

Slag Characterization and Removal Using Pulse Detonation Technology During Coal Gasification

**Quarterly Report
January 1 - March 31, 1998**

**By
Ziaul Huque; Daniel Mei
Paul O. Biney; Jianren Zhou**

Work Performed Under Contract No.: DE-FG22-95MT95010

For
U.S. Department of Energy
Office of Fossil Energy
Federal Energy Technology Center
P.O. Box 880
Morgantown, West Virginia 26507-0880

By
Department of Mechanical Engineering
Prairie View A&M University
P. O. Box 397
Prairie View, Texas 77446

Disclaimer

This report was prepared as an account of work sponsored by an agency of the United States Government. 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.

QUARTERLY RESEARCH REPORT
(Reporting Period: 01/01/98 - 03/31/98)

ON

**Slag Characterization and Removal Using Pulse Detonation Technology During
Coal Gasification**

Program Identification Number: DE-FG22-95MT95010 -09

Submitted To:

**Document Control Center
U.S. Department of Energy
Pittsburgh Energy Technology Center
P.O.Box. 10940, MS 921-143
Pittsburgh, PA 15236-0940**

Submitted By:

**Dr. Ziaul Huque, Dr. Daniel Mei,
Dr. Paul.O. Biney and Dr. Jianren Zhou**

**Department of Mechanical Engineering
Prairie View A&M University
P.O.Box. 397
Prairie View, TX 77446**

Tel: (409)-857-4023 Fax: (409)-857-4395

April 30, 1998

Abstract

The main activity in the first quarter of 1998 was concentrated on understanding the detonation code, so that it can be linked with the in-house CFD code NPARC for simulation. The objective is to obtain the velocity and pressure distribution inside the detonation tube and compare with the experimental data that we have obtained from the experiments. Once the code is validated, the simulation will be extended to obtain the pressure and velocity fields in the large chamber, i.e., outside the exit of the detonation tube where the slag samples are attached.

Introduction

Pulse detonation technology takes advantage of the gas dynamics and thermodynamic processes associated with detonative combustion for use in propulsive systems, energy conversion, materials production, waste disposal, and thermal coatings applications. Another possible industrial application of pulse detonation technology is the removal of slag deposits on the utility boiler tubes. The technology is based upon the rapid combustion via a detonation wave of a pre-mixed fuel/oxidizer mixture contained in a tube, which is open at one end and closed at the other. The fuel/oxidizer mixture is introduced at the closed end and is detonated once the tube is completely filled. The detonation produces a high pressure and temperature reservoir of combustion products. Once the high-pressure combustion products have expanded out the open end, the process is repeated in a rapid, cyclical manner, producing a quasi-steady flow of high pressure and temperature products. The present project is studying the feasibility of using pulse detonation wave in removing boiler slag deposits as an efficient and cheap alternative to conventional slag removal methods.

Results and Discussion

During this period the research is focused on developing a numerical system to simulate the pressure and velocity fields developed due to the generation of the detonation wave. For the purpose we are using numerical codes. This system works by linking two separate codes one is (Pulse Detonation Engine) PDE code and other is (Computational

Fluid Dynamics) CFD code. These two codes work in tandem i.e. output of one is frozen and is utilized as initial condition for the next. The two codes are:

- 1-D code based on algebraic model which processes the detonation chemical reaction and predicts the properties of PDE.
- 2-D/ 3-D CFD code NPARC (obtained from NASA) to calculate the velocity and pressure fields

Currently we are on the process of understanding the 1-D detonation code. The following are what the detonation code does.

Working of 1-D Code :

The 1-D code starts with pulse.f program file which takes the input for the problem to be analyzed. These input parameters are:

- Fuel Option
- Inert Gas Concentration
- Geometry
 - Chamber Length.
 - Chamber Cross-Section Area.
 - Ignition Location.

□ Initial Condition

- Temperature of Unburned Reactant.
- Free Stream Pressure.
- Initial Mach No.
- Pressure Ratio Reactant to Free Stream.

□ Chemical Reaction

- Fuel Oxidizer Equalance Ratio.
- Percent Combustion.
- Gamma of Unburned Reactants.
- Gamma of Burned Products.

These input parameters are then transferred to a subroutine called combust (combust.f file for combustion) . The function associated with this subroutine are:

- Setting the terms associated with the various fuel.
- Finding the molecular weight and heat of formation of stoichiometric product (excluding N₂).
- Finding the stoichiometric and actual fuel to oxygen mass ratio.

- Finding mass fraction of fuel, oxygen, nitrogen and product before and after reaction.
- Calculating the change in zero point energy.
- **Calling subroutine deton (for detonation) or deflag (for deflagration) based on specified parameters.**
- Determining the time, pressure thrust and thrust for curves.
- Calculating average thrust and specific fuel consumption.
- Estimating average temperature at exit and wall.
- Returning the values to pulse.f program.

One of the functions of subroutine combust (as separate file combust.f) is to call the sub-subroutine deton (for detonation) or deflag (for delagation). The function associated with these sub-subroutines are almost same except the equations for the process are different.

These functions are:

- Finding the PULSE modal properties.
- Calling the subroutine thrustpeq and pulseth.
- Estimating duration of lag, pulse, steady state, decay and refill
- Estimating the thrust contribution of each.

The PULSE modal properties (pressure, temperature etc.) are calculated on the following states:

- Behind the detonation wave.
- Behind ignition expansion

- At wall after reflected detonation wave.
- At exit during evacuation expansion
- At the exit after reflected evacuation expansion
- On the wall after evacuation expansion reflection.

The function of these subroutine thrustpeq and pulseth that deton subroutine calls are to calculate ideal thrust parameters and average properties (pressure,temperature, pressure thrust and their ratios) respectively.

All the calculated data are then returned to pulse.f which generates output file of PDE code. The out are:

- Speed of ignition pulse head and tail.
- Lag, Pulse, Steady, Decay, Refill valuse of Time, Mass Flow and Exit thrust.
- Pressure ratio, Temperature ratio, density ratio and Mach no of different states during the process.
- Exit wall temperature.
- Thrust, Specific Fuel Consumption and Specific Thrust.

In order to see the effect of varying the input parameter on the output we have initially simulated the program by changing only two parameter for input. These are:

- Fuel option
- Ignition length. (which is in the form of ratio to whole chamber length).

EFFECT OF CHANGE IN FUEL & IGNITION POINT

FUEL	IGNITION LOCATION	SFC	Max. PRESS. RATIO	EXIT TEMP.	THRUST (LB)	MACH #
HYDROGEN	0	0.729314	38.85	2541	54257.1	1.0
DO	0.25	0.811351	DO	2663	48771	DO
DO	0.5	0.914184	DO	2373	43285	DO
DO	0.75	1.04687	DO	3180	37798.9	DO
JP4	0	1.75213	44.51	2610	70056.9	DO
DO	0.5	2.18888	DO	2325	56081.6	DO
DO	0.75	2.5004	DO	2325	49093.9	1.0
ACETYLENE	0	1.70846	53.2	6574	49093.9	1.0
DO	0.5	2.12512	DO	6574	63357	1.0
DO	0.75	2.42	DO	6574	55631.6	1.0

The results that we are getting are not reasonable because practically the Mach No. should have higher value i.e. more than one. Thus our current emphasis is to work for correction of these problems. Besides this we are also trying to understand how the output of this code is used to start the CFD code. We expect to furnish the analysis by the end of June, 1998.

Conclusion

Currently we are working on understanding the algorithm and simulation of the PDE code. As of now we are not getting the expected results, specifically the maximum Mach NO. Efforts are underway to resolve this problem.