# Small-Scale Engineered High Flexibility Gasifier

DOE Award No. DE-FE0031531

2019 Annual Project review Meeting

*Crosscutting Research, Rare Earth Elements, Gasification Systems and Transformative Power Generation*

*Pittsburgh,PA*
*April 9-11,2019*

# Project Team

SOUTHERN RESEARCH

Santosh Gangwal, PhD – PI
Mikhail Granovskiy, PhD– Co-PI
Swananda Tupsakhre, PhD
Kevin McCabe

REACTION ENGINEERING INTERNATIONAL

Hong-Shig Shim, PhD
Martin Denison, PhD
Kevin Davis, PhD
Jost Wendt, PhD

unitel technologies
Your Partner in the Pursuit of Process Innovations

Ravi Randhava, PhD

# Project Goals

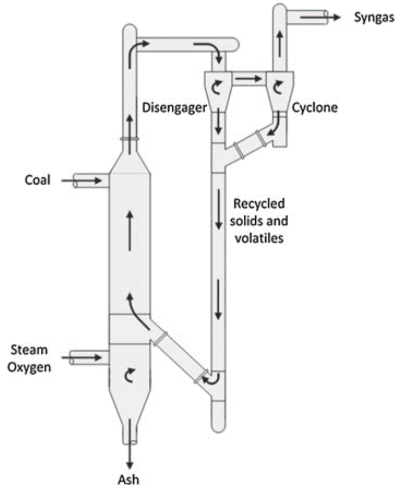
- Develop a fuel flexible and modular/shop fabricated oxygen-blown small-scale coal gasifier to produce medium BTU syngas with
  - Tar < 10 ppmw
  - Ammonia < 1 ppmv

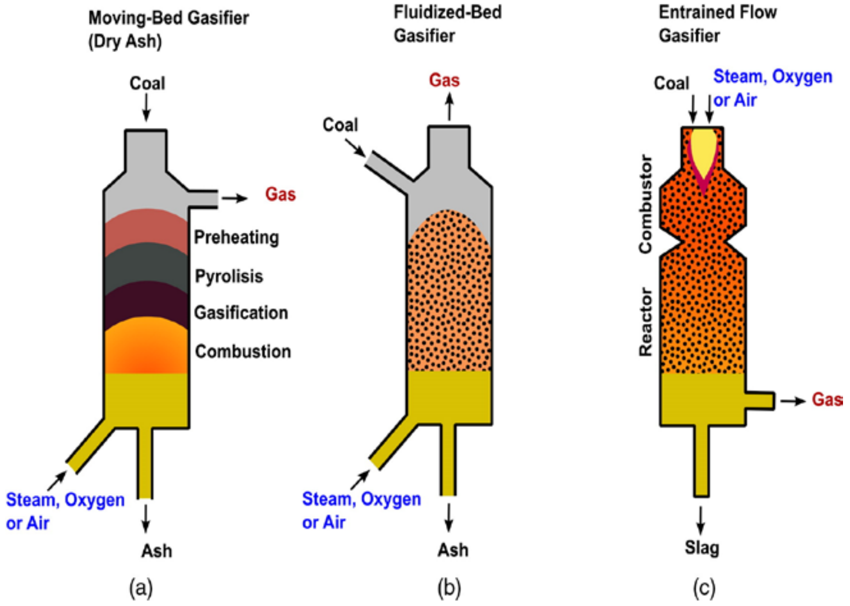
- Demonstrate gasifier performance to meet target at bench-scale (10-50 lb/h)

- Design a 1-5 MW combined heat and power (CHP) system and conduct a technoeconomic evaluation (TEA)

# Commercial Coal Gasifiers

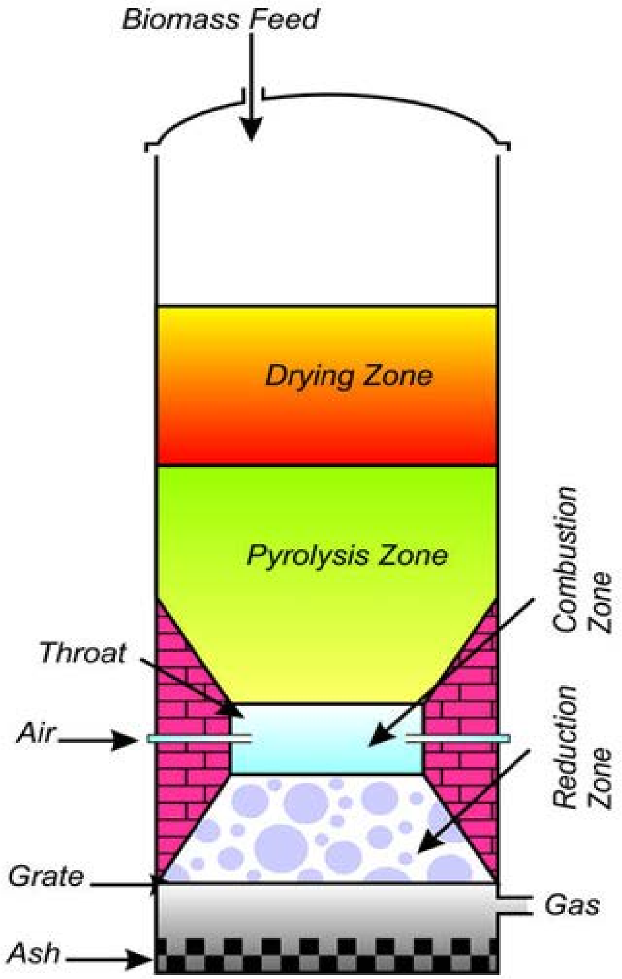
- Large scale commercial coal gasifiers
  - Entrained flow (GE/Texaco, E-Gas/CBI, Shell and others)
  - Updraft moving bed (Lurgi)
- Other large scale coal gasifiers
  - Fluidized bed
  - Transport
- Commercial small-scale coal gasifiers do not exist



# Small-scale Wood Gasifiers are Commercial

- Downdraft moving bed
  - Many small commercial installations
    - Air blown, sub-atmospheric
  - Used mainly for producing heat
  - Very few successful power applications, mostly 40 KWe or smaller
- Reduced tar formation
  - Volatiles pass through a combustion zone
  - Tar make is typically reduced to 100 ppmw
  - Ammonia typically not reported



# Downdraft Design Chosen for Project

- Develop oxygen-blown pressurized coal gasifier suitable for small scale distributed applications
  - Modular, standardized factory construction
- Construct computational model to optimize design
- Optimally designed to
  - Produce medium BTU syngas
  - Manipulate char make, quality, reactivity
  - Mitigate/reform tars, decompose $NH_3$
- Design for fuel flexibility – coal, biomass, MSW

# Comparison to State of the Art

| | State of the Art-commercial | This project |
|---|---|---|
| Fuel | Mostly wood | Non-caking coal |
| Scale | 40 KW | Bench-scale; Ultimate goal--1-5 MW |
| Oxidant | Air | Oxygen |
| Steam | No | Yes |
| Pressure | Subatmospheric | 3-5 atm |
| Gasification zone temp | ~750-800$^{o}$C | ~950-1100$^{o}$C |
| Feed flexibility | Low | High |
| Product flexibility | Mostly heat, char | Char, Heat, power, fuel, chemicals |
| Syngas | Low BTU | Medium BTU |
| Tar | 200 ppmw | 10 ppmw |
| Ammonia | Not reported | 1 ppmv |

# Project Tasks

- Computational modeling to optimize gasifier design
- Laboratory testing to obtain model input parameters
  - Chars produced at relevant gasification conditions
  - Gasification reactivity measurements to develop a kinetic expression
- Design and construct gasifier based on modeling results
- Commission & test gasifier, demonstrate performance, update computational model
- Design 1-5 MW energy conversion system
- Develop Aspen-based model for integrated 1-5 MW energy conversion system, conduct TEA

# Combination of High T and Char Catalysis are Keys

- Maintain 1000-1050$^o$C + for sufficient depth in gasification zone to fully reform tar and decompose ammonia. Is this possible?
- Based on literature Information
  - It can be concluded that essentially complete tar reforming should be achieved over coal chars at ~1000$^o$C within <1 sec [e.g. D.Fuentes-Cano et al., Chem Engg. J, 228 (2013) 1223]
  - Results from **multi-stage multi-vessel** biomass gasifier (pyrolysis-partial oxidation-char gasification) indicate that tar can be reduced to <15 ppmw [e.g. P.Brandt et al., Energy Fuels 2000, 14, 816]
- Our mass/energy balance and modeling efforts indicate that it is possible to maintain the required temperature in the gasification zone of our **simpler, single vessel** downdraft gasifier with proper management of the heat release from combustion

# PRB Coal Selected for Modeling and Testing

| | |
|---|---|
| Moisture | 24.29 |
| C | 52.32 |
| H | 3.95 |
| N | 0.8 |
| S | 0.26 |
| Ash | 4.99 |
| O by difference | 13.39 |
| Total | 100 |

Initial Ash Fusion temperature: 1210°C

Major Ash Components (Wt%)

| | |
|---|---|
| $SiO_2$ | 30.2 |
| $Al_2O_3$ | 15.4 |
| $Fe_2O_3$ | 5.9 |
| CaO | 24.3 |
| MgO | 4.8 |
| $SO_3$ | 13 |

# Mass Balance for Desired Wet Syngas Composition

| Input (lb/h) | | Output (lb/h) | |
|---|---|---|---|
| Coal | 25.00 | Syngas | 74.75 |
| steam | 36.70 | Char | 1.59 |
| Oxygen | 14.65 | | |
| | | | |
| Total | 76.34 | | 76.34 |

| | vol %** | Wt % |
|---|---|---|
| $CO_2$ | 7.1 | 16.3 |
| CO | 20.2 | 29.5 |
| $H_2$ | 18.1 | 1.9 |
| $H_2O$ | 54.6 | 52 |
| $N_2$ | | 0.27 |
| $H_2S$ | | 0.05 |
| Total | 100 | 100 |
| | ** N,S free | |

S/C = 1.47

O/C = 0.59

# Gasification Kinetics

- Steam and CO2 gasification measurements were made on chars produced  by pyrolysis under various time and temperature conditions using TGA
- These data were used to develop a best fit rate equation
- Two kinetic equations from recent literature were used:
  - Wang, Y, D. A. Bell "Competition between $H_2O$ and $CO_2$ during gasification of Powder River Basin coal" Fuel 187 (2017) 94-102.
  - Umemoto, S., Kajitani, S., Hara, S., "Modeling of coal char gasification in coexistence of $CO_2$ and $H_2O$ considering sharing of active sites," Fuel 103 (2013) 14-21.
- Best fit parameters were determined by non-linear optimization (Matlab)

# Kinetic Equations

$$\frac{dX}{dt} = \left\{\frac{K_1 p_{H_2O}}{1 + K_2 p_{H_2O}} + (1 - \theta_{H_2O})\frac{K_4 p_{CO_2}}{1 + K_4 p_{CO_2}}\right\}(1 - X)\sqrt{1 - \Psi ln(1 - X)}$$

Wang and Bell Competing Sites Model

$$\frac{dX}{dt} = \left\{\frac{K_{21} p_{H_2O}}{1 + bcK_{12} p_{CO_2} + bcK_{13} p_{CO} + K_{22} p_{H_2O}} + \frac{K_{11} p_{CO_2}}{1 + K_{12} p_{CO_2} + K_{13} p_{CO} + \frac{a}{c} K_{22} p_{H_2O}}\right\}(1 - X)\sqrt{1 - \Psi ln(1 - X)}$$

Umemoto Shared Active Sites Model

# Umemoto Shared Sites Equation Provided a Better Fit

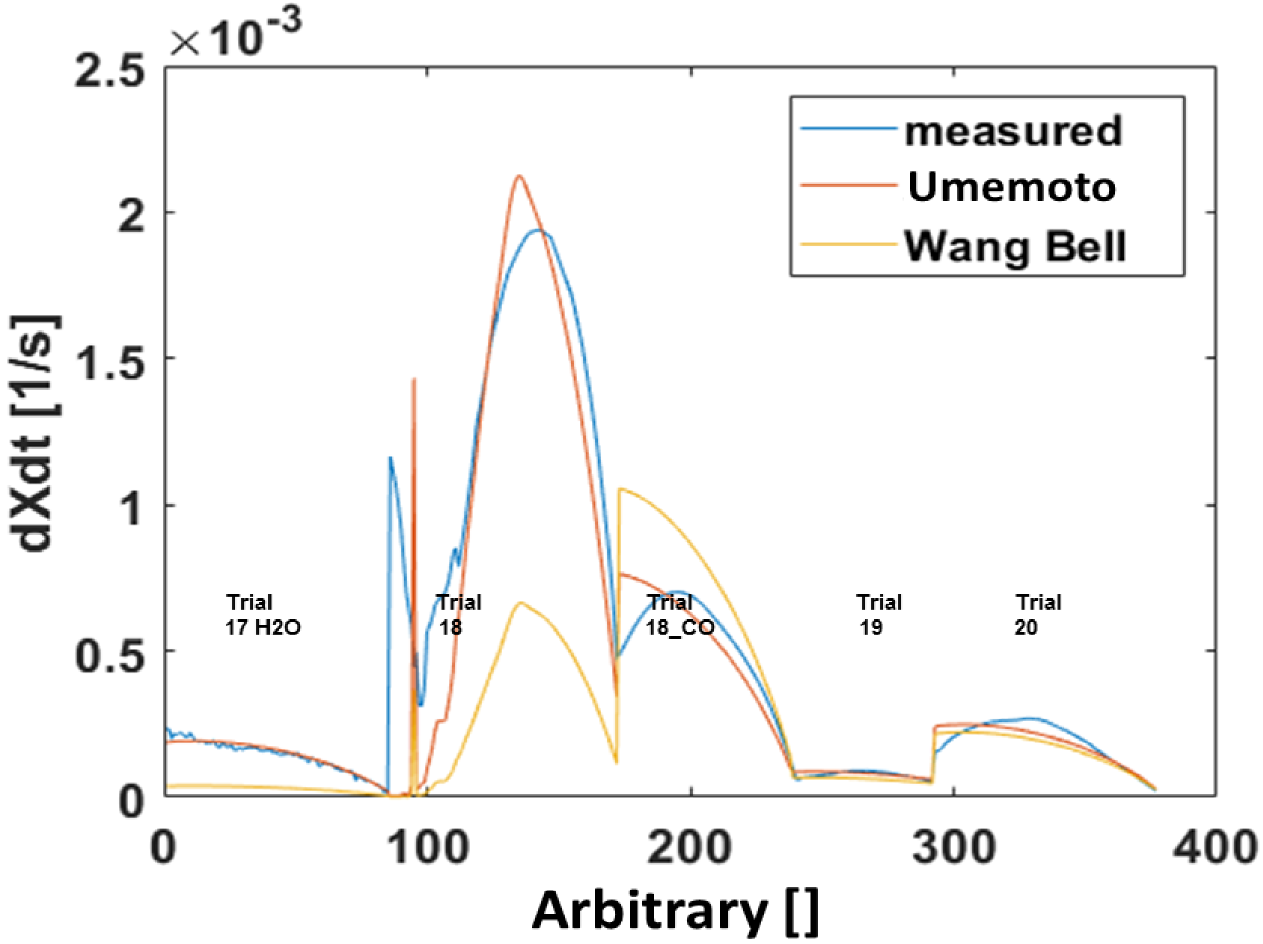



*Figure 1. Kinetics model fits for Umemoto and Wang Bell for 5 trials data sets*

*Optimal kinetic model parameters for Umemoto model*

| | |
|---|---|
| $A_{11}$ | 2.65e9 |
| $A_{12}$ | 9.451e7 |
| $A_{13}$ | 2989 |
| $A_{21}$ | 1.001e9 |
| $A_{22}$ | 2.681e12 |
| $A_{23}$ | 0.1620 |
| $E_{11}$ | 231.3 |
| $E_{12}$ | 129.70 |
| $E_{13}$ | 20.521 |
| $E_{21}$ | 206.4 |
| $E_{22}$ | 236.6 |
| $E_{23}$ | 280.3 |
| a | 0.999995 |
| b | 4.0645e-05 |
| $\Psi_1$ | 4.2980 |

# REI Modeling Effort

- Based on prior work REI employed a two-stage approach to modeling the SR modular gasifier
  - **Stage 1** adapted an existing, one-dimensional, zonal model. The purpose of the zonal model was to help establish process parameters, rather than details of the micro processes and mixing within each zone (addressed in Stage 2).
  - **Stage 2** used a porous-media CFD approach to explore multi-dimensional mixing of injected oxygen & steam into the porous bed
- 15 cases involving variations in amounts and positions of steam and oxygen injection were investigated. Gasifier exit results are presented for cases 8 and 9. Modeling effort is complete. Models will be adjusted by REI for scale up based on bench-scale gasification results

# Exit Conditions from Gasifier Model Results

| | Case 8 | Case 9 |
|---|---|---|
| Temperature, °C | 456 | 466 |
| H2, % vol wet | 16.66 | 15.06 |
| CO, % vol wet | 20.87 | 18.12 |
| CO2, % vol wet | 6.29 | 7.16 |
| H2O, % vol wet | 55.79 | 59.40 |
| CH4, % vol wet | 0.154 | 0.052 |
| Gas Mass Flow, kg/s | 0.00885 | 0.00974 |
| Density, $kg/m^3$ | 0.957 | 0.954 |
| Volume Flow, actual $m^3/s$ | 0.009247 | 0.01021 |
| Char Mass Flow, kg/s | 5.99e-5 | 4.55e-5 |
| Carbon Content, % | 42.2 | 32.0 |

# Work in Progress

- Based on the kinetic studies and modeling efforts, a design of the 25 lb/h modular gasifier has been carried out.  The design is highly flexible to achieve the desired syngas composition, guided by the model.
- Discussions were initiated with experts at Unitel and TR Miles, inc, and CUNY for assistance with critical components, in particular, for gasifier start up, selection of coal feeder, char withdrawal, materials of construction, temperature measurements within gasifier.  Balance of plant components have been determined, they are fairly straight forward and will be obtained from commercial vendors
- Gasifier construction task  is about 4 months behind because of move of our laboratory from RTP to Birmingham, Alabama.  A site has now been established at the  new location.
- Aspen simulations and preliminary TEA efforts have been carried out.  TEA indicates reduced cost due to standard factory components.  Potential sale of char byproduct can make small distributed systems economical

# Conclusions and Future Work

- Modeling efforts and flexible input capability for oxygen and steam have confirmed the ability to manipulate temperature distribution within gasifier and achieve the desired syngas composition, char composition, tar, and ammonia levels.
- Gasifier design and construction will be completed and testing should begin in late 2019.

# Disclaimer

This presentation was prepared as an account of work sponsored by an agency of the United States Government (DOE-NETL, Office of Fossil Energy). Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

# Thanks for Listening!  Questions?

REACTION ENGINEERING INTERNATIONAL

SOUTHERN RESEARCH

Solving the world's hardest problems.

unitel technologies

Your Partner in the Pursuit of Process Innovations