GASIFICATION OF WASTE TIRE: SYSTEMATIC ANALYSIS AND NUMERICAL SIMULATION

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Problem definition

- Of the 1.2 billion generated tires only 50% of waste tire are being recycled worldwide [Rubber Div., 2008]
- None bio-degradable and can last 100 years or more if no proper handling is carried out
- Illegal dumping/burning can be seen everywhere and incorrect disposal is environmentally hazardous
- Wasted resources/business opportunities:
  - Rereading and granulation
  - Energy & chemicals
  - Carbon black
  - Metal
  - Liquid and gas fuel etc.!

Melbourne Australia 2006, tire pile fires lasted over a month sending up an acid black plume that seen miles away contains toxic chemicals and air pollutants just as toxic chemicals are released into surrounding water supplies by oily runoff from tyre fires

WORLD ENERGY CONSUMPTION 2013

Billion BTU's

CHINA	15,522,296
UNITED STATES	14,590,365
RUSSIA	4,409,567
INDIA	3,344,285
JAPAN	3,254,716
GERMANY	2,035,958
CANADA	2,016,837
FRANCE	1,608,236
WORLD TOTAL	76,668,568

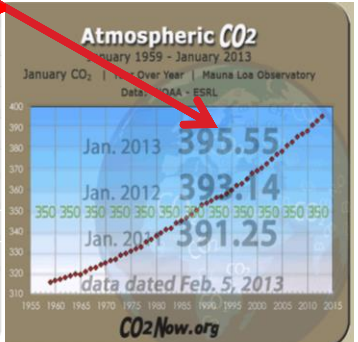
OilPrice.com

WORLD ENERGY PRODUCTION 2013

Billion BTU's

CRUDE OIL	25,000,768
COAL	23,813,681
NATURAL GAS	18,388,511
NUCLEAR	3,995,532
HYDROELECTRIC	4,946,611
WIND	950,575
BIOFUELS	377,916
SOLAR	189,210
GEOTHERMAL	51,831
TOTAL PRODUCTION	76,605,547
TOTAL CONSUMPTION	76,670,547

OilPrice.com



Stock availability and potential

- Worldwide, an estimated 1.2 billion waste tiers are generated every year. Only a fraction of these tyres are currently recycled with the majority being incinerated, dumped or stockpiled.

Location	Generation (million)	Stockpile (million)
USA	240	500 to 3,000
Australia	8	20
Japan	100	100
Europe	250	3,000

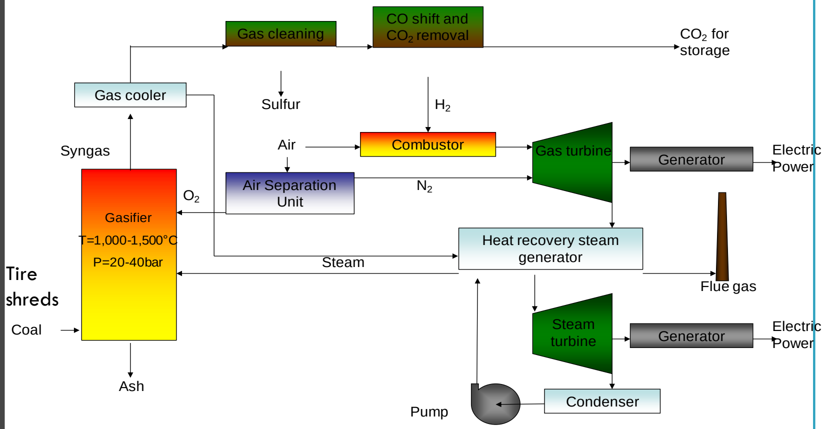
- UAE: 2,500 tiers is collected in Sharjah per day or 63 tons/daily, [Sharjah Municipality, 2012]
  - Abu Dhabi available stock over 5,000,000 tiers or 126,000 tons [CWM, 2012]
  - 120 tons daily gasifier ensure stocks for 3 years, but within these three years another 69,000 is collected,
  - This quantity will last for 19 months, by the end of this 19 months another 35,910 tons is collected
  - This will last for approxmately10 months…and so on.
- Other 4 Emirates: Ajman, Umm Alqaiwain, Ras AL Khaima and Al Fujaira together produce and have in stock twice as much as the Emirate of Abu Dhabi at this moment [Beah, 2012].
- Sharjah Emirate has at this moment over 5,000,000 tires in stock [Beah, 2013]
- Dubai Emirate has over 5,000,000 ties in stock [Duabi Municipality, 2011]
- Emirates have got all the potential to have their own plants as Abu Dhabi.

* Small tire weight/availbility 12kg/60%, large 45kg/60% production is based on 345 days per year).

Motivation and Objective

Motivation

- Gasification:
  - Efficient way to convert solid feedstock to fuel (syngas & chemicals)
  - Feedstock /product flexibility
  - Syngas is used in IGCC as fuel



Objective

- Material characterization
  - Proximate, ultimate and calorific value analysis
- Low fidelity simulation
  - Thermodynamic analysis of gasification
- High fidelity simulation
  - Coupled CFD analysis with radiation and reaction kinetics

Gasification

- Gasification is a thermo-chemical pathway to convert any carbonaceous feedstock into syngas.

Global Gasification Reaction

$$\underbrace{CH_xO_yN_z}_{\text{Feedstock}} + m\,(\underbrace{O_2 + 3.76\,N_2}_{\text{Oxidizer}}) + n\,\underbrace{H_2O/CO_2}_{\text{Moderator}} \rightarrow \underbrace{x_1\,CO + x_2\,H_2 + x_3\,CH_4}_{\text{Syngas}} + \underbrace{x_4\,CO_2 + x_5\,H_2O}_{\text{Combustion products}} + 3.76m\,N_2$$

Intermediate Gasification Reactions [Higman et. al.]

1) Combustion reactions

$$C + \tfrac{1}{2}O_2 = CO \quad -111\ MJ/kmol$$

$$CO + \tfrac{1}{2}O_2 = CO_2 \quad -283\ MJ/kmol$$

$$H_2 + \tfrac{1}{2}O_2 = H_2O \quad -242\ MJ/kmol$$

2) Boudouard reaction

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3) Water gas reaction

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4) Methanation reaction

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5) CO shift reaction

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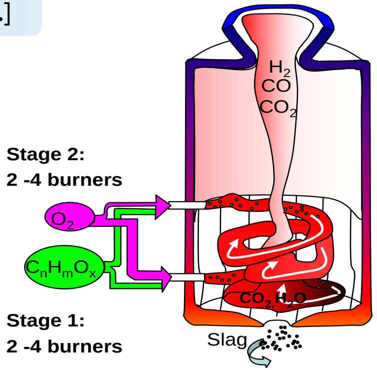
6) Steam methane reforming reaction

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \quad +206\ MJ/kmol$$



Material Characterization

- Proximate analysis
- Ultimate analysis
- Calorific value analysis

Composition	Tire
Proximate (Wt.%)	
Moisture	1.0
Volatile Matter	68.0
Fixed Carbon	23.2
Ash (dry)	8.8
Ultimate (Wt.%) (dry)	
C	73.8
H	6.8
N	0.3
S	1.3
O	9.0
Ash	8.8
HHV (MJ/kg)	36.0
MW (kg/kmole)	14.83
$CH_{1.1057}O_{0.0915}N_{0.0035}S_{0.0066}$	

Thermodynamic model of gasification through

Gibbs Energy Minimization Lagrange multiplier method

- A relatively easy method to formulate a large number of product species as compared to Equilibrium constant method.
- Function: $\Delta G^{o}_{f,i} + RT \ \ln(\frac{x_i}{x_{total}}) + \sum_k \lambda_k a_{ik} = 0 \ \ (i = 1, \ 2, \ ... \ number \ of \ \ species, k = C, H, O, N, S)$

Reactants

$$\underbrace{CH_xO_yN_zS_w}_{\text{Feedstock}} + \underbrace{m \ (O_2 + 3.76 \ N_2)}_{\text{Oxidizer}} + \underbrace{n \ H_2O}_{\text{Moderator}} + \underbrace{Q}_{\text{Heat Input}}$$

Products

44 species: Product of gasification										
C(g)	CH	CH_2	CH_3	CH_4	C_2H_2	C_2H_4	C_2H_6	C_3H_8	H	H_2
O	O_2	CO	CO_2	OH	H_2O	H_2O_2	HCO	HO_2	N	N_2
NCO	NH	NH_2	NH_3	N_2O	NO	NO_2	CN	HCN	HCNO	S(g)
S_2(g)	SO	SO_2	SO_3	COS	CS	CS_2	HS	H_2S	C(s)	S(s)

Thermodynamic model of gasification through

Gibbs Energy Minimization Lagrange multiplier method

Model formulation:

- Elemental balance
  - Carbon balance
  - Hydrogen balance
  - Oxygen balance
  - Nitrogen balance
  - Sulfur balance

  → 5 Equations
- Gibbs Energy functions → 44 Equations
- Energy balance → 1 Equation
- Total 50 Equations

$$\Delta G^o_{f,i} + RT \ \ln(\frac{x_i}{x_{total}}) + \sum_k \lambda_k a_{ik} = 0$$

Examples of Gibbs Energy Function:

for Methane,

$$G^o_{f,CH4} + RT \ \ln(\frac{x_{CH4}}{x_{total}}) + (\lambda_1 + 4\lambda_2) = 0$$

for hydrogen,

$$G^o_{f,H2} + RT \ \ln(\frac{x_{H2}}{x_{total}}) + 2\lambda_2 = 0$$

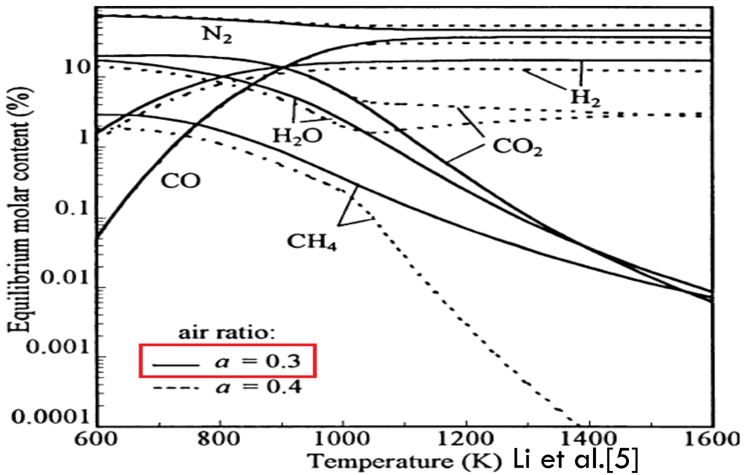
for carbon monoxide,

$$G^o_{f,CO} + RT \ \ln(\frac{x_{CO}}{x_{total}}) + (\lambda_1 + \lambda_3) = 0$$

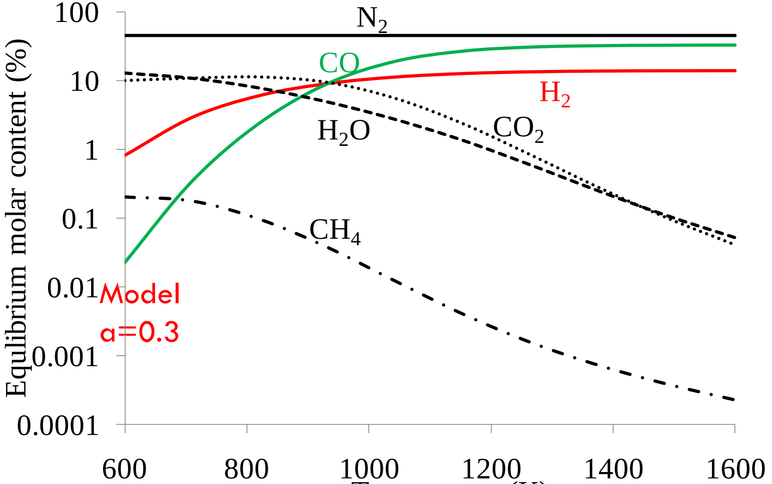
Thermodynamic model of gasification through

Gibbs Energy Minimization Lagrange multiplier method

- Model validation (air ratio (a)=0.3 kmole)
  - Feedstock: high vale coal [5]
  - Empirical formula: $CH_{0.6923}O_{0.2124}N_{0.0105}S_{0.0013}$
  - Higher heating value: 21.1 MJ/kg



Li et al.[5]



Temperature (K)

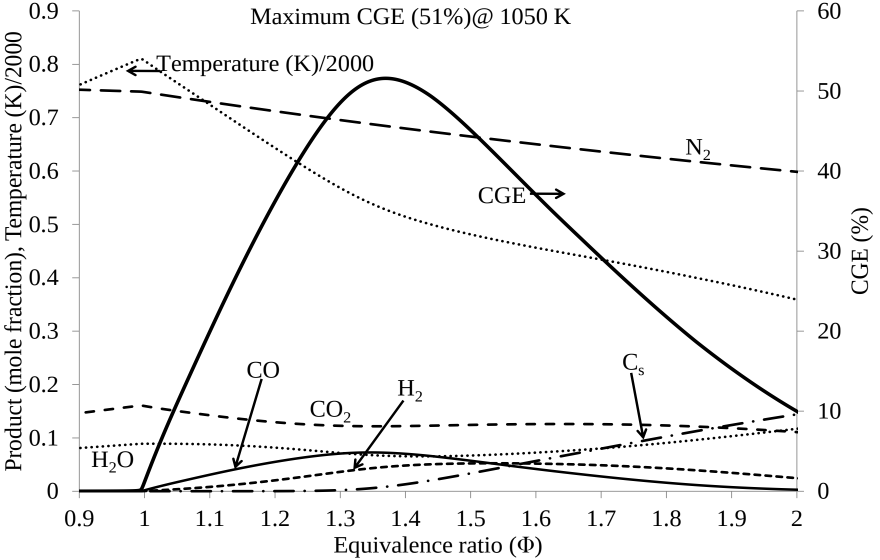
[5] Li, X., et al., Equilibrium modeling of gasification: a free energy minimization approach and its application to a circulating fluidized bed coal gasifier. Fuel, 2001. 80(2): p. 195-207.

Gibbs Energy Minimization Lagrange multiplier method

- Results

H_2O gasification

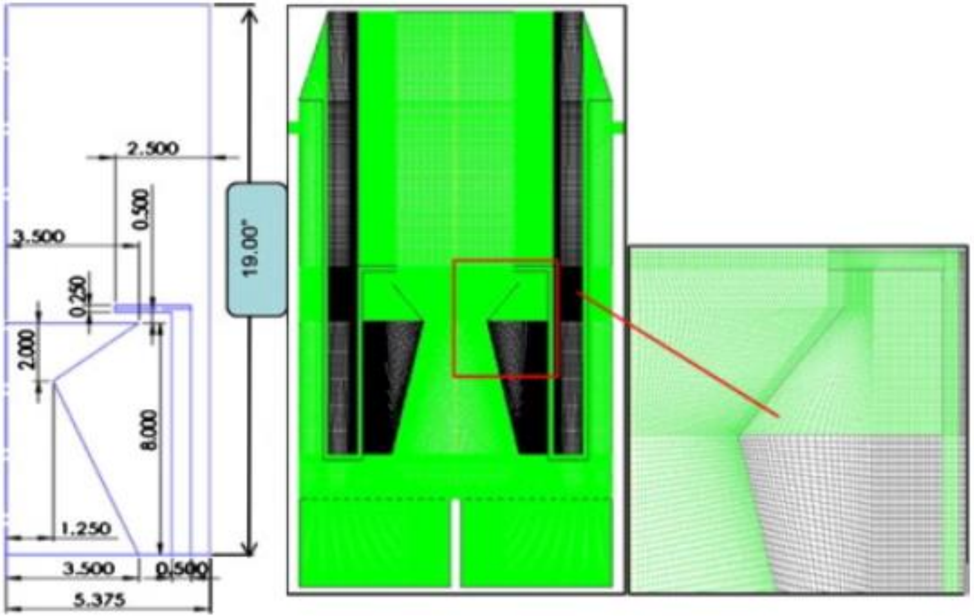
$$CH_{1.1057}O_{0.0915} + 0.9085\ H_2O + m(O_2 + 3.76N_2)$$



Species	Syngas mole (%)
CO	7.2
CO_2	12.2
H_2	4.57
H_2O	6.63
O_2	0
N_2	68.4
CH_4	0
Temperature (K)	1051
Equivalence ratio (Φ)	1.37
CGE	51%

Coupled thermo-chemical simulation with CFD

- Gasifier geometry and boundary conditions



Gasifier Inlet Conditions

Tire inlet condition	
Inlet temperature (K)	300
Inlet velocity (m/s)	1.70E-04
Diameter (mm)	0.1
Air inlet condition	
Inlet temperature (K)	300
Inlet velocity (m/s)	0.195

Coupled thermo-chemical simulation with CFD

Governing Equations:

- Mass, momentum and energy

$$\frac{\partial}{\partial t}(\Theta) + \frac{\partial}{\partial x_i}(u_i \Theta) = -\frac{\partial}{\partial x_i}\left(\Gamma_\Theta \frac{\partial \Theta}{\partial x_i}\right) + S_\Theta$$

Time rate   *advective*   *diffusion*   *source*

$\Theta \equiv$ density, velocity, temperature

- Reaction terms and kinetics

$$\sum_{i=1}^{N} v'_{i,r} S_i \underset{k_{b,r}}{\overset{k_{f,r}}{\Leftrightarrow}} \sum_{i=1}^{N} v''_{i,r} S_i$$

Reaction		Kinetic Parameters Aj , Ej [kJ/mol]
R1	$2\,CO + O_2 \rightarrow 2\,CO_2$	$A = 10^{17.6}$[(m3mol-1)-0.75s-1], $E = 166.28$
R2	$2\,H_2 + O_2 \rightarrow 2\,H_2O$	$A = 1e11$ [m3mol-1s-1], $E = 42$
R3	$CO + H_2O \leftrightarrow CO2 + H_2$	$A = 0.0265$, E= 65.8
R4	$C_{(s)} + O_2 \rightarrow CO_2$	$A = 5.67e9$ [s-1], $E = 160$
R5	$C_{(s)} + CO_2 \rightarrow 2\,CO$	$A = 7.92e4$ [m3mol-1 s-1], $E = 218$
R6	$C_{(s)} + 2\,H_2 \rightarrow CH_4$	$A = 79.2$ [m3mol-1 s-1]$E = 218$
R7	$C_{(S)} + H_2O \rightarrow CO + H_2$	$A = 7.92e4$ [m3mol-1 s-1], $E = 218$
R8	$vol + 0.4\,O_2 \rightarrow 1.317\,CO + 2.09\,H_2 + 0.064\,N_2$	$A = 1E15$ [m3mol-1 s-1], $E = 1E8$

$$\hat{R}_{i,r} = \Gamma(v''_{i,r} - v'_{i,r})\left(k_f \prod_{j=1}^{N} C_{j,r}^{v^*_{,rj}} - k_b \prod_{j=1}^{N} C_{j,r}^{v'^*_{j,r}}\right) \text{ and } R_i = M_i \sum_{r=1}^{n} \hat{R}_{i,r}$$

- Transport equation

$$\frac{\partial}{\partial t}(\rho m_i) + \frac{\partial}{\partial x_i}(\rho u_i m_i) = \frac{\partial}{\partial x_i}(\rho D_{i,m} + \mu_t / Sc_t)\frac{\partial m_i}{\partial x_i} + R_i + S_i$$

- Discrete particle interaction

$$\frac{d\vec{u}_P}{dt} = F_D(\vec{u} - \vec{u}_P) + \vec{g}(\rho_P - \rho)/\rho_P \; ; \; \frac{d\vec{x}_P}{dt} = \vec{u}_p$$

$$-\frac{dm_p}{dt} = Ae^{-(E/RT)}[m_p - (1 - f_v^0)m_p^0]$$

$$m_p c_p \frac{dT_p}{dt} = hA_p(T_\infty - T_p) + \frac{dm_p}{dt} h_{fg} + \varepsilon_p A_p \sigma(T_R^4 - T_p^4)$$

Calculation procedure of feedstock conversion:

(a) Solve the continuous phase
(b) Introduce and solve for the discrete phase
(c) Recalculate the continuous phase flow using the inter-phase exchange of momentum, heat, and mass
(d) Recalculate the discrete phase trajectories
(e) Repeat c and d steps until a convergence is attained

Numerical approach

Coupled thermo-chemical simulation with CFD

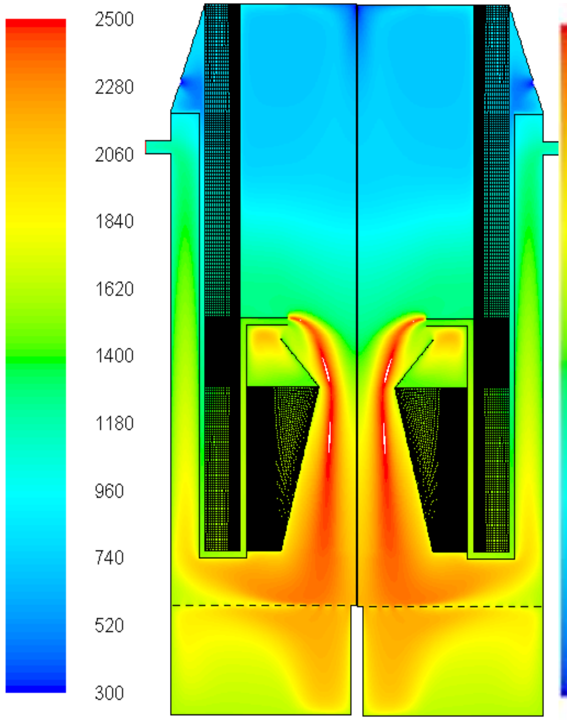


Figure: Temperature (K) distribution inside gasifier

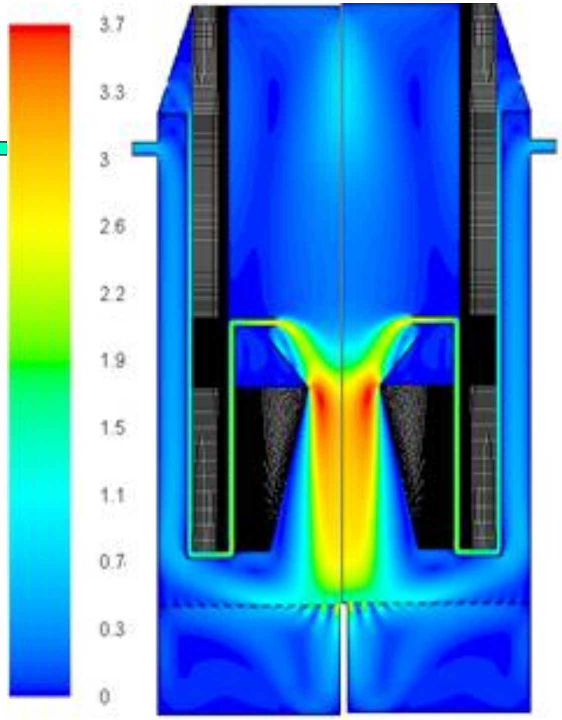
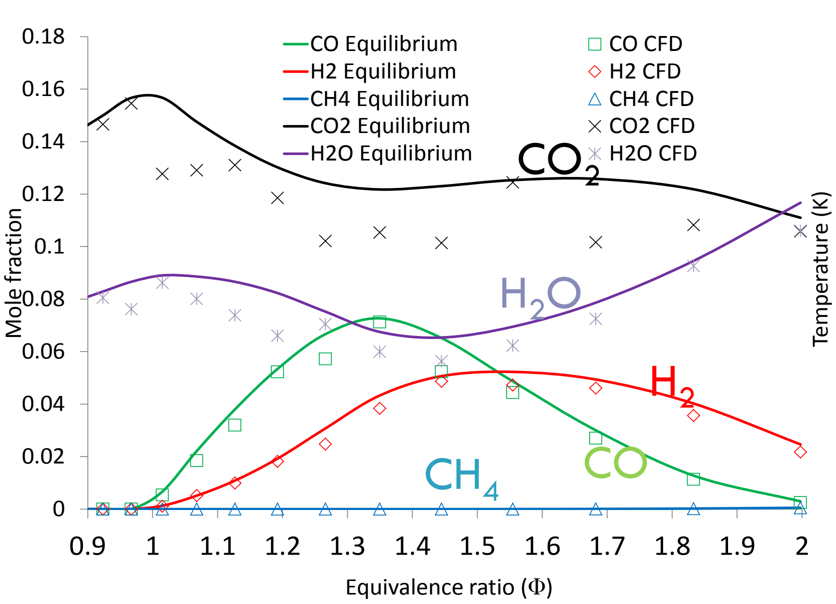
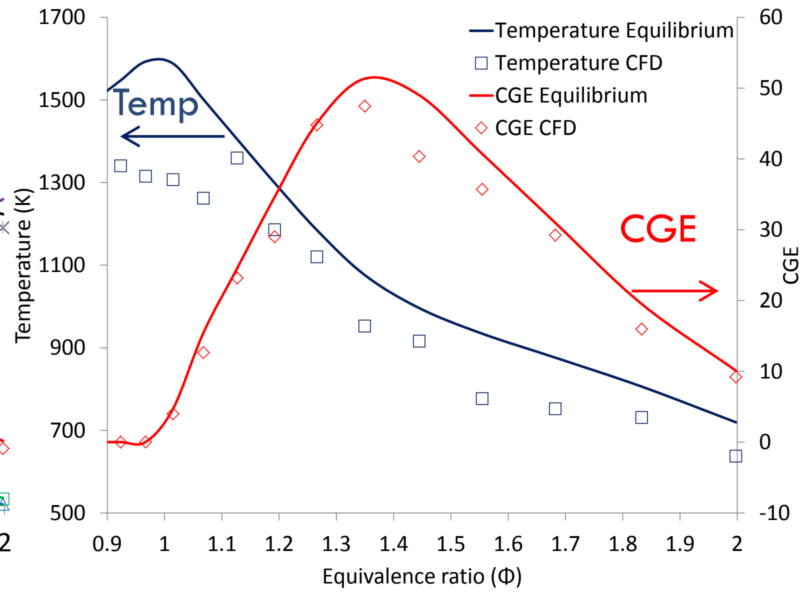


Figure: Velocity (m/s) distribution inside gasifier

Numerical approach

Coupled thermo-chemical simulation with CFD



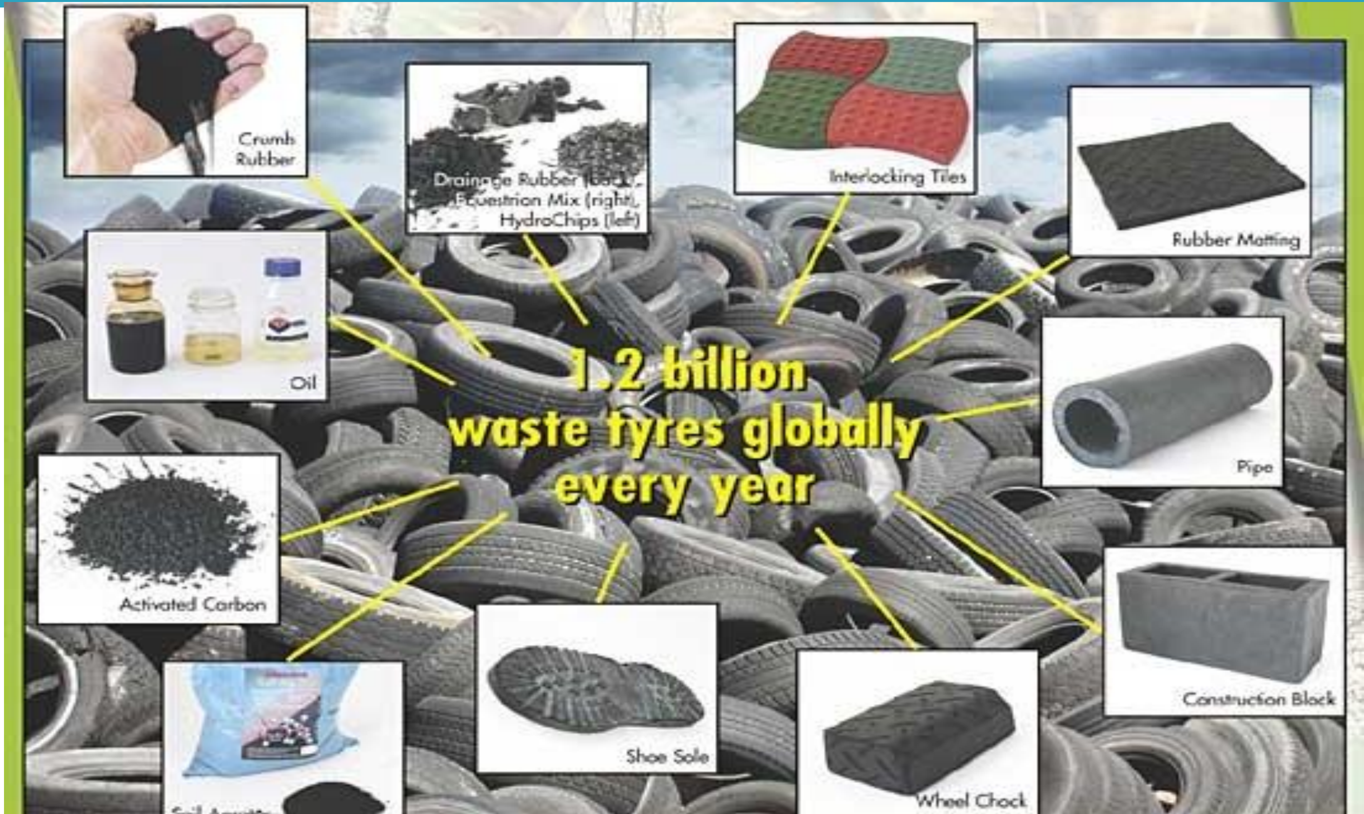


Conclusions

- Material characterization is performed to measure the proximate and ultimate composition of tire along with its high heating value.
- Simulation low vs high fidelity:
  - Low fidelity Gibbs minimization approach shows the maximum tire cold gasification efficiency is 51%.
  - High fidelity CFD simulation is favorably compared to the results of Gibbs energy minimization model
  - The Gibbs energy minimization model can be use initially to predict the quality of syngas without going for tedious CFD simulation or experimental approach.
- What you need to know:
  - Thermochemical conversions is making a strong comeback as sustainable energy source and efficiency enhancement.
  - This technology can be deployed as renewable source for million of tons of waste streams disposed of at landfill and risking our ecological system.
  - Modeling ad simulations are needed at the conceptual level to increase the process efficiency and throughput.

Acknowledgement:

The financial sponsorship of Masdar institute is highly acknowledged. Thank you ….Questions ?



Backup slide:

Global Gasification reaction

$$CH_xO_yN_z + m(O_2 + 3.76N_2) + nH_2O + pCO_2 \rightarrow x_1H_2 + x_2CO + x_3CO_2 + x_4H_2O + x_5C + \left(\frac{z}{2} + 3.76m\right)N_2$$

Intermediate Gasification Reactions [Higman et. al.]

1) Combustion reactions

$C + \frac{1}{2}O_2 = CO \quad -111 \ MJ/kmol$

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$C + CO_2 \leftrightarrow 2CO \quad +172 \ MJ/kmol$

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$C + H_2O \leftrightarrow CO + H_2 \quad +131 \ MJ/kmol$

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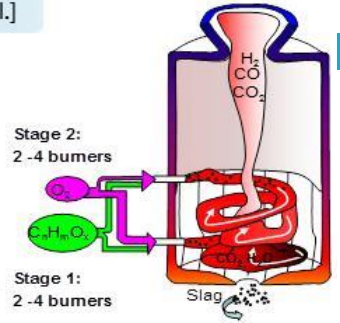

- Elemental balance
  - Carbon balance
  - Hydrogen balance
  - Oxygen balance
  - Nitrogen balance
- Equilibrium constant equation
  - For Bouduard reaction:
  - For CO shift reaction:
  - For Methanation reaction:
- Energy balance between reactant and product

$$\sum_{i\_prod=1}^{N} n_i(\bar{h}_o + \bar{h}_s) + Q = \sum_{i\_react=1}^{N} n_i(\bar{h}_o + \bar{h}_s)$$

- Conversion Metrics

$$CGE = \frac{x_1(283800) + x_2(283237.12) + x_5(889000)}{HHV_{feedstock}}$$

$$K_1 = \frac{x_2^2}{x_3 x_{total}} \quad (Equilibrium\ const.\ for\ Boudouard\ reaction)$$

$$K_2 = \frac{x_1 x_3}{x_2 x_4} \quad (Equilibrium\ const.\ for\ CO\ shift\ reaction)$$

$$K_3 = \frac{x_5 x_{total}}{x_1^2} \quad (Equilibrium\ const.\ for\ Methanation\ reaction)$$

$$x_{total} = x_1 + x_2 + x_3 + x_4 + x_5 + \left(\frac{z}{2} + 3.76m\right)$$