Advancing Coal Catalytic Gasification to Promote Optimum Syngas Production

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Proposed Work

- Novel approach will be the use of red mud catalysts to improve the gasification process.
- Adding small fractions of biomass feedstock will help increase hydrogen content for quality syngas suitable for hydrocarbon synthesis.
- The proposed research will focus on:
  - bench-scale and pilot-scale experiments to measure key reactive properties,
  - developing kinetic models that predict the product formation, and
  - CFD modeling that incorporates the reaction kinetics for catalytic coal gasification.
- Collaboration consists of a unique team with expertise in experiments, modeling reaction kinetics, combustion and CFD of multiphase flows.

Specific Objectives

1. Measure syngas composition
   - Perform experiments to determine gas composition of sub-bituminous coal with red mud catalysts and modified with nickel
   - Investigate catalytic gasification to reduce methane
   - Add small quantities of biomass to increase hydrogen content of syngas
2. Model detailed reaction kinetics and product formation
   - Analyze reactions from catalytic gasification to understand major pathways involved
   - Identify necessary reaction mechanisms needed for the computational models
   - Implement reaction kinetics into MFIX CFD code.
   - Validate with the experiments

Summary

- Red mud promoted better cracking of char and tars into gas product compared to silica sand.
- Product gas yields obtained using red mud were higher than product gas yields from silica sand experiments.
- Gasification of coal improved with increasing temperature and addition of biomass feedstock.
- Gasification experiments provided data to develop a chemical kinetics model, and reaction rates were tuned for implementation into CFD.
- Coal gasification simulations using an earlier version of the lumped kinetic model demonstrated the need for parameter tuning to validated well with experiments.
- C3M-HPTR pyrolysis model validates well at 900°C but yields over-prediction of CO at lower temperatures.

Final kinetics models will be tuned according to co-gasification experiments and CFD input

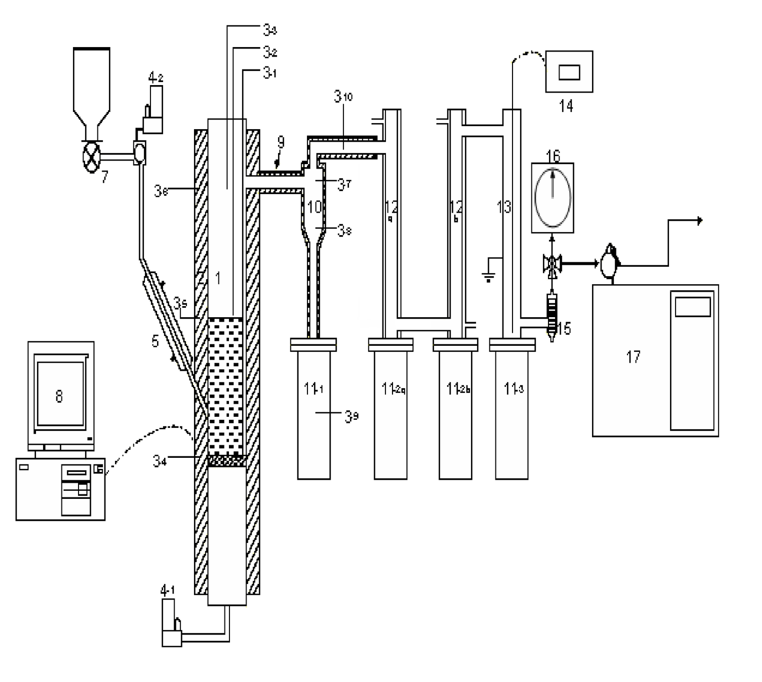
Gasification of Coal/Biomass Mixtures on RM

Sub-bituminous Coal CO_2, NO_X, and SO_X | Red Mud | Biomass

- Coal gasification is an alternative to mitigate pollutant emissions
- Blending coal with biomass allows to control the H_2 to CO ratio

Synthesis Gas – Electricity generation
Sub. Natural Gas – Substitute for diesel, petrol
Fischer-Tropsch – Hydrocarbons: gasoline, diesel
Chemical Feedstock – Methanol, ammonia

Bench-scale Fluidized Bed Reactor



1 - Fluidized bed reactor
3 - Thermocouple
4 - Mass flow controller
5 - Jacketed air-cooled feeder tube
6 - Hopper
7 - Screw feeder
8 - Computer
9 - Heating tape
10 - Hot gas filter
11 - Reservoir
12 - Condenser
13 - ESP
14 - AC power supply
15 - Filter
16 - Wet gas meter
17 - Gas chromatograph

Coal Gasification under Steam on RM

Product gases (mol, %) for coal gasification on RM under N_2 and under N_2 & Steam

Temp, °C	H_2 : CO	H_2	CH_4	CO	CO_2	C_2-C_4	O_2	N_2	Σ_{Gases}
Product gases for coal gasification on RM under N_2									
700	3.5 : 1	5.032	0.809	1.442	1.988	0.480	0.059	89.690	99.50
800	2.5 : 1	5.939	0.862	2.373	2.933	0.121	0.036	86.521	98.79
900	1.6 : 1	8.264	0.938	5.161	3.010	0.367	0.040	80.052	97.83
Product gases for coal gasification on RM under N_2 & Steam									
700	4.7 : 1	8.563	1.195	1.826	5.258	0.703	0.058	81.954	99.56
800	2.4 : 1	16.94	1.641	7.069	6.725	0.785	0.027	66.017	99.21
900	1.8 : 1	24.17	1.944	13.81	8.298	0.555	0.027	49.949	98.76

Product liquids, solids, and gases (wt, %)

	Coal on RM under N_2				Coal on RM under N_2 & Steam			
Temp, °C	Moist., %	Liquid	Solid	Gas	Moist., %	Liquid	Solid	Gas
700	24.19	29.58	43.20	27.22	23.96	19.36	54.06	26.58
800	24.33	27.57	42.78	29.65	22.52	17.08	40.81	42.11
900	24.94	20.97	29.61	49.42	21.55	13.94	31.87	54.19

Coal Gasification under CO_2 and Steam on RM

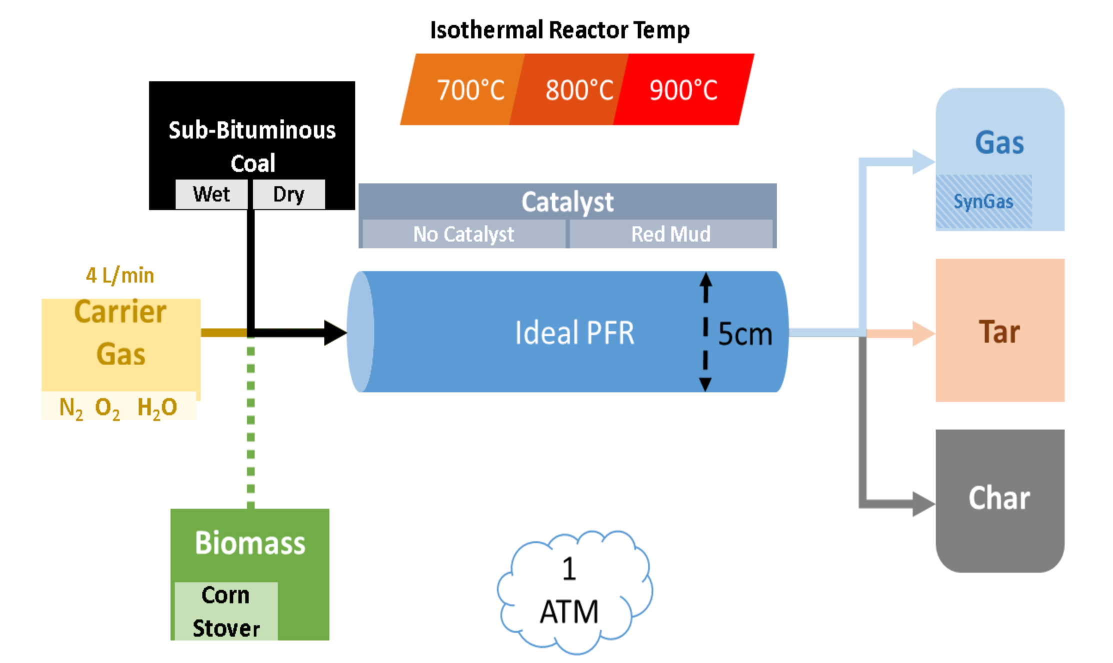
Product gases (mol, %) for wet coal gasification under N_2 and CO_2 on RM

Temp, °C	H_2 : CO	H_2	CH_4	CO
Product gases (mol, %) for wet coal gasification under N_2 on RM				
800	2.5 : 1	5.94	0.86	2.37
900	1.6 : 1	8.26	0.94	5.16
Product gases (mol, %) for wet coal gasification under CO_2 on RM				
800	1 : 3.1	6.11	1.81	18.97
Product gases for wet coal gasification on RM under N_2 & Steam				
800	2.4 : 1	16.94	1.64	7.07
900	1.8 : 1	24.17	1.94	13.81
Product gases (mol, %) for wet coal gasification under CO_2 and Steam on RM				
800	1 : 1.3	19.43	1.94	25.05
900	1 : 1.95	17.88	2.20	34.91

Product liquids, solids, and gases (wt, %)

Temp, °C	Moisture, %	Liquid	Solid	Gas by dif.
Wet Coal on RM under N_2				
800	24.33	27.57	42.78	29.65
900	24.94	20.97	29.61	49.42
Wet Coal under CO_2 on RM				
800	24.11	37.03	43.56	19.41
Wet Coal on RM under N_2 & Steam				
800	22.52	17.08	40.81	42.11
900	21.55	13.94	31.87	54.19
Wet Coal on RM under CO_2 and Steam				
800	24.90	26.34	34.03	39.63
900	21.99	15.84	5.76	78.40

Modeling the Kinetics of Product Formation



Kinetics Strategy and Reaction Network

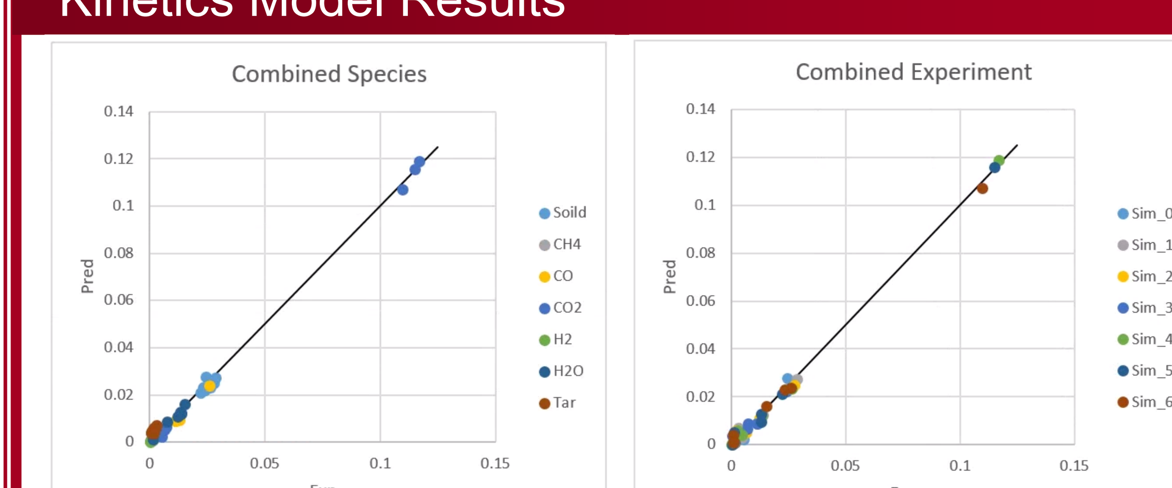
Lump	MW (g/mol)	Density (g/L)	OBJ Lump	OBJ Weight a
Coal	1000	1300	Solid	1
CharH (C2H)	25	2000		
CharC (C)	12	2000		
Tar	182	---	Tar	100
H_2O	18	---	H_2O	1
CH_4	16	---	CH_4	1
CO	28	---	CO	0.1
CO_2	44	---	CO_2	1
H_2	2	---	H_2	0.1

$$OBJ = \sum_{i}^{n} \left(\frac{exp_i - mdl_i}{exp_i * \alpha} \right)^2 = 1.47$$

Reaction	Type	logA	E*
Coal → a CharH + b CH_4 + c CO + d CO_2 + e H_2 + f H_2O	Pyrolysis	4.70	24.20
Coal → g Tar + h CO_2 + i H_2O	Pyrolysis	-0.37	1.69
Tar → j CharC + k CH_4 + l H_2 + m H_2O	Condensation	2.22	11.39
CharH → 2 CharC + ½ H_2	Pyrolysis	4.77	29.48
CharC + H_2O → CO + H_2	Gasification	-0.22	3.37
CharC + CO_2 → 2 CO	Gasification	-0.002	0.030
CharC + 2 H_2 → CH_4	Gasification	-6.77	9.93
CO + H_2O ↔ CO_2 + H_2	Water-Gas-Shift	2.45	1.22

a	25.8		e	10.8		i	4.4	m	1.1
b	1		f	0.11		j	11.5		
c	8.2		g	4.7		k	1.5		
d	1.9		h	1.3		l	0.45		

Kinetics Model Results

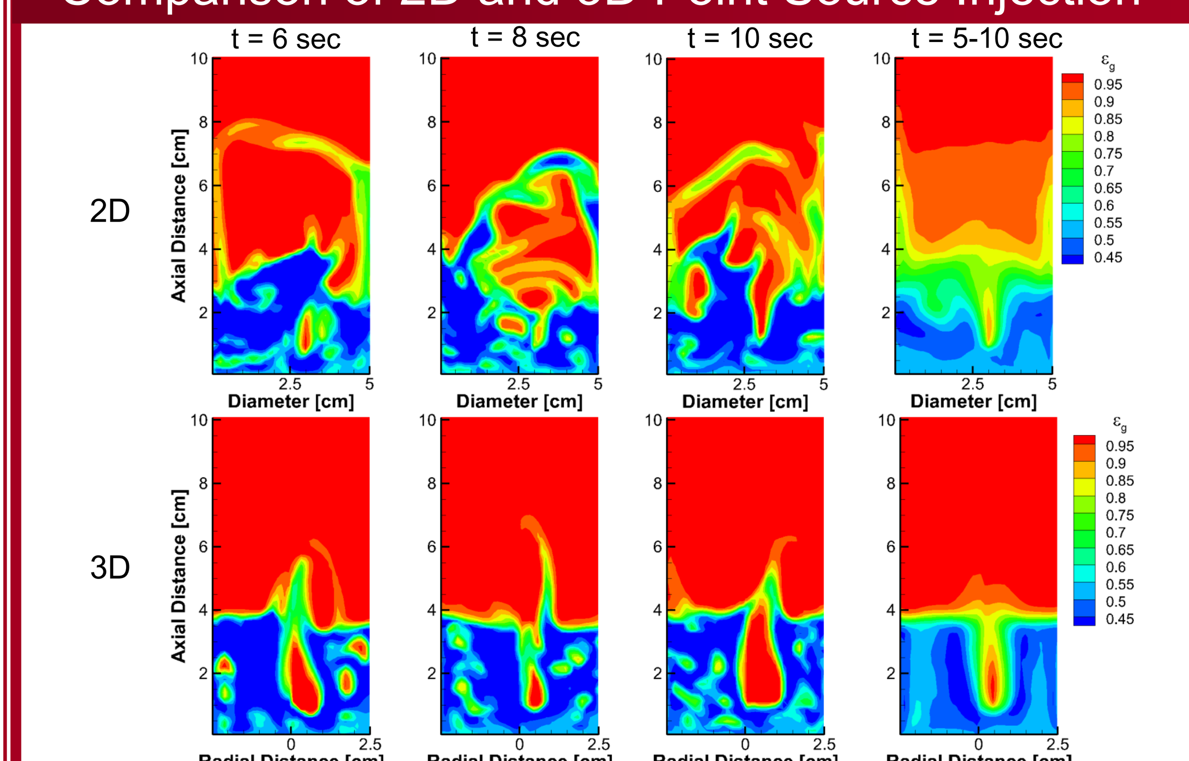


	Sim_0	Sim_1	Sim_2	Sim_3	Sim_4	Sim_6	Sim_6
Temp °C	900	700	800	900	700	800	900
Carrier Gas	N_2	N_2	N_2	N_2	CO_2	CO_2	CO_2
Fuel	Dry Coal	Wet Coal	Wet Coal	Wet Coal	Wet Coal	Wet Coal	Wet Coal

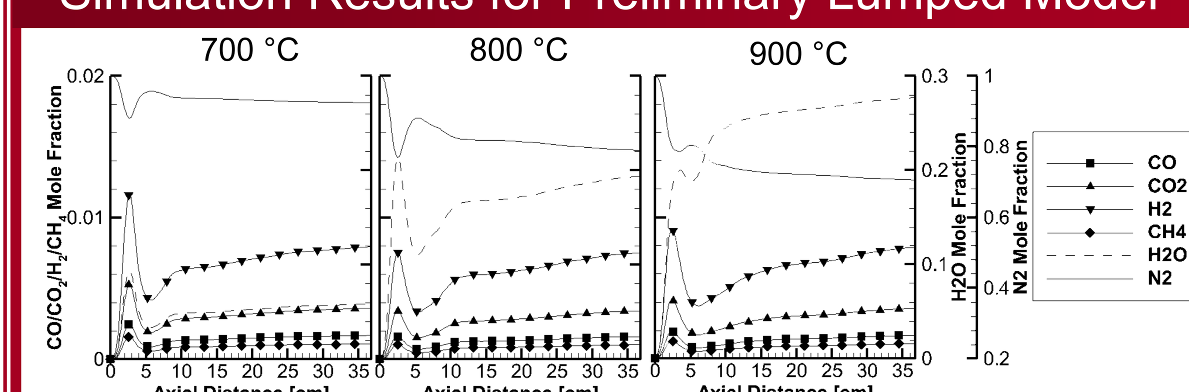
Computational Fluid Dynamics Simulations

- Simulations were performed in MFiX (2014-1) using the Two-Fluid (Eulerian-Eulerian) Model
- Coal is introduced directly into the sand bed using a point source strategy where experimental carrier stream velocities and mass flow rates are preserved
- Preliminary simulations were performed under an N_2 atmosphere implementing the lumped drying and pyrolysis reactions to assist in kinetics model tuning
- C3M-HPTR chemistry model was also tested because of fuel similarity

Comparison of 2D and 3D Point Source Injection



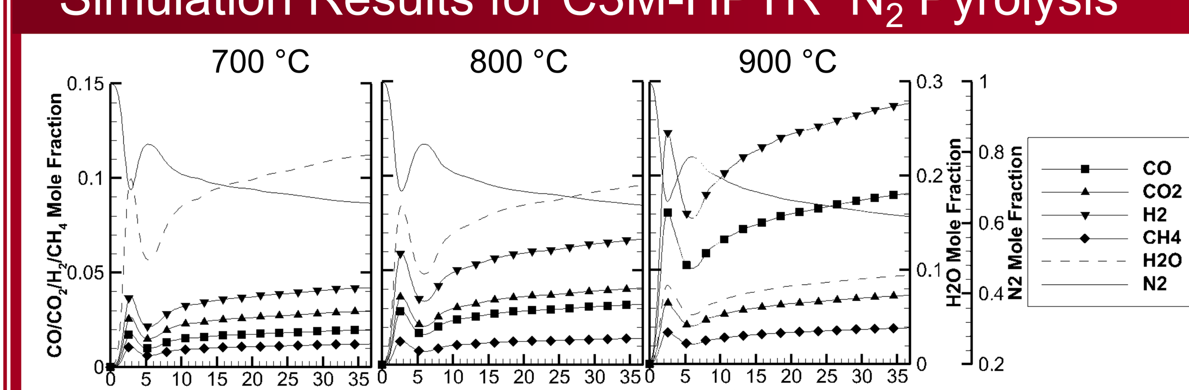
Simulation Results for Preliminary Lumped Model



Comparison of N_2/H_2O/Tar Free Gas Phase Mole Fractions and Relative Error

	700 °C			800 °C			900 °C		
	Exp.	Sim.	% RE	Exp.	Sim.	% RE	Exp.	Sim.	%RE
CO	0.190	0.118	38.2	0.209	0.118	43.8	0.318	0.118	63.8
CO_2	0.286	0.252	11.8	0.265	0.252	5.0	0.128	0.252	96.2
H_2	0.407	0.555	36.8	0.434	0.555	27.9	0.485	0.555	14.3
CH_4	0.118	0.076	36.1	0.092	0.078	17.6	0.068	0.078	11.1

Simulation Results for C3M-HPTR N_2 Pyrolysis



Comparison of N_2/H_2O/Tar Free Gas Phase Mole Fractions and Relative Error

	700 °C			800 °C			900 °C		
	Exp.	Sim.	% RE	Exp.	Sim.	% RE	Exp.	Sim.	% RE
CO	0.190	0.323	70.0	0.209	0.310	48.2	0.318	0.303	4.8
CO_2	0.286	0.239	16.4	0.265	0.172	35.2	0.128	0.137	6.2
H_2	0.407	0.329	18.8	0.434	0.417	3.9	0.485	0.463	4.7
CH_4	0.118	0.108	8.6	0.092	0.102	10.5	0.068	0.098	43.8