation with time.
The solution for char conversion has a logarithmic dependence on time

This difference explains what is observed – much longer durations
for char conversion compared to ignition. Dependences on density
of fuel and diameter are captured.

# Summing up

- Quantitative minimalism refers to extracting the appropriate elements in a mathematical functional form to create (or help) understanding.

- It forces one to reduce "excesses" – opposite of "taking all things into account"

- Example: for one may compute in all detail – like DNS for instance – may reveal little of primal causes – unless of course, efforts are made to extract the behavior based on hypothesis. An example of very slow progress is understanding turbulent flows.

- Working towards quantitative minimalism will allow deeper, awkward questions to be asked with oneself that will surely bring greater understanding and of course, sobriety – scientific (combustion science here) or whatever one cares to think about!

*Thanks…..*