Waste 2 Energy Labortory

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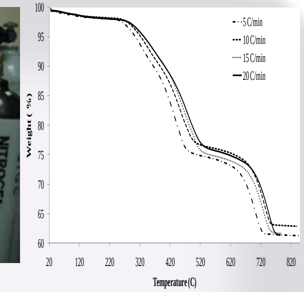
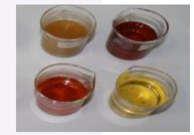
Main research activities

❑Material Characterization:



- Proximate (TGA)
- Ultimate (CHNSO-Flash)
- Chemical Kinetics (TGA)
- Thermal properties: Bomb Cal/Cp(STA)
- Impurities (GC-MS, ICP)
- Species determination (Drop. Tube)

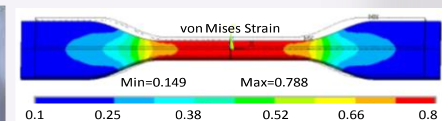


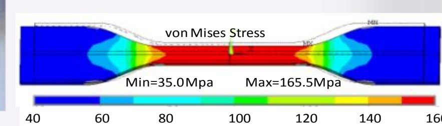
❑Low Temp. Pathway

- Transesterification
- Plastic recycling:

  -Decrossing-Extruding-Injection

  -Tensile testing &modeling/Simulation





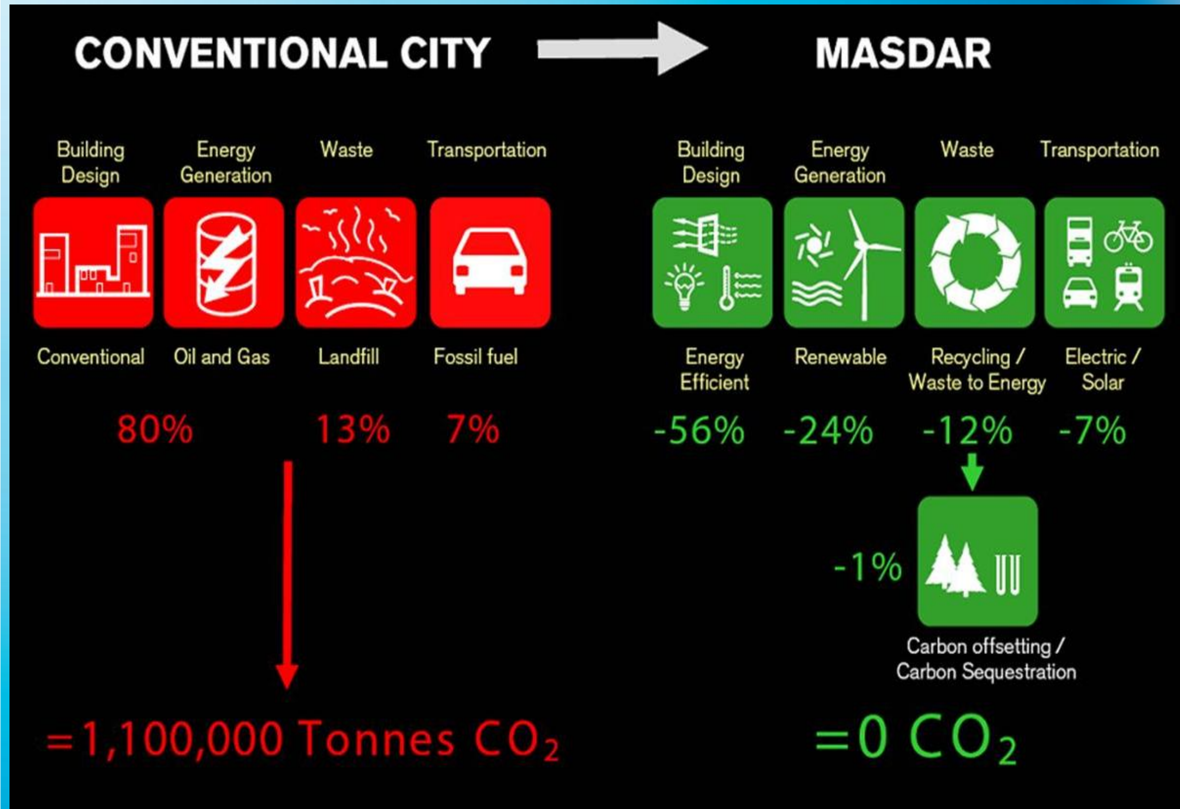
❑High Temp. high Temp. pathway:

- Incinerations/Combustion
- Pyrolysis (Buchi Reactor)
- Gasification (GEK)

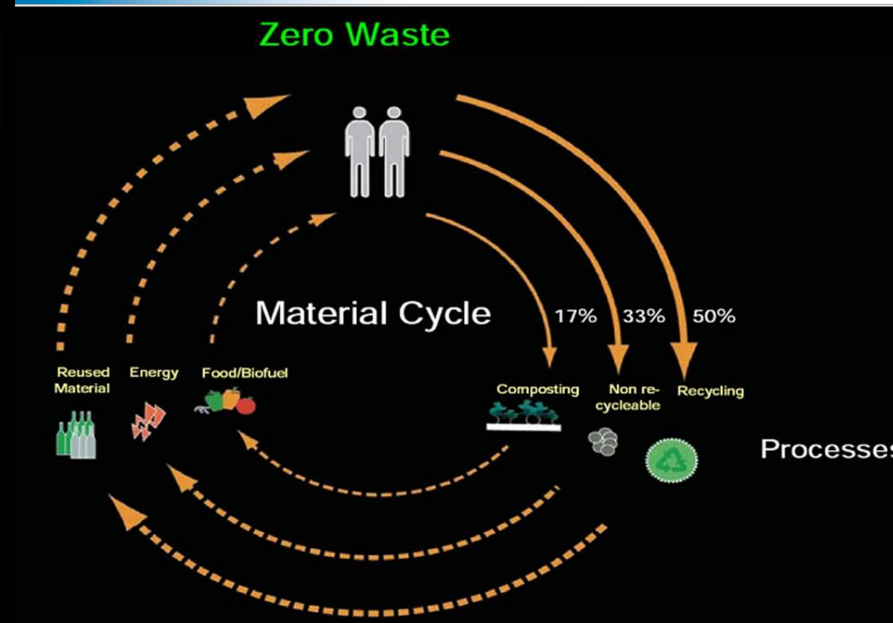
Outlines

- Overview, Challenges, Objectives
- Material characterization
  - Proximate analysis
  - Ultimate analysis
  - Calorific value analysis
- Low fidelity simulation
  - Equilibrium constant approach
  - Gibbs energy minimization approach
- High fidelity simulation
  - Reaction kinetics using Arrhenius equation
  - Numerical simulation using CFD (Cold Flow Analysis)
  - Numerical simulation using coupled CFD with Discrete particle in reactive flow Env.

Overview :



Advocating zero waste

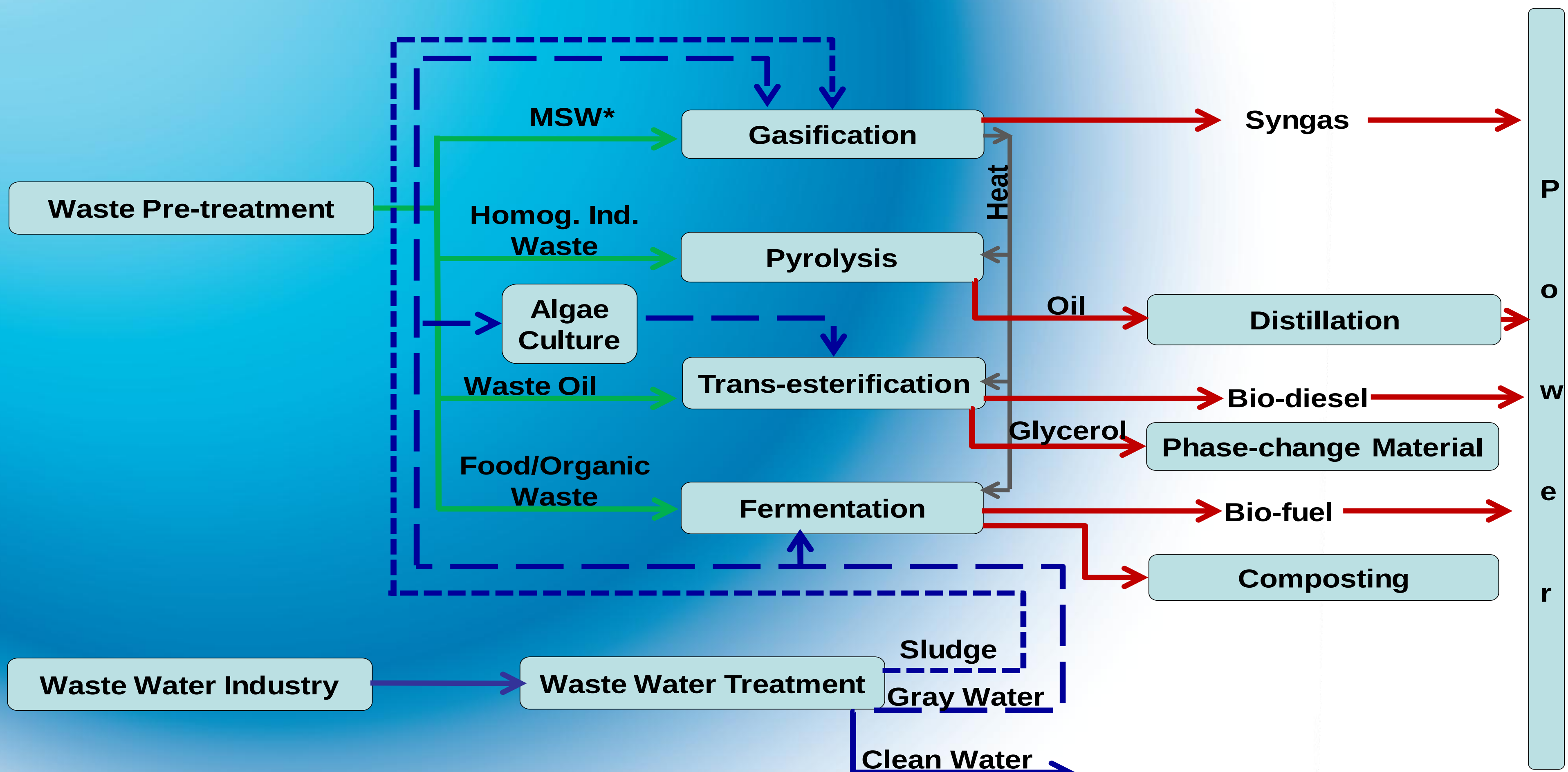


Country	MSW (Kg/person/day)	Country	MSW (Kg/person/day)
Bahrain	1.3	Austria	0.89
EU-7	1.4	Belgium	0.93
India	0.45	Egypt	0.81
Italy	0.95	France	0.89
Japan	1.12	Jordan	0.6
Kuwait	1.4	Oman	0.7
Qatar	1.3	Portugal	0.7
Spain	0.88	Tunisia	0.41
UAE	1.2	Turkey	0.95
US	2	UK	0.95

	Type of Waste Thousands tons/year)								
Year	Organics	Fiber	Wood	Plastic	Paper	Glass	Metal	Others	Total
1995	422	41	41	109	178	29	23	11	854
2000	492	47	47	124	203	32	26	13	984
2005	558	53	53	141	231	37	29	15	1,117
2010	662	63	63	167	273	44	35	17	1,324
2015	**736**	**71**	**71**	**185**	**303**	**49**	**38**	**19**	**1, 472**
2020	830	80	80	209	342	55	43	22	1,661

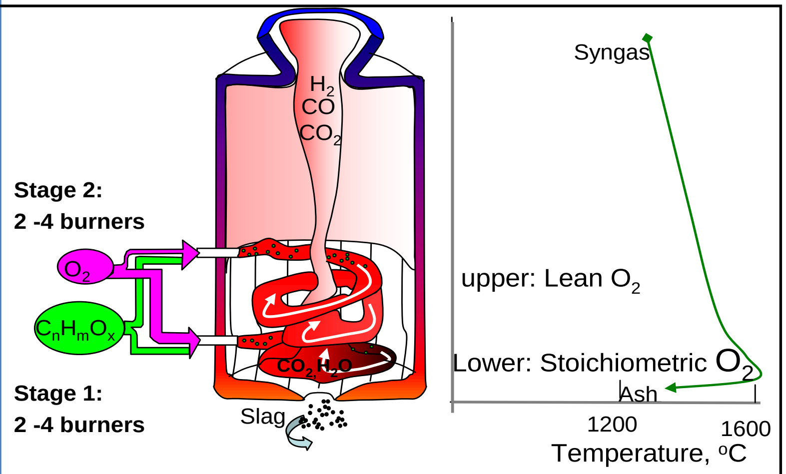
Objectives:

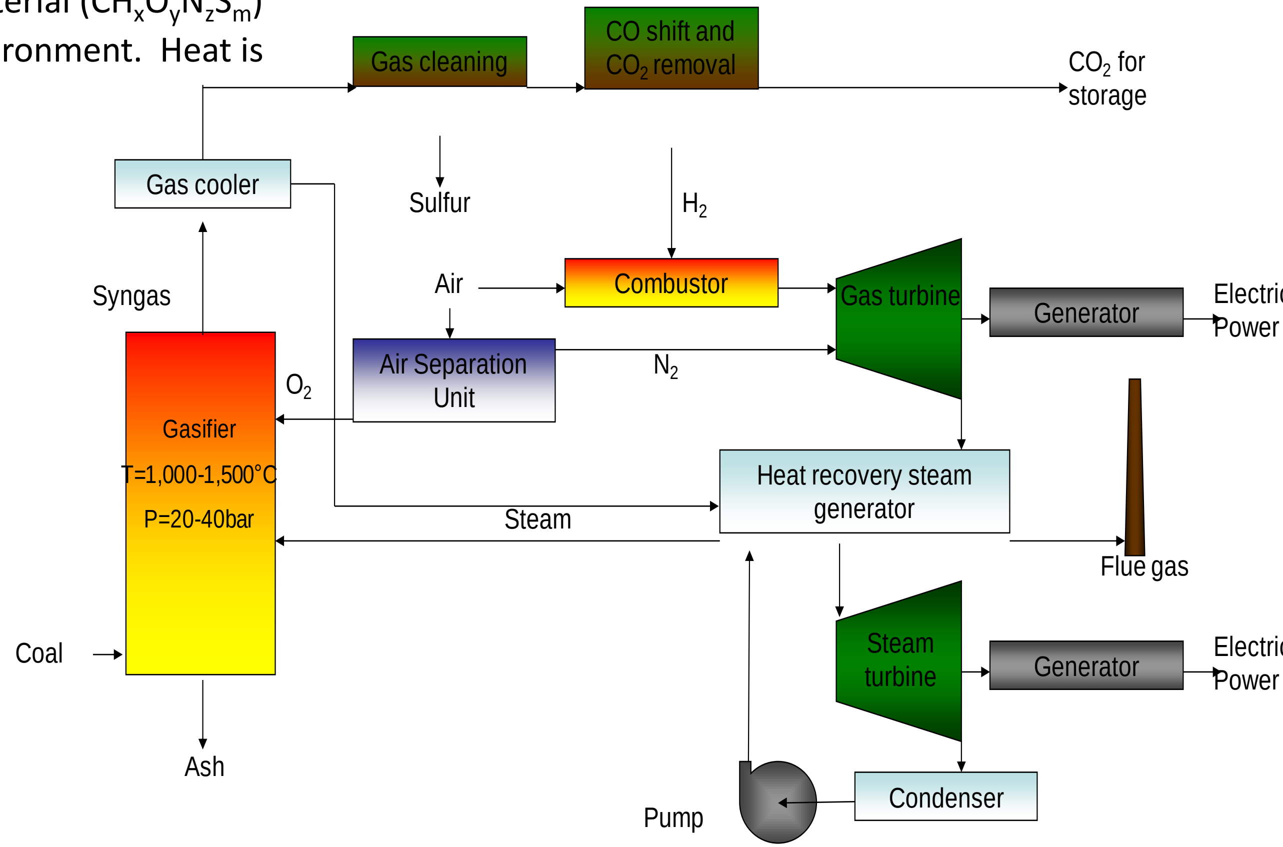
- ❑Provide sustainable routes to maximize resource utilization by converting waste to energy and Reduce MENA 's emission foot print (CO2, NOX, SOX, CH4, etc)
- ❑Fulfill the emerging stringent environmental regulations and reduce landfill deposits
- ❑Promote IGCC as the cleanest and most efficient (50%) power generation technology amenable to CO_2 capturing
    - ❑Explore high temperature conversion including gasification and pyrolysis of waste stream into syngas
    - ❑ Use trans and esterification of waste cooking and algae oil into biodiesel (2nd and 3rd Generation)
    - ❑ Use fermentation processes to convert organic waste into bio-fuel and compost



To Gasify, or Not to Gasify?

Definition: To convert carbonaceous solid material ($CH_xO_yN_zS_m$) into a mixture of CO and H2 in an O2 deprived environment. Heat is provided by combusting part of the fuel.





Advantages

- Control over produced energy
- Capability for carbon capture and storage.
- Flexibility in feedstock and products.
- Alternative to “bury or burn” policy.
- Hydrogen-based energy systems (near zero-CO_2 emissions).
- Small scale gasifiers for distributed generation.

Gasification	versus	Combustion
CO	C	CO_2
H_2	H	H_2O
N_2	N	NO_x
H_2S	S	SO_x

To Gasify, or Not to Gasify?

Challenges

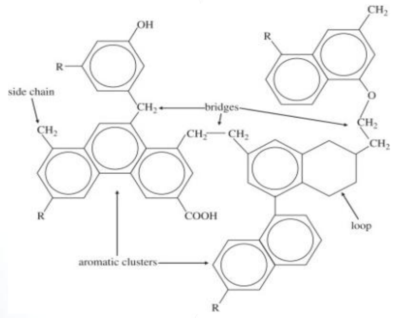
Current needs & technology challenges	Physical aspect	Modeling implementation
Feedstock flexibility	•Dynamic and intrinsic behavior •Feedstock and char characterization –proximate&ultimate analysis	Accurately models fuel switching and associated reactions
Slag blockage/removal	•Turbulence-chemistry-radiation interactions •Accurate Slag characterization	Accurately models slag flow, composition and temperature distribution and turbulence
Downstream fouling and poisoning	•Particle dispersion and inhomogeneous distribution •Agglomeration, swelling and fragmentation particle mechanisms •Nitrogen and sulfur production	Accurately flow modeling, conversion, ash distribution and pollutant formation
Wall/refractory failure	•Particle dispersion and inhomogeneous heat distribution •Turbulence-chemistry-radiation interactions •Slag wall build up	Accurately model wall interactions, thermal stresses, pressure effects and abrasion
Injector failure	•Turbulence-chemistry-radiation interactions	Accurately model flow and temperature distribution
Space efficiency	•Particle dispersion •Turbulence-chemistry-radiation interactions	Accurately model flow and conversion

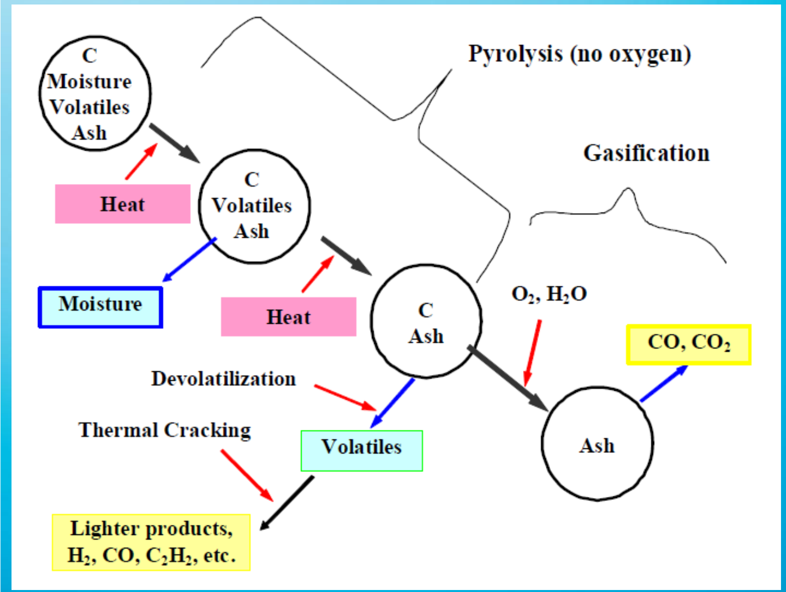
Cycle	Fuel	Temp low (oC)	Temp High (oC)	Carnot (η)	Actual (η)	Car(η)/Act(η)%
Conventional Steam Power Plant	Coal	27	540	63	40	63
Ditto Ultra Super Critical	Coal	27	650	67	45	67
IGCC	Coal	27	1350	82	46	56
Open Gas Turbine Cycle	Gas	27	1210	80	43	54
Combined Cycle	Gas	27	1350	82	58	71
Low Speed Marine Diesel (LSMD)	Heavy Fuel Oil	27	2000	87	48	55
LSMD with Super Charger	Heavy Fuel Oil	27	2000	87	53	61

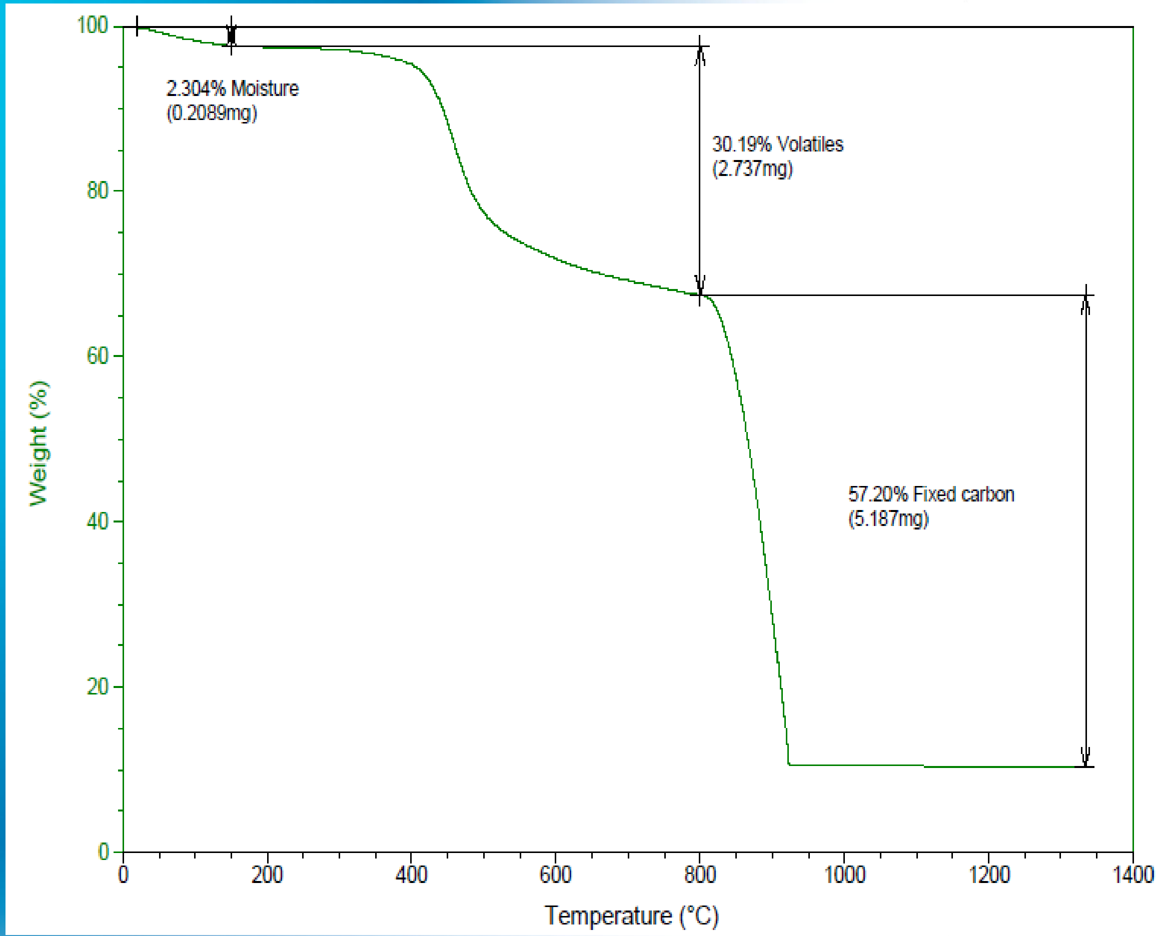
Material Characterization

- What does the feedstock compose of?

Carbonaceous fuel is a complex collection of organic polymers consisting mainly of aromatic chains.

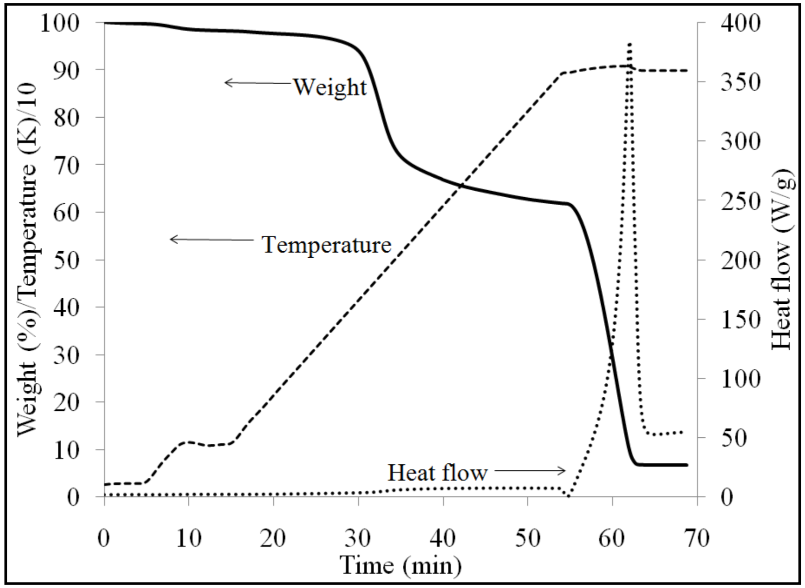






- Drying
- Pyrolysis
- Combustion
- Gasification

MATERIAL CHARACTERIZATION
Proximate Analysis



DSC/TGA curve of RTC-Coal with respect to time.

Summary of the proximate analysis

Composition	Weight (%)
Moisture	0.3001
Volatiles	37.8147
Fixed Carbon	54.6571
Ash	7.2281
Total	100

Simultaneous DSC/TGA Q600

Proximate analysis is used to calculate the weight percentage of moisture, volatiles, fixed carbon and Ash present in the sample.

MATERIAL CHARACTERIZATION

Ultimate analysis

Sample ID	Nitrogen Wt(%)	Carbon Wt(%)	Hydrogen Wt(%)	Sulphur Wt(%)	Oxygen Wt(%)	Ash Balance Wt (%)
1	2.2926	76.5178	5.3233	0.8075	8.1136	6.9452
2	2.1930	73.2217	5.0185	1.0848	7.7913	10.6908
3	2.2319	73.8664	5.0861	1.0148	7.6337	10.1671
4	2.1340	66.7894	4.6437	1.0004	7.8425	17.5901
5	2.1348	71.1166	4.7098	1.0794	7.7338	13.2257
Average	**2.1972**	**72.3024**	**4.9563**	**0.9974**	**7.8230**	**11.7238**

Results of ultimate analysis for RTC-coal

Flash 2000 CHNSO analyzer (TCD)

Ultimate analysis is used to calculate the elemental composition of the sample

Ultimate analysis	Wt(%) Previous	Wt(%) New	Molar number	Carbon normalization
Nitrogen	2.49	2.50	0.1784	0.0260
Carbon	81.90	82.17	6.8475	1.0000
Hydrogen	**5.58**	5.60	5.5967	0.8173
Sulfur	1.13	1.13	0.0354	0.0052
Oxygen	**8.57**	8.60	0.5376	0.0785
Total	99.68	100		

Empirical formula of RTC-coal using ultimate analysis $CH_{0.8173}O_{0.0785}N_{0.0260}$

MATERIAL CHARACTERIZATION

Calorific value analysis

Sample ID	Weight (gms)	HHV (MJ/Kg)
1	3.4027	30.2205
2	1.7868	30.8207
3	1.7145	30.4197
4	1.6064	30.2232
Average HHV (MJ/Kg)		30.4210

Higher heating value of RTC-Coal

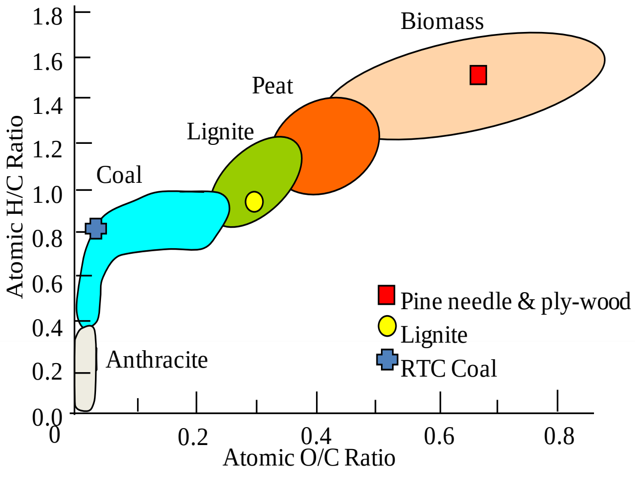
$$HHV\left(\frac{MJ}{Kg}\right) = -0.03(Ash) - 0.11(Moisture) + 0.33(Volatiles) + 0.35(Fixed\ Carbon)$$

$$HHV\left(\frac{MJ}{Kg}\right) = 0.3491\ C + 1.1783\ H + 0.1005\ S - 0.1034\ O - 0.0151\ N - 0.0211\ A$$

Parr 6100 Bomb calorimeter

Feedstock	C %Wt	H %Wt	O %Wt	N %Wt	S %Wt
RTC coal	83.36	5.52	7.44	2.53	1.15
Pine needles	48.58	6.30	43.64	1.48	0.00
Ply-wood	49.59	6.28	43.74	0.39	0.00
Lignite	66.03	4.65	25.64	2.07	1.62

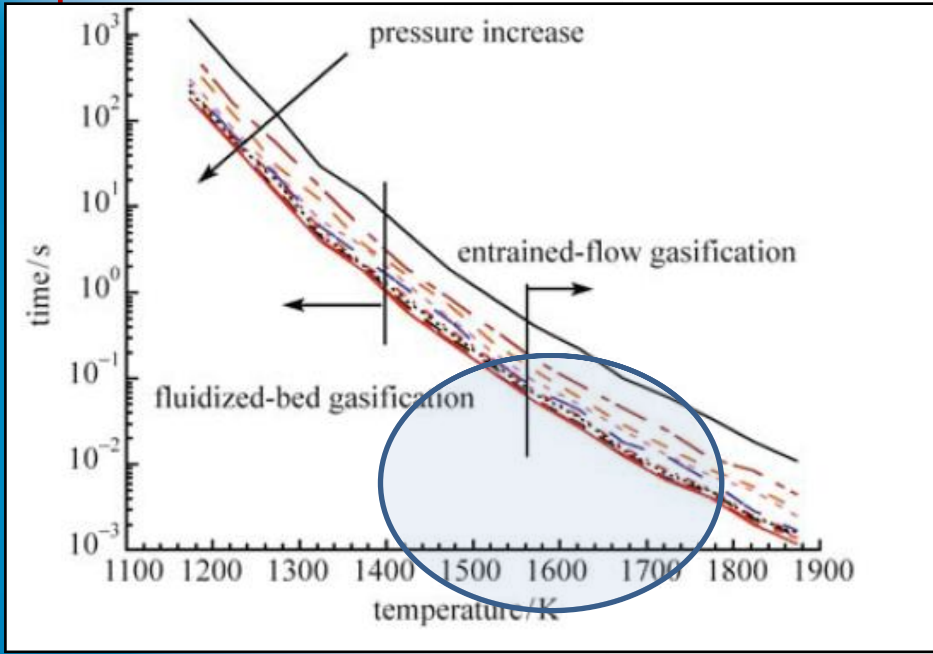
Feedstock	Empirical formula	HHV KJ/Kmole	HHV MJ/Kg
RTC coal	$CH_{0.7946}O_{0.0670}N_{0.0260}$	502928	35.34
Pine needles	$CH_{1.5550}O_{0.6736}N_{0.0261}$	489784	19.83
Ply-wood	$CH_{1.5196}O_{0.6615}N_{0.0067}$	487566	20.14
Lignite	$CH_{0.8450}O_{0.2912}N_{0.0268}$	469939	26.28



Low Fidelity Model

Can a zero dimensional model predict the gasifier performance?

- Simplest level of modeling.
- No dimension nor time is variable.
- Entrained flow gasifiers are amenable to equilibrium.



Category	Moving Bed		Fluid Bed		Entrained-Flow
Ash condition	Dry Ash	Slagging	Dry Ash	Agglomerating	Slagging
Typical processes	Lurgi	BGL	Winnkler, HTW, CFB	KRW, U-Gas	Shell, Texaco, E-Gas, Noell, KT
Feed characteristics					
Size	6-50mm	6-50mm	6-10mm	6-10mm	<100 μm
Acceptability of fines	Limitted	Better than dry ash	good	better	unlimitted
Acceptability of caking coal	yes (with stirrer)	yes	possibly	yes	yes
Prefered coal rank	any	high	low	any	any
Operating characteristics			l		
Outlet Gas Temperature	low (425-650C)	low (425-650C)	moderate (900-1050C)	moderate (900-1050C)	high (1250-1600C)
Oxidant demand	low	low	moderate	moderate	high
Steam demand	high	low	moderate	moderate	low
Other characteristics	hydrocarbone in gas	hydrocarbone in gas	lower carbon	lower carbon	pure gas, high c conversion

Source: Adapted from Simbeck et al. 1983

LOW FIDELITY SIMULATION
Equilibrium constant approach

Global Gasification reaction

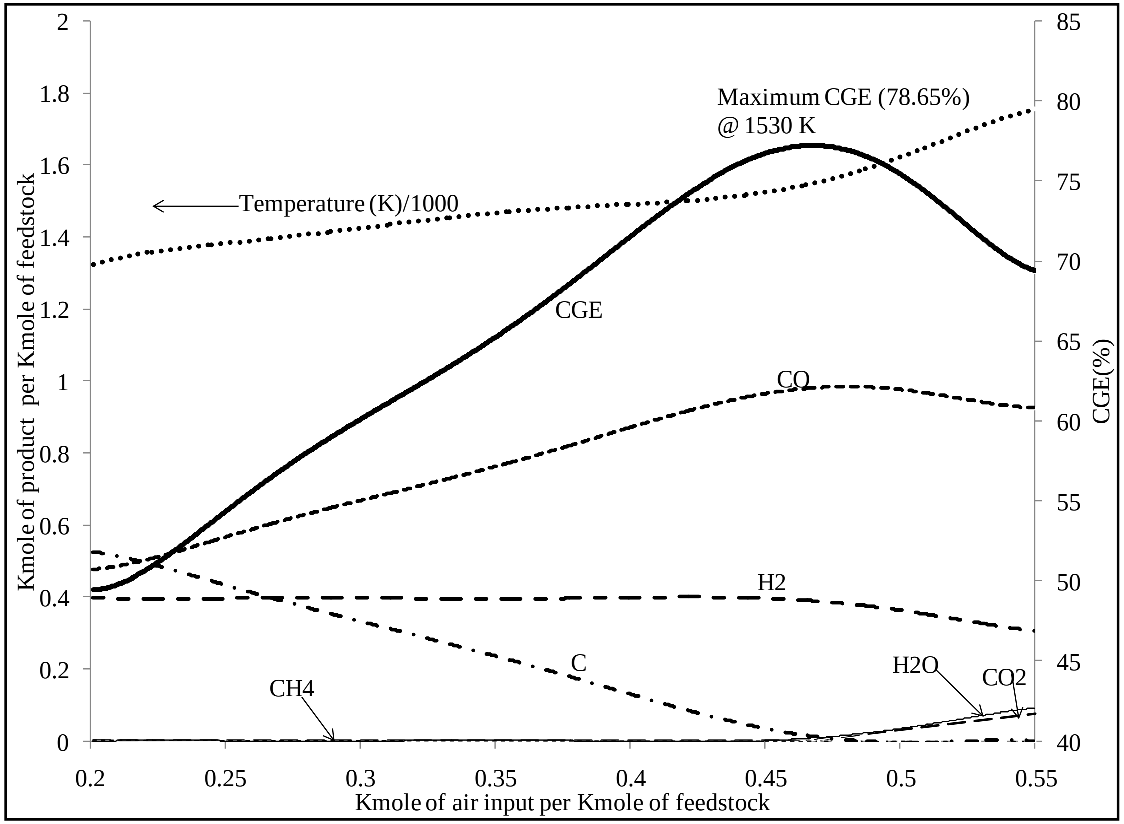
$$CH_xO_yN_z + m(O_2 + 3.76\ N_2) \rightarrow x_1H_2 + x_2CO + x_3CO_2 + x_4H_2O + x_5CH_4 + x_6C + (z/2 + 3.76m)\ N_2$$

- Elemental balance
  - Carbon balance
  - Hydrogen balance
  - Oxygen balance
  - Nitrogen balance
- Equilibrium constant equation
  - For Bouduard reaction: $C_{(s)} + CO_2 <=> 2CO$
  - For CO shift reaction: $CO + H_2O <=> CO_2 + H_2$
  - For Methanation reaction: $3H_2 + CO <=> CH_4 + H_2O$
- 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

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



Equilibrium analysis for RTC coal showing CGE, Temperature and product gas composition

LOW FIDELITY SIMULATION
Gibbs energy minimization approach

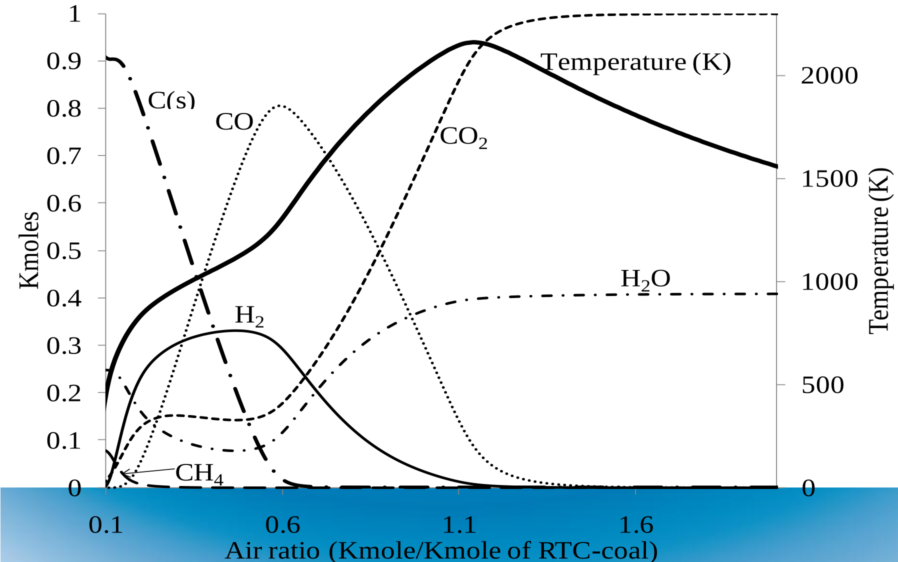
Gibbs Energy minimization using Lagrange multiplier : $G^t_{T,P} = g(n_1, n_2, ..., n_N)$

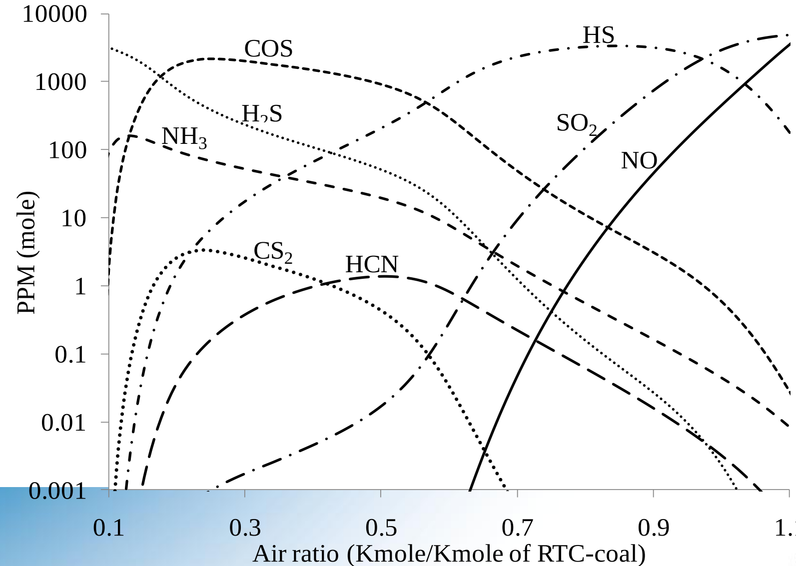
$$\Delta G^o_{fi} + RT \ln\left(\frac{n_i}{n_{total}}\right) + \sum_k \lambda_k a_{ik} = 0, \quad (i = 1,2, \dots, n)$$

List of species considered in the model

Species										
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)

	Air gasification	Air-steam gasification	solar gasification
Maximum CGE	70.94%	71.64%	90.67%
Temperature (K)	1247	1087	1516
CO (Kmoles)	0.7985	0.4562	0.9488
H_2 (Kmoles)	0.3113	0.6609	1.306
CO_2 (Kmoles)	0.1611	0.4969	0.0141
Feedstock consumption (weight %)	16.60%	46.52%	1.32%
Air input (Kmoles)	0.57	0.56	0
H_2O input (Kmole)	0	0.95	0.95
Additional Heat input (KJ/Kmole)	0	0	264070





HIGH FIDELITY SIMULATION

Reaction kinetics via Arrhenius equation

Arrhenius Equation

$$\frac{dX}{dt} = K(1 - X)^n ; K = Ae^{(-E/RT)}$$

- Integral method:

$$\ln\left[-\frac{\ln(1-X)}{T^2}\right] = -\frac{E}{RT} + \ln\frac{AR}{\beta E}$$

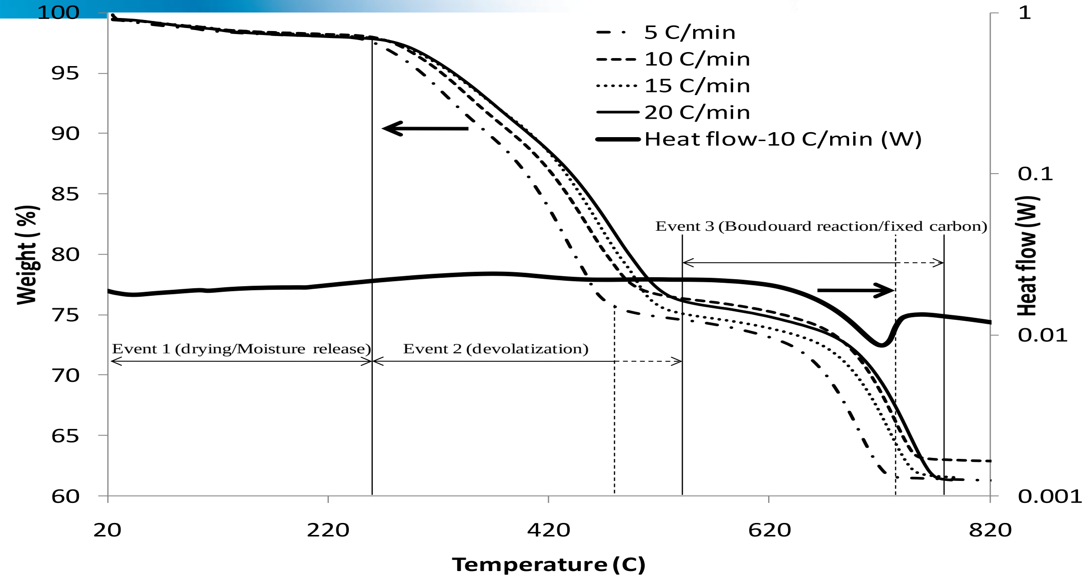
- Direct Arrhenius plot method:

$$\ln\left[-\frac{1}{1-x}\left(\frac{X_{T_2} - X_{T_1}}{T_2 - T_1}\right)\right] = -\frac{E}{R}\left(\frac{1}{T}\right) + \ln\frac{A}{\beta}$$

- Method of approximate temperature integral:

$$\frac{d\ln P(u)}{du} = b + \frac{c}{u}$$

A and *E* can be used in high Fidelity simulation



METHODS:		INTEGRAL METHOD		DIRECT ARRHENIUS PLOT METHOD		APPROX. TEMP. INTEGRAL METHOD	
Heating Rate	Events	E (KJ/mol)	A (sec^{-1})	E (KJ/mol)	A (sec^{-1})	E (KJ/mol)	A (sec^{-1})
20 K/min	Drying	15.9	2.22E-01	8.3	3.26E-02	17.0	3.97E-01
	Devolatization	64.5	2.19E+02	60.7	1.51E+02	66.7	3.02E+02
	Boudouard	152.0	4.71E+05	172.0	7.98E+06	155.8	5.59E+05
15 K/min	Drying	5.9	4.70E-03	8.0	1.96E-02	6.9	1.16E-02
	Devolatization	65.8	2.13E+02	64.2	2.16E+02	68.0	2.92E+02
	Boudouard	173.8	8.03E+06	182.2	2.76E+07	177.8	9.18E+06
10 K/min	Drying	5.6	2.30E-03	4.7	3.90E-03	6.6	5.80E-03
	Devolatization	65.3	1.73E+02	60.5	9.66E+01	67.6	2.38E+02
	Boudouard	171.2	3.25E+06	145.3	1.16E+05	175.3	3.76E+06
5 K/min	Drying	10.9	5.80E-03	5.0	1.60E-03	11.9	1.18E-02
	Devolatization	65.8	1.17E+02	56.2	2.62E+01	68.0	1.60E+02
	Boudouard	168.1	1.61E+06	122.2	4.19E+03	172.2	1.87E+06

HIGH FIDELITY SIMULATION

Coupled CFD and reaction kinetics

<u>Mathematical System:</u>

1) Continuity, Momentum, Energy, TKE (k), TDR (ε):

$$\underbrace{\frac{\partial}{\partial t}(\phi)}_{Time\ rate} + \underbrace{\frac{\partial}{\partial x_i}(u_i\phi)}_{advective} = \underbrace{-\frac{\partial}{\partial x_i}\left(\Gamma_\phi \frac{\partial \phi}{\partial x_i}\right)}_{diffusion} + \underbrace{S_\phi}_{source}$$

2) Transportation equation for m_i species:

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

3) Reaction kinetics:

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

$$R_{i,r} = M_{i,r}\left(v''_{i,r} - v'_{i,r}\right)\left(k \prod_{j=1}^{N} C_{j,r}^{\eta^*_{,rj}}\right)$$

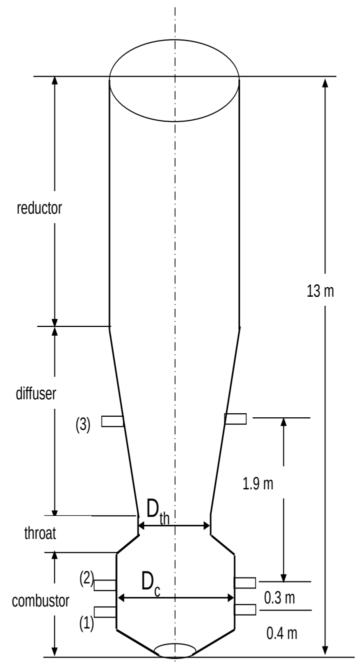
$$k = Ae^{(-E/RT)}$$

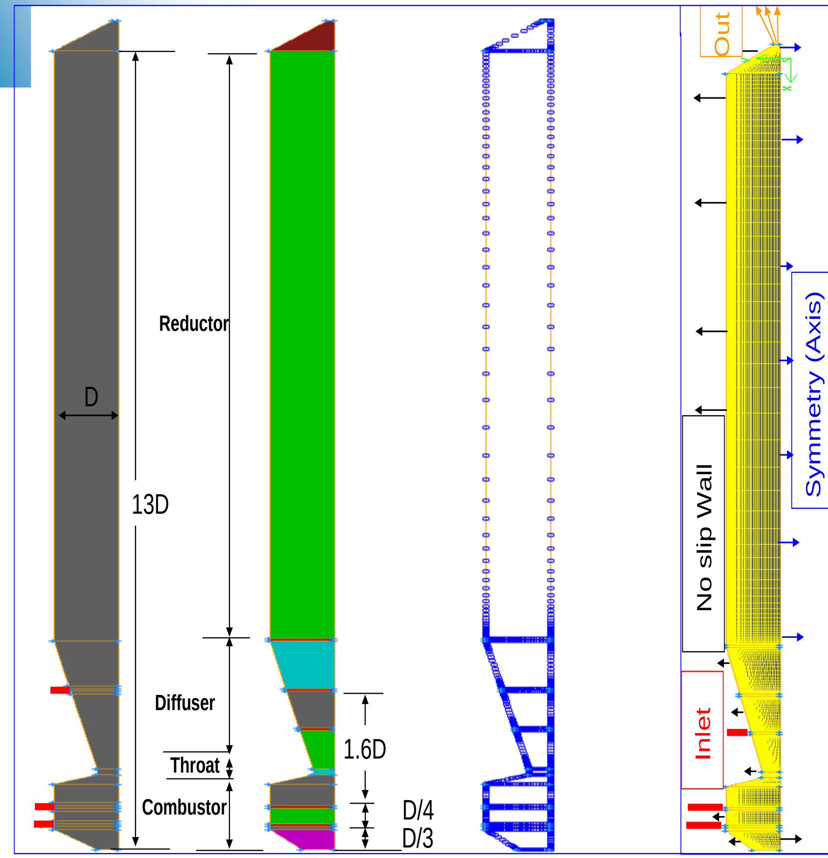
4) Discrete Lagrangian particle:

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

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

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





The procedure for the calculation of pulverized 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 determined during the previous particle calculation;
(d) Recalculate the discrete phase trajectories in the modified continuous phase flow field;
(e) Repeat the previous two steps until a convergence solution

HIGH FIDELITY SIMULATION

Geometry & Mesh Generation

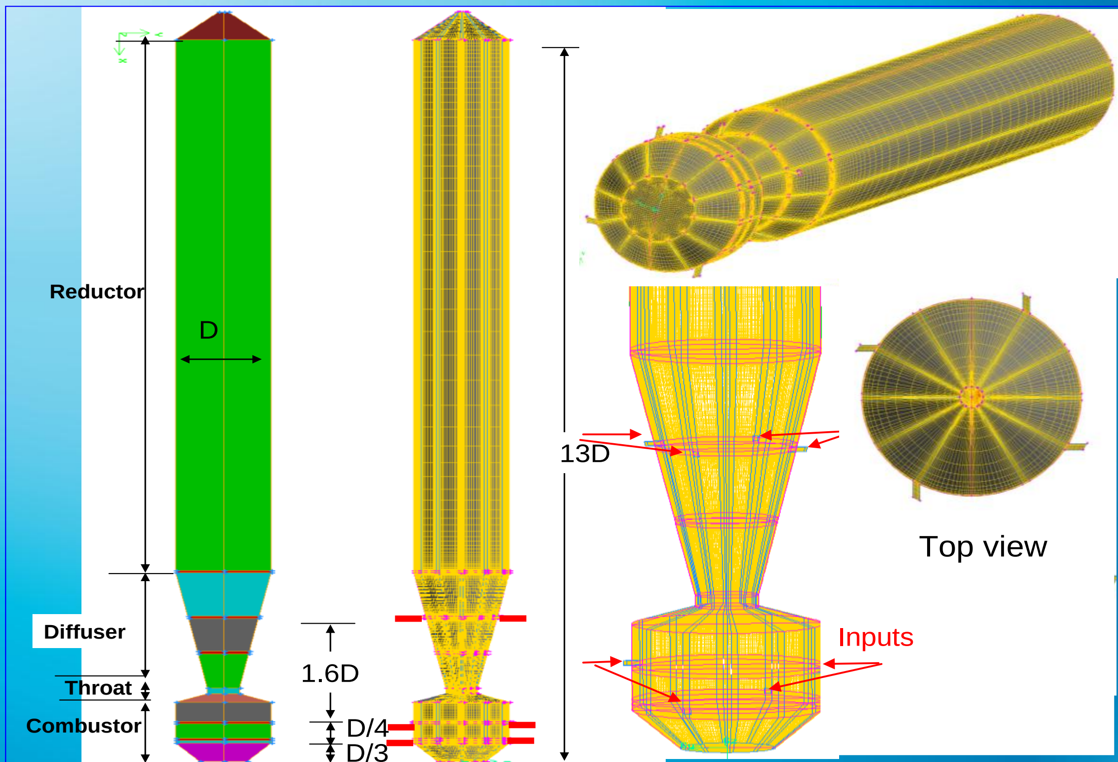


Figure 1: (a) 200t/d two-stage air blown gasifier and nozzle geometry showing blocking topology and the resulted 3D mesh. [Chen et al. and Bockelie et al]

Mesh Information

- The 3D mesh consists of 1,427,896 finite volumes.
- Fitted within 30 volumes of surface sweep with appropriate axial scaling.
- Boundary layer adjacent to the gasifier refractory walls.
- Sufficient near-wall resolution to allow for wall-function rather than direct resolution (i.e. $y^+<20$).
- Captures the exact gasifier topography.

Model Boundary and Operating Conditions

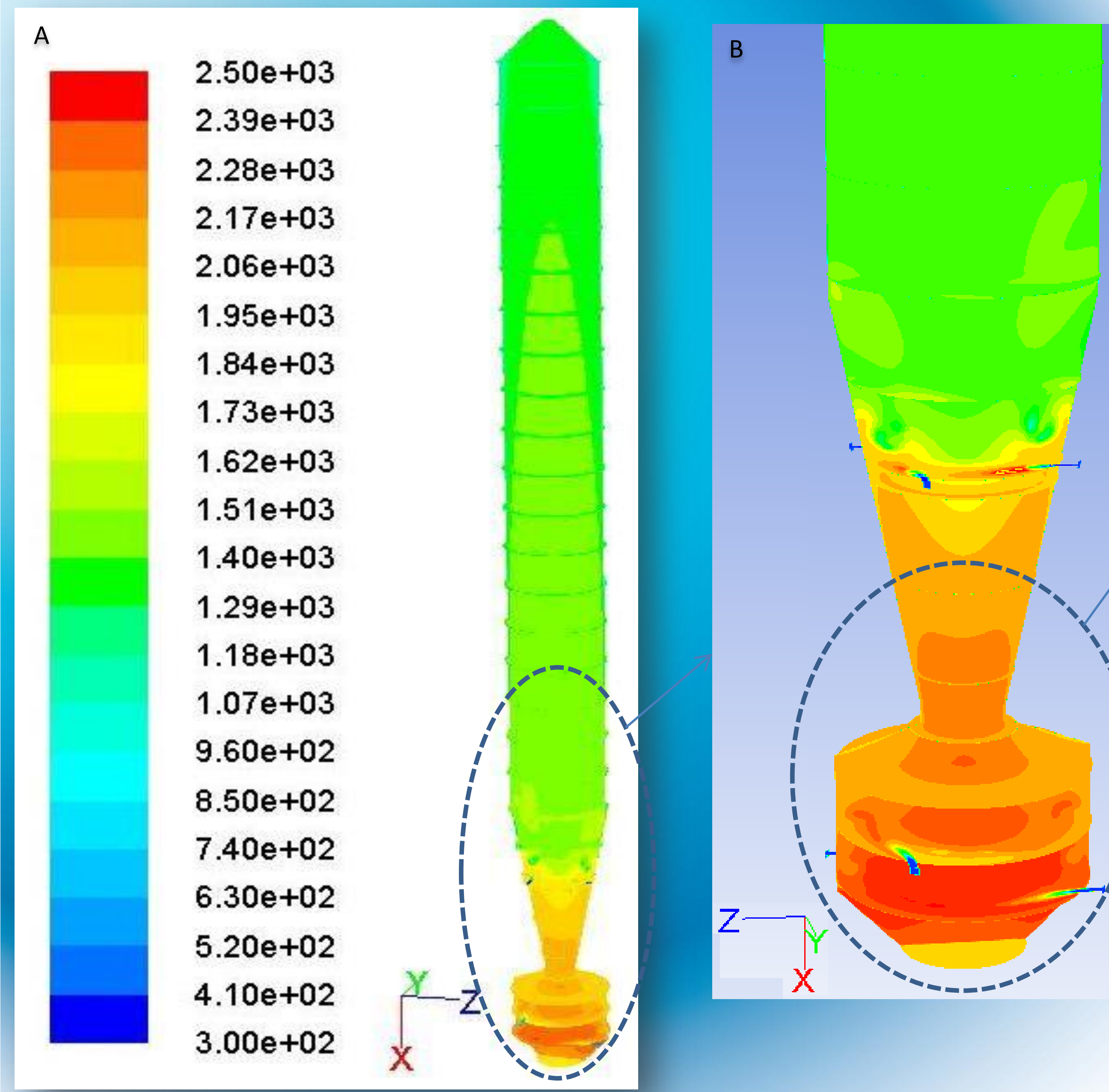
Selected Model Parameters & Operating Conditions:

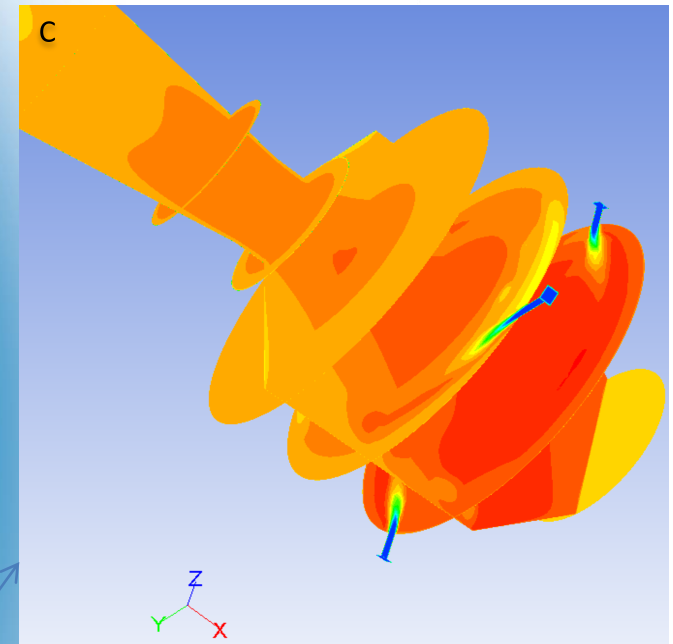
Feedstock Composition	Taiheiyo Bituminous Coal
Ultimate (wt%)	
C	77.6
O	13.9
H	6.5
N	1.13
S	0.22
Proximate (wt%)	
FC	35.8
V	46.7
M	5.3
A	12.1
HHV (MJ/kg)	27.4
Gas flow rate (kg/s)	
Combustor burners 1	4.708
Combustor burners 2	4.708
Diffuser burners	1.832
Particle loading (kg/s)	
Combustor burner 1	0.472
Combustor burner 2	1.112
Diffuser burner	1.832
Wall Temperature (K)	
Combustor	1897
Diffuser	1073
Reductor	873
Pressure (MPa)	2.7
Turbulence Model	K-e Standard

Modeled Reactions:

Volatile decomposition	$C_{0.87}H_{1.95}O_{0.26}N_{0.0245}S_{0.002} \rightarrow 0.239\ CO + 0.002\ H_2S + 0.443\ CH_4 + 0.027\ H_2O + 0.057\ H_2 + 0.012\ N_2 + 0.219\ C_{0.87}H_{0.13}$
CO Combustion	$CO + 0.5\ O_2 \rightarrow CO_2$
Water-gas shift	$CO + H_2O \leftrightarrow CO_2 + H_2$
H_2 Combustion	$H_2 + 0.5\ O_2 \rightarrow H_2O$
CH_4 Combustion	$CH_4 + 1.5\ O_2 \rightarrow CO + 2\ H_2O$
CH_4 Reforming CH_4 Reforming	$CH_4 + H_2O \rightarrow CO + 3\ H_2$ $CO + 3\ H_2 \rightarrow CH_4 + H_2O$
Tar Combustion	$C_{0.87}H_{0.13} + 0.902\ O_2 \rightarrow 0.87\ CO_2 + 0.065\ H_2O$
Tar Reforming	$C_{0.87}H_{0.13} + 0.87 H_2O \rightarrow 0.87 CO + 0.935 H_2$
Char Oxidation	$C_{(s)} + O_2 \rightarrow CO_2$
CO_2 Gasification	$C_{(s)} + CO_2 \rightarrow 2\ CO$
H_2O Gasification	$C_{(s)} + H_2O \rightarrow CO + H_2$
H_2 Gasification	$C_{(s)} + 2\ H_2 \rightarrow CH_4$

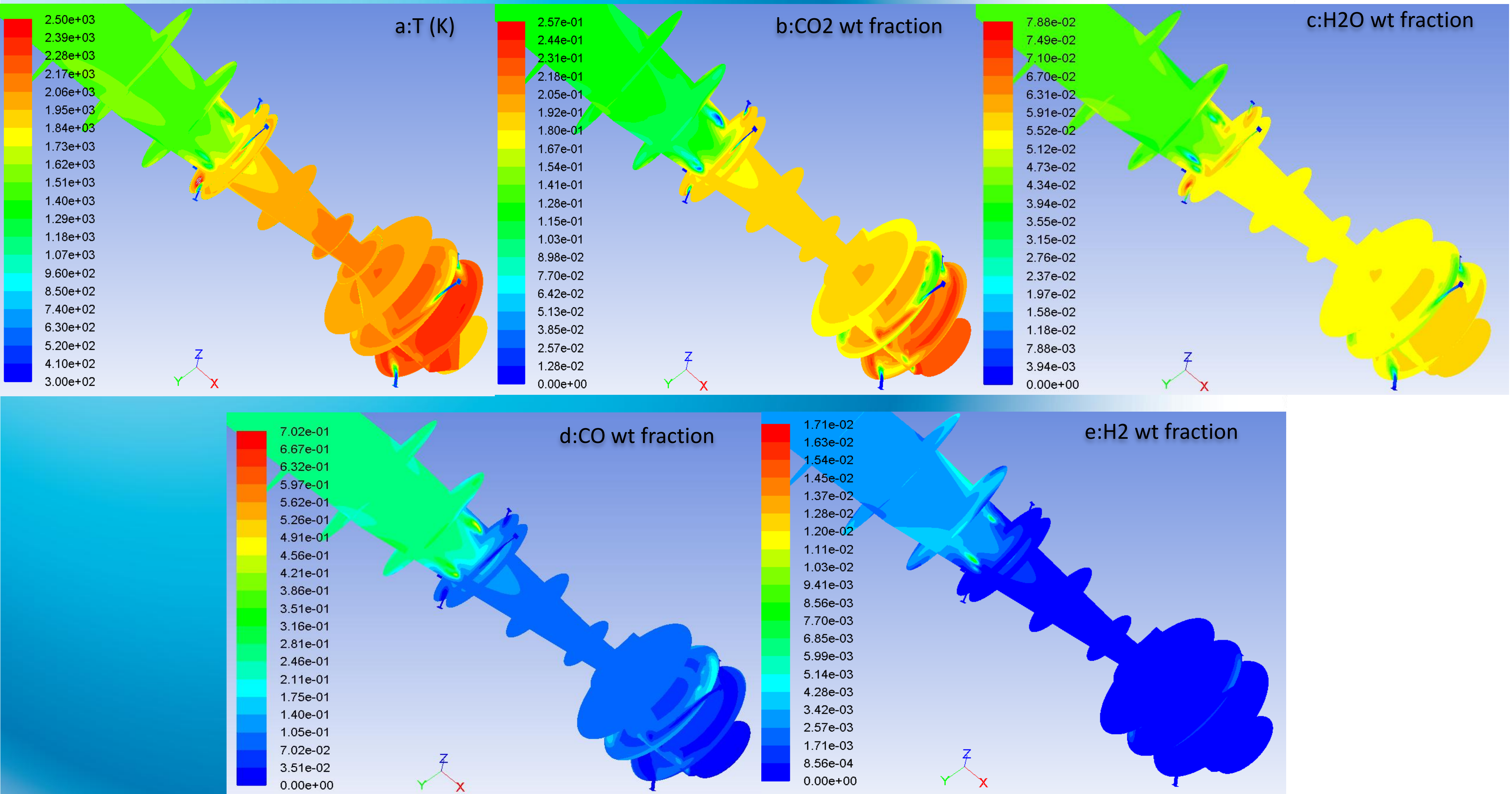
Model Sample Results



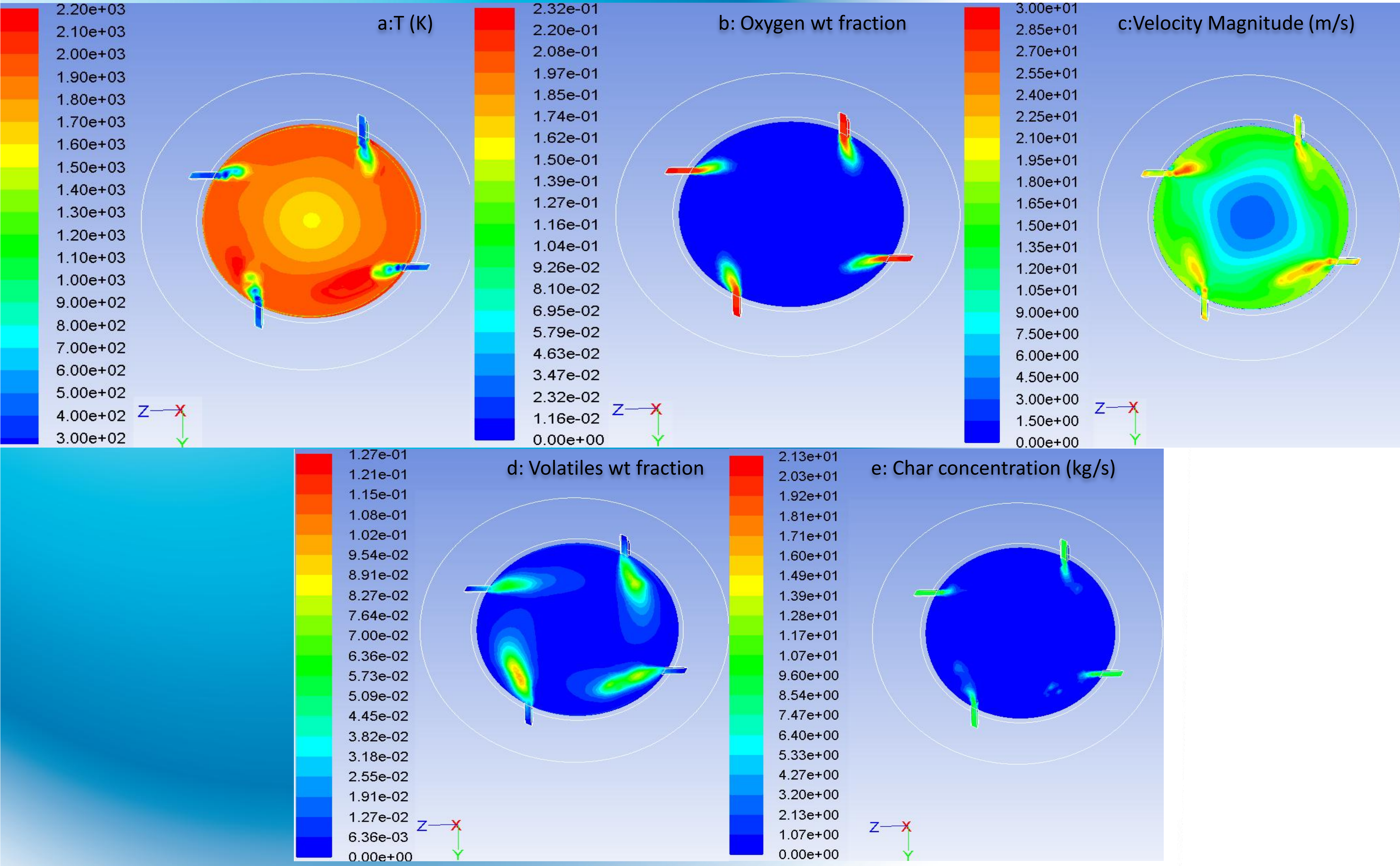


- Temperature field distribution. (a) Showing complete geometry. (b, C) Closer look at the combustor and diffuser.
- Average gasifier temperature = 1493 K

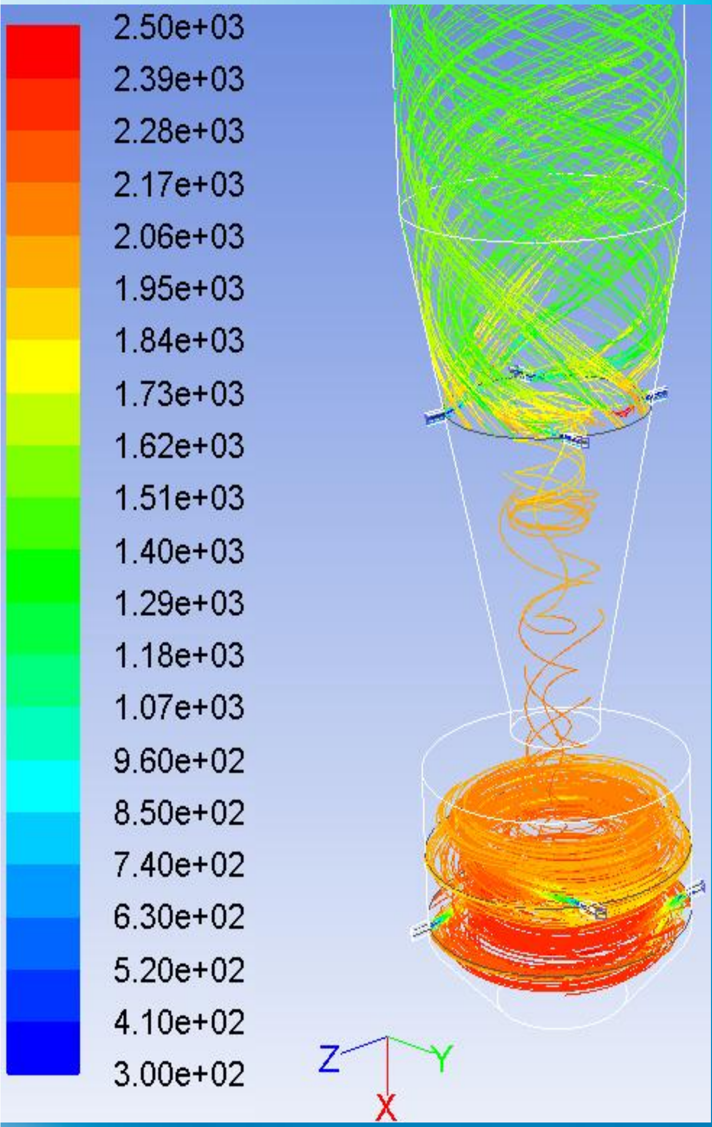
Model Sample Results



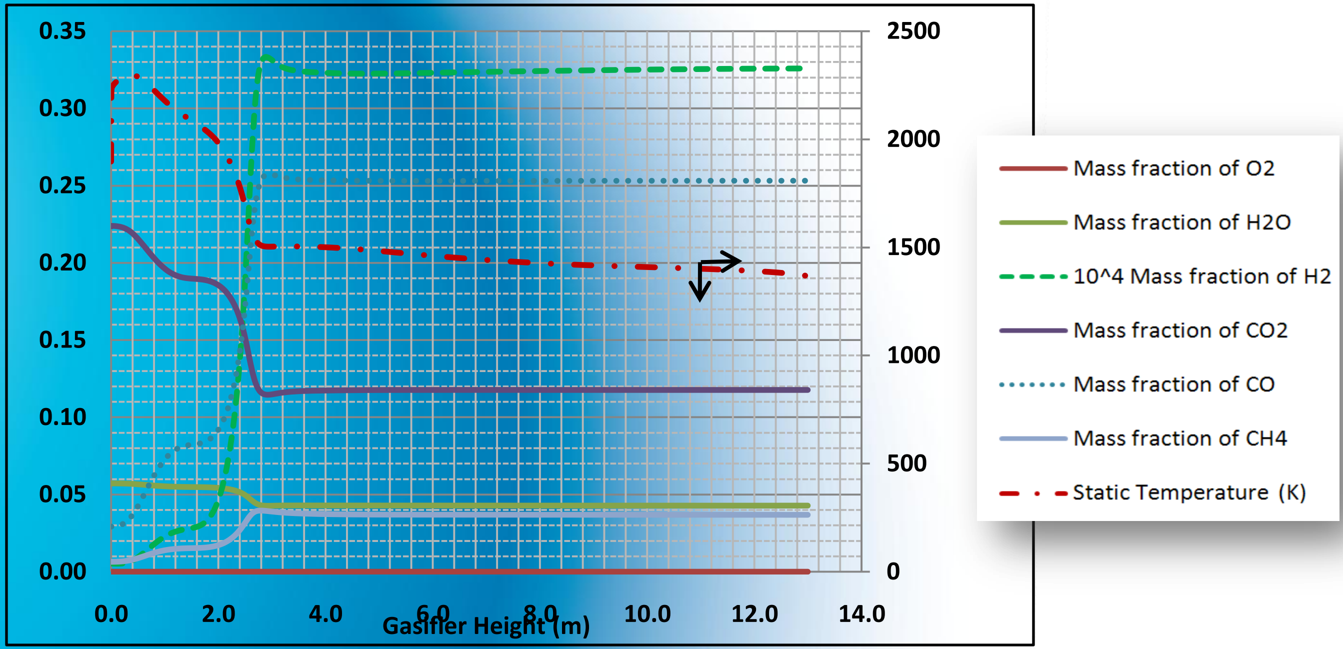
Model Sample Results



Model Sample Results



Particle temperature pathlines showing the effect of swirl.



Axial temperature and species profile along the center line of the gasifier.

Species	% Mass fraction	% Mole fraction
CO	0.253	0.235
H_2	0.003	0.042
CO_2	0.116	0.069
H_2O	0.043	0.062
CH_4	0.037	0.060
Tar	0.017	0.041
N_2	0.530	0.491

Produced gas composition at gasifier exit.

What you need to know

- Gasification 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.
- High fidelity analyses and simulations are needed at the conceptual level to increase the process efficiency and throughput.