

Catalytic Combustor for Fuel-Flexible Turbine

Technical Progress Report

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ABSTRACT

Under the sponsorship of the U. S. Department of Energy's National Energy Technology Laboratory, Siemens Westinghouse is conducting a three-year program to develop an ultra low NO_x, fuel flexible catalytic combustor for gas turbine application in IGCC. The program is defined in three phases: Phase 1- Implementation Plan, Phase 2- Validation Testing and Phase 3 – Field Testing. The Phase 1 program has been completed. Phase II was initiated in October 2004.

In IGCC power plants, the gas turbine must be capable of operating on syngas as a primary fuel and an available back-up fuel such as natural gas. In this program the Rich Catalytic Lean (RCL™) technology is being developed as an ultra low NO_x combustor. In this concept, ultra low NO_x is achieved by stabilizing a lean premix combustion process by using a catalytic reactor to react part of the fuel, increasing the fuel/air mixture temperature.

In Phase 1, the feasibility of the catalytic concept for syngas application has been evaluated and the key technology issues identified. In Phase II the catalytic concept will be demonstrated through subscale testing. Phase III will consist of full-scale combustor basket testing on natural gas and syngas.

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EXECUTIVE SUMMARY

The Rich Catalytic Lean (RCL™) technology, Figure 1, is being developed as an ultra low NO_x gas turbine combustor for Integrated Gasification Combined Cycle (IGCC). In this concept, ultra low NO_x is achieved by stabilizing a lean premix combustion process by using a catalytic reactor that produces a nominal gas temperature increase in the fuel/air mixture (by converting part of the fuel).

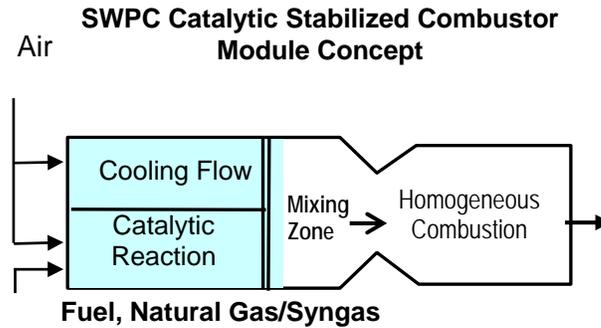


Figure 1 – SWPC Catalytic Stabilized Combustor

A key challenge in developing a fuel flexible catalytic combustor is the ability to provide one base design that will accommodate the different process flow conditions that are indicative of different IGCC plant designs. Cold vs hot gas cleaning, degree that the gas turbine is integrated with the IGCC plant and how the plant might be optimized for efficiency vs power output all impact the process flows that must be managed within the combustor. In Phase 1, the feasibility of the concept for syngas applications was evaluated, benchmarked and a validation test program (Phase 2) is defined. Specifically,

Catalytic module and combustor design concepts are defined for fuel flexible operation which minimize changes to the current catalytic reactor design, thus retaining the product of prior engineering and development. The proposed module design options are summarized in Table 1. In phase 2 these design options will be evaluated in detail.

Table 1 – Summary of Catalytic Combustor Design Options for IGCC

Concept Approach	Syngas Operation	Natural Gas Operation
No change to the current catalytic module design.	Options include staging or bypassing syngas and nitrogen to increase fuel conversion on the reactant side.	No impact
No change to the current catalytic	Syngas air split can be optimized but will require	No impact

module design. Utilize an eductor to control air split.	higher syngas pressure to drive the eductor.	
Modify current catalytic module for syngas.	Can be optimized for syngas conversion.	Requires device to control air split during natural gas operation.

During Phase II these concepts will be developed and tested. The catalytic combustor and module product definition will be further developed for the IGCC W501FD engine application. The focus will be on improvements required for syngas and the higher firing temperature of the W501FD engine. Highlights of this phase of the project were testing of SWPC catalytic coatings on natural gas and syngas, down selection of an alternative catalytic coating, redesign and testing of the baseline catalytic module with dual fuel capabilities for natural gas and syngas and development of alternative reactor concepts.

TASK II.2 – FUEL FLEXIBLE CATALYST DEVELOPMENT:

Because the RCL combustion design does not have a preburner, light off temperature is critical to successful operation. Light off is defined as the temperature at which the catalyst surface initially becomes active. Once the catalyst is lit it will remain active even if the temperature is reduced below the initial light off temperature. Testing in the combustor basket rig has shown that combustor dynamics are high at loads in excess of 80% when the catalyst was not active. To insure sufficient margin, the target light off temperature was set to be 50% load on the SGT-6-5000F engine. This corresponds to an inlet temperature of roughly 350 C. All catalyst coatings are initially screened for light off. Those with acceptable light off are then tested for durability. All coatings are compared to the baseline coating developed by Precision Combustion Inc. (PCI). The PCI coating light off is consistently between 300 and 330 C.

The main development focus for this program has been traditional coatings, ceramic washcoat with precious metal catalyst. The PCI coating is an example of a traditional catalytic coating. The catalyst is applied to a Haynes 230 tube. Haynes 230 was chosen because of its resistance to oxidation. Oxidation is a concern because the tube is only 0.010 in thick. The active metal catalyst can be platinum, palladium, rhodium or a mixture of these compounds. Preliminary testing has shown that pure platinum catalysts have a light off temperature of greater than 450 C and therefore do not satisfy the light off requirements for this program. Development on this program has focused on palladium and palladium based mixtures for the catalyst. Figure 2 shows the catalyst system for the traditional ceramic catalyst. In addition to the traditional ceramic coatings an internal Siemens ceramic metal coating has been developed as shown in Figure 3.

The catalytic coating development on this program is pursued with the following industrial partners:

- ACS Advanced Catalyst Systems
- Engelhard
- Guild Associates Inc.
- Miratech
- CFI/CTI Coatings for Industry/Coating Technologies Inc

Dr. Larry E. Campbell
Dr. Tom Giroux, Dr. Bob Farrauto
Dr. Joseph Rossin
Don Newburry
Dr. Basil Mucha

The first 4 companies are involved in the production of traditional ceramic catalyst materials. CFI/CTI is involved in the design of the Siemens metal ceramic coating.

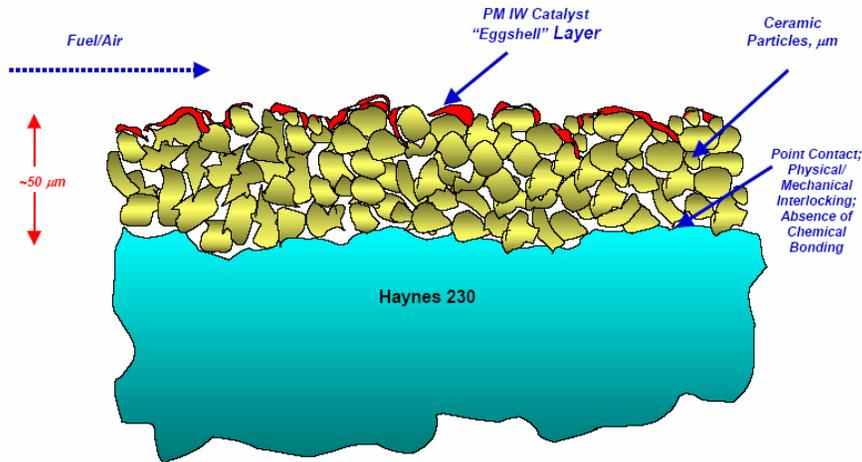


Figure 2 Traditional Ceramic Coating

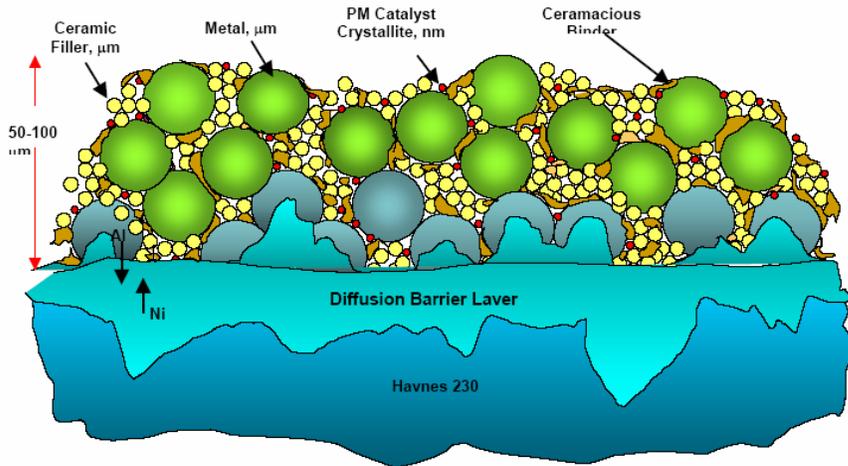


Figure 3 Siemens Metal Ceramic Coating

TESTING OF CATALYSTS

The following criteria were set up for initial ranking of catalysts: 1) final stabilized lightoff temperature; 2) fuel conversion and oxygen conversion rates; 3) coating durability properties. For catalysts which would demonstrate the acceptable screening properties, additional poisoning, adhesion, and durability studies were planned.

Screening of catalyst light-off properties and fuel conversion characteristics are conducted in the Single tube rig at Siemens' Casselberry labs where the fuel, split air, and main air flows, temperatures and pressure parameters were designed to simulate the conditions of the catalytic combustor operating in the SGT-6-5000F engine. Figure 4 represents the catalyst testing conditions in the Single Tube rig. Figure 5 shows the instrumented test of the single tube catalytic rig used for the screening tests.

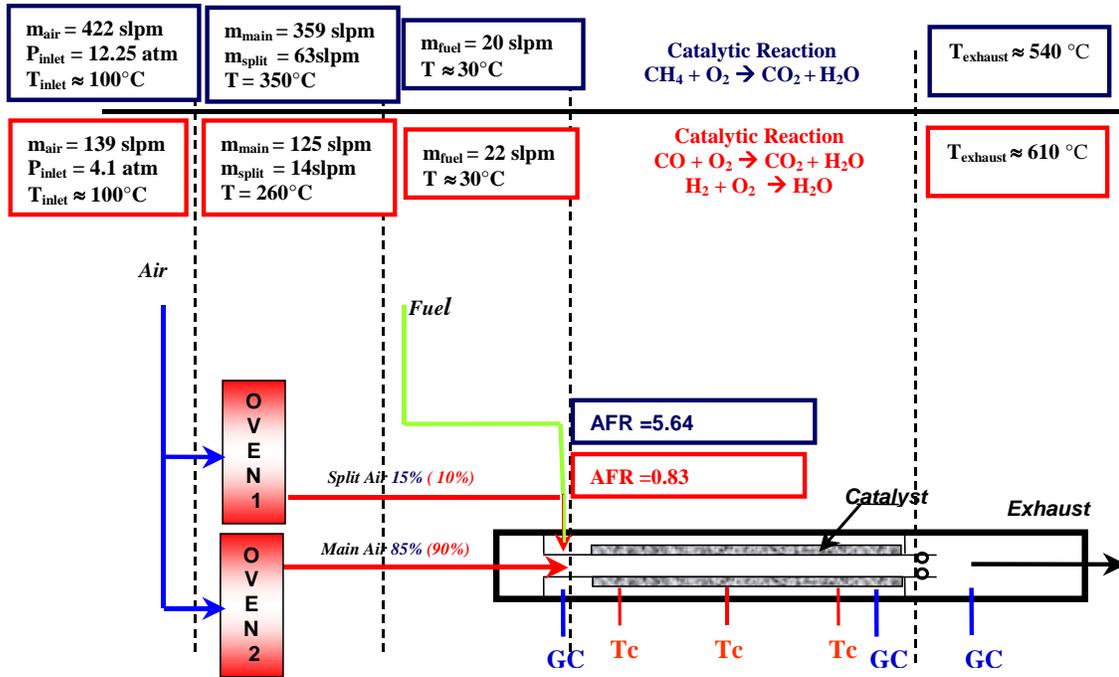


Figure 4. Testing Conditions in the Single Tube Rig (Casselberry Labs)

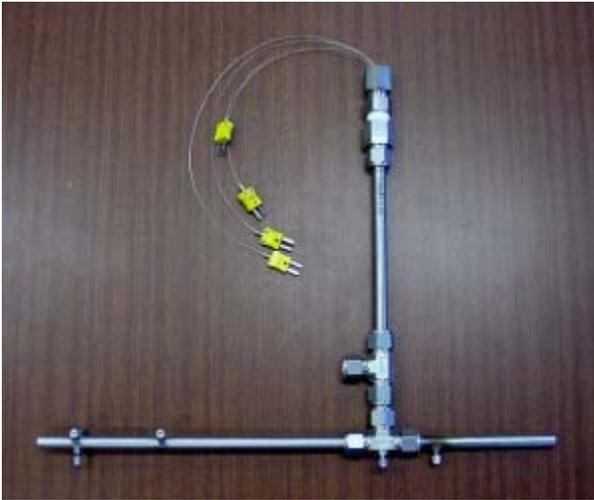


Figure 5 Instrumented Test Section of the Single Tube Rig

Because the lightoff temperatures on syngas and hydrogen are significantly lower than those of natural gas, the initial coating screening tests were conducted on natural gas. As a rule, any catalyst which would light off in natural gas at the acceptable temperature range of 350 °C, will light-off at even lower temperatures with syngas. Lightoff temperatures in hydrogen are even lower than syngas or natural gas.

Three thermocouples were attached to the catalyst surface at the following sample locations: just after the beginning of the catalyst, the middle of catalyst, and close to the exit of the catalyst. Catalyst light-off temperature was determined as the temperature at which a sudden increase of temperature on catalyst by 200-300°C was observed. Three GC ports were installed at the rig to monitor the gas fractions: at the catalyst inlet; at the catalyst outlet, and at the reactor exhaust. Fuel conversion rates and/or oxygen conversion rates were calculated from gas composition differences obtained between second and first GC ports, which represented post-catalyst and pre-catalyst mixtures, respectively. For most tests the oxygen conversion is reported because it has been verified by both the gas chromatograph and the Ultramat Emissions Analyzer.

Precision Combustion Inc. (PCI) has developed the initial catalyst for use in the RCL catalytic combustor. The PCI catalyst demonstrated stable light-off properties (LOT) and fuel conversion rates in the acceptable ranges. All new catalyst formulations are compared to the PCI data. Newly developed catalysts were prepared by collaborative interactions with four companies: Advanced Catalyst Systems (ACS), Guild Associates Inc., Miratech Corporation, and Engelhard Corporation. Approaches in the development of catalysts were undertaken in two directions: adjustment of washcoat composition in order to develop the high-surface-area and sintering resistant catalyst support; adjustment of catalyst combination and concentrations in order to find the best catalytic system. All comparison data on catalyst performance was obtained from the single tube rig. An overview of the approaches undertaken with each company and the properties of each of the catalysts are discussed in the Appendix.

CATALYST DEVELOPMENT CONCLUSIONS

Figure 6 represents the Pugh diagram with evaluation of all recently prepared best catalysts according to various selection criteria (LOT performance, fuel conversion, estimated durability, cost, etc).

			Catalysts																				
			1		2		3		4		5		6		7		8		9		10		
			Current PCI Catalyst		ACS 27-3 Catalyst Al2O3 (180) Pd-5 mg/in2		ACS 102-2 Catalyst Al2O3 (180) Pd-Pt-Rh - 5.5 mg/in2		Guild 12 Pd Pt = 75:25		Guild 108 Pd Rh = 9:1		Guild 111 PdPtRh = 6.5,2.5:1		Miratech Durab.7 Pd-7 mg/in2		Miratech DOE3 Pd-6 mg/in2, Pt-1.5 mg/in2, Rh-0.6 mg/in2		Engelhard COM 7		Engelhard COM 8		
CTX			Rating	Weighted Score	Rating	Weighted Score	Rating	Weighted Score	Rating	Weighted Score	Rating	Weighted Score	Rating	Weighted Score	Rating	Weighted Score	Rating	Weighted Score	Rating	Weighted Score	Rating	Weighted Score	
Weighting																							
SELECTION CRITERIA	1	Initial Light Off Temperature in Natural Gas (Goal - 350 Deg C or less)	3	3	9.0	1	3.0	3	9.0	3	9.0	3	9.0	3	9.0	2	6.0	3	9.0	3	9.0	3	9.0
	2	Second Light Off Temperature in Natural Gas (Goal - 350 Deg C or less)	3	3	9.0	2	6.0	1	3.0	1	3.0	3	9.0	3	9.0	2	6.0	3	9.0	2	6.0	1	3.0
	3	Stabilized Light Off Temperature in Natural Gas (Goal - 350 Deg C or less)	5	5	25.0	4	20.0	3	15.0	5	25.0	4	20.0	5	25.0	4	20.0	5	25.0	4	20.0	3	15.0
	4	Oxygen Conversion Rate in Natural Gas (Goal - 40-60 %)	5	4	20.0	5	25.0	5	25.0	3	15.0	3	15.0	3	15.0	5	25.0	5	25.0	5	25.0	5	25.0
	5	Stability of Oxygen Conversion Rates in Natural Gas	3	3	9.0	3	9.0	3	9.0	3	9.0	2	6.0	2	6.0	3	9.0	3	9.0	3	9.0	3	9.0
	6	Syngas Performance Data ("1" - Catalyst was not tested in Syngas)	3	3	9.0	1	3.0	1	3.0	1	3.0	1	3.0	1	3.0	1	3.0	1	3.0	3	9.0	1	3.0
	7	Visual Discoloration of Catalyst after Testing	2	1	2.0	1	2.0	1	2.0	1	2.0	1	2.0	1	2.0	1	2.0	1	2.0	1	2.0	1	2.0
	8	Coating Durability / Spallation after Initial Testing Trials	5	5	25.0	5	25.0	5	25.0	5	25.0	5	25.0	5	25.0	1	5.0	1	5.0	4	20.0	4	20.0
	9	Performance Reproducibility on Parallel samples ("1" - Catalyst was not Reproduced)	4	4	16.0	1	4.0	2	8.0	1	4.0	1	4.0	1	4.0	3	12.0	1	4.0	3	12.0	3	12.0
	10	Catalyst Cost / per Tube (Goal - ~ \$25 / per Element or less)	5	1	5.0	1	5.0	1	5.0	2	10.0	2	10.0	2	10.0	4	20.0	4	20.0	5	25.0	5	25.0
	11	Vendor Manufacturing Availability	5	5	25.0	1	5.0	1	5.0	1	5.0	1	5.0	1	5.0	5	25.0	5	25.0	5	25.0	5	25.0
	12	Information Availability about Catalyst to Siemens	5	1	5.0	5	25.0	5	25.0	5	25.0	5	25.0	5	25.0	2	10.0	2	10.0	3	15.0	3	15.0
Raw Score			159.0000		132.0000		134.0000		135.0000		133.0000		138.0000		143.0000		146.0000		177.0000		163.0000		
Rank			9		7		6		8		5		4		3		1		2				
Decision or Outcome			Compared														Selected						

Figure 6 Pugh Concept Matrix for Catalyst Selection

Three catalysts (Engelhard, Miratech and Guild) showed promise of achieving the program goal of 350 C lightoff. The Engelhard COM7 catalyst was preliminary selected as the primary candidate for further studies towards final evaluation as a catalyst for Siemens catalytic combustor. The Miratech DOE-3 catalyst showed very promising lightoff characteristics but additional work is required to resolve a coating adhesion issue. Guild 111 and other Guild catalysts demonstrated some promising properties. Planned simultaneous correlation of precious metals loadings in SiO₂-Al₂O₃ – stabilized washcoat should provide some improvement in catalyst properties.

Further tests are planned towards final evaluation of COM7 catalyst. Extensive syngas testing with determination of catalyst tolerance against sulfur poisoning are planned. A ten day catalyst durability test will be performed on both the PCI and COM 7 catalysts using syngas fuel from the bench scale gasification unit at the EERC at the University of North Dakota. This test will be performed with varying levels of sulfur contamination. In addition thermocycling tests will be performed on natural gas for the expected 400 cycle life of the catalyst. Additionally, COM7 catalyst performance properties in hydrogen fuel environment

will be evaluated. Currently a 100 hr durability test is ongoing for catalysts from Engelhard, Miratech, Guild and ACS. Results are expected next month.

In parallel, catalyst poisoning studies are planned at Siemens Corporate Technology in Erlangen. Two sets of COM7 and Miratech coupons were submitted to SCT for the poisoning studies. Initial poisoning studies will be conducted towards evaluation of catalysts tolerance against sulfur poisoning and catalyst tolerance against coking. Upon determination of further possible catalytic candidates, additional catalysts will be nominated for precise performance characteristics and poisoning effect studies.

TASK II.3 – DEVELOPMENT OF CATALYTIC REACTOR

The proper design of the catalytic reactor section requires modeling tools for the aerodynamics, heat transfer and homogeneous and heterogeneous chemical kinetics of the reactor section. The most challenging aspect of this design is the understanding of the surface chemical kinetics. This controls the heat release at the catalyst section which is critical to the design of the reactor. These tools are necessary in order to extend the design from the current tubular reactor to the alternative corrugated plate geometry. In order to model the reactor in detail the surface Chemistry options of CHEMKIN were investigated.

CHEMKIN solves the surface chemistry reactions in detail and uses several simplifications to the fluid mechanics. The available models are the perfectly stirred reactor model (PSR), the plug flow reactor model (PFR) and the boundary layer model (CRESLAF). Both the PSR and PFR models assume one dimensional flow and a kinetic controlled process. In the PSR the entire volume of the reactor is assumed to be completely mixed. This model is used to represent a region of intense mixing such as a recirculation zone. The PFR models a channel with perfect mixing in the radial direction but no mixing in the axial direction. The PFR model is often used as an approximation for turbulent flow in a channel. The CRESLAF models a laminar flow channel and includes gradients in both the axial and radial direction. The radial gradients in this model are based on the laminar flow equations. All of these models can incorporate heat loss to the reactor walls.

None of these models is directly applicable to the RCL catalytic reactor. Because the reactor operates under rich conditions the reaction rates are controlled by diffusion of the oxygen to the surface of the catalyst. Since neither the PSR nor PFR include radial gradient of temperature and concentrations, they tend to over estimate the reaction rates at the catalyst surface. The CRESLAF model has the radial gradients but they are calculated based on laminar flow properties. Because laminar transport properties are significantly lower than turbulent transport properties, this model tends to under estimate the reactions at the surface of the reactor. Two modeling techniques were investigated for the RCL catalytic reactor using CHEMKIN.

THREE LAYER CLUSTER MODEL

The three layer, 5 stage PSR cluster model is shown in Figure 7. In this model the reactor is divided into 5 axial zones and 3 radial zones each represented as a PSR. The 3 Layer Model divides the mass flow through the catalytic combustor into three layers. The first two layers represent the reacting flow and the third layer simulates the air used to cool the catalyst. The turbulent flow field in the reacting region is represented by two PSR layers with proper exchange rate between them. The first PSR represents the turbulent core. This is a perfectly

mixed region with a macroscopic axial flow. Only gas phase reactions can be considered in this volume.

The second PSR represents the stationary boundary layer. Both surface and gas phase reactions can occur in this region. There is no axial flow into or out of this reactor. This approximation is based on the fact that if the thickness of the boundary layer is low enough then the axial mass transfer within this layer is negligible compared to the turbulent core. There is a mass transfer in radial direction specified as an exchange rate between the boundary layer PSR and the core turbulent PSR. This exchange rate is a critical parameter and is set to represent the convective transport of mass and energy from the boundary layer to the turbulent core.

The cooling air is modeled as a PSR with no chemical reactions. It is linked to the reacting flow PSRs by a heat transfer coefficient. This coefficient is calculated separately from CHEMKIN. By modeling the cooling flow as a PSR reactor it is possible to solve for the variation in catalyst surface temperature along the length of the reactor.

The five axial stages of this model were the maximum number of stages which could be practically solved in the CHEMKIN cluster. Adding additional reactors to the model made convergence almost impossible.

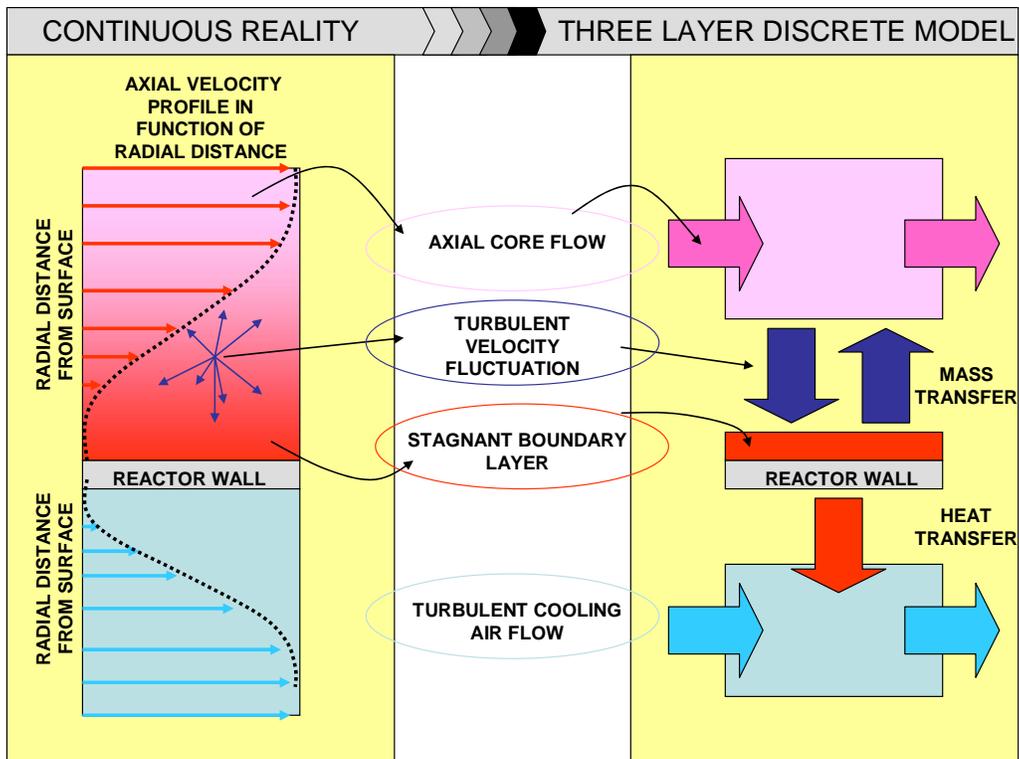


Figure 7 Three Layer PSR Model of the RCL Reactor

The main task for this model is to find an accurate value for the exchange rate between core and boundary layer reactors. As a first guess the turbulent intensity was used for the exchange rate. The turbulent intensity is given by the turbulent fluctuations traverse to the main flow direction divided by the core velocity. Measurements on a flat plate with a turbulent

boundary layer suggested that the maximum turbulent intensity in the boundary layer is 0.04. Therefore 4% was initially chosen for the exchange rate. When this exchange rate was used the heat and mass exchange was clearly under estimated. These observations led to a different approach to the exchange rate. The exchange between boundary layer and the core flow were determined by comparing the calculated exchange rate with that calculated by standard turbulent heat and mass transfer correlations. An exchange rate of 20% was found to be the best fit to the data.

The three layer model has the advantage that the heat transfer between the cooling channel and the reacting flow can be explicitly modeled. One disadvantage is that because all of the reactors are solved simultaneously in one cluster, the problem becomes very stiff and difficult to solve as the number of reactors is increased. The 3 layer model is limited to 5 axial stages because this is the largest number of reactors which could be practically solved. This limits the special resolution of the catalyst in the model. The cluster model is only available in the Reaction Design version of CHEMKIN.

Figure 8 shows the oxygen concentrations in the boundary layer and core flow zones of the 3 layer model. This calculation clearly demonstrates how the surface reaction rate is controlled by both the surface reaction rates as well as the diffusion of oxygen to the reaction zone. In this model the oxygen concentration in the boundary layer region is significantly lower than it is in the core flow region. Accurate modeling of the RCL reactor requires modeling of both the mass diffusion and kinetics of the system.

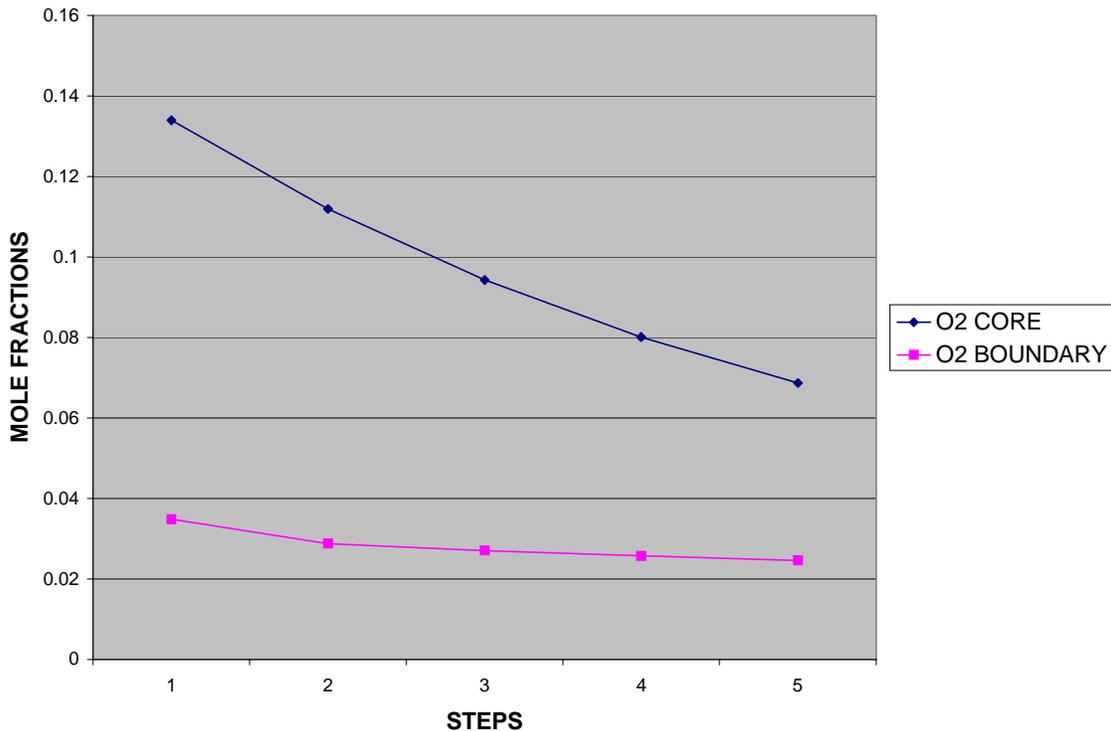


Figure 8 Calculated Oxygen Concentrations In the Reactor

THE SHEAR FLOW MODEL

The shear flow model (CRESLAF) simulates the reacting flow along the catalytic surface. This program solves the momentum equation, assuming laminar flow field. In order to simulate turbulent mixing in this model, the viscosity, diffusivity and conductivity are multiplied by a constant factor. This module does not include the heat loss due to the backside cooling air cooling air flow. A heat loss term can be added to the equations but it would be dependent on the cooling air temperature which increases with axial distance along the reactor. It was decided that when using the shear flow model the experimental temperature profile would be used as a boundary condition. The resultant exit gas temperature and concentration of gas species will be compared with the experimental results. As with the exchange factor in the 3 layer model, the turbulent enhancement factor used in this model will be determined experimentally.

To include the effects of the backside cooling air in the model, an iterative solution is necessary. An initial surface temperature profile would be assumed and CHEMKIN used to calculate the heat release. This heat release would then be used as an input to a thermal model of the catalyst reactor. With this heat release rate a new surface temperature profile would be calculated and CHEMKIN would be rerun.

REACTION KINETICS

Platinum, palladium and rhodium are considered as most promising catalytic metal. Table 2 lists the available surface reaction mechanisms in the literature. Notice most of the available mechanisms are based on platinum catalysts. In addition these mechanisms are based on low pressure data.

TABLE 2 Surface Reaction Mechanisms.

Active Metal	Fuel	Reference
Pt, Rh	CH ₄	1
Pt	C1 species	2
Pt, Pd	CH ₄	3
Rh	CH ₄	4
Pt, Pd	CH ₄	5

Pt	H2	6
Pt	H2	7
Rh	H2/CH4	8

For the modeling studies conducted under this program the mechanism of Deuschmann (3) was chosen to represent the surface kinetics. This mechanism is based on platinum experiments.

Data from the single tube rig is used for validation of the reaction mechanism. The original Deuschmann mechanism did not reproduce the lightoff data obtained experimentally. This is not entirely surprising in that it is based on platinum data and platinum has a significantly higher lightoff than palladium. To match the experimental data the Deuschmann mechanism was modified to reduce the lightoff temperature. The mechanism changes were studied using a two dimensional CFD calculation with Star-CD including the surface reaction model from CHEMKIN. In order to match the lightoff data from the single tube rig the rates of the following reactions were modified.

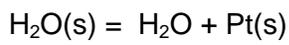
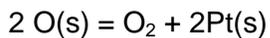
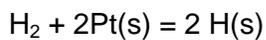


Figure 9 shows that with these modifications the experimental lightoff conditions in the single tube rig were reproduced. Current modeling studies have been performed with the modified Deuschmann mechanism. Optimization of the surface reaction mechanism will be the subject of future work.

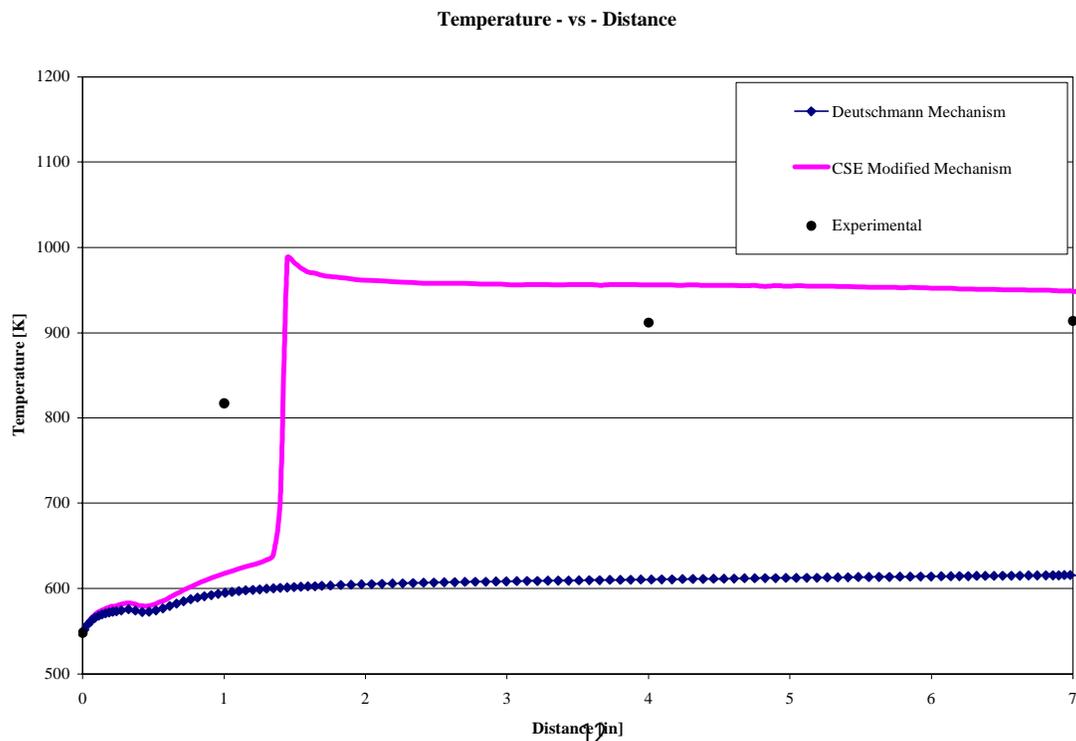


Figure 9 Calculated Catalyst Temperature with Revised Kinetics

MODELING RESULTS

The calculations from the 3 layer model and the shear flow model were compared with data generated in the single tube rig. The basic components of the single tube rig are shown in Figure 9. The catalytic tube is inside of the reactor tube hence the reacting side is an annulus between the two tubes. The cooling side is the cross sectional area of the inner tube. In addition to thermocouples on the tube, the mixed gas temperature at the exit to the catalyst is measured. Gas chromatograph ports are located at the entrance before the catalyst, at the exit of the catalyst zone and in the mixed gas zone.

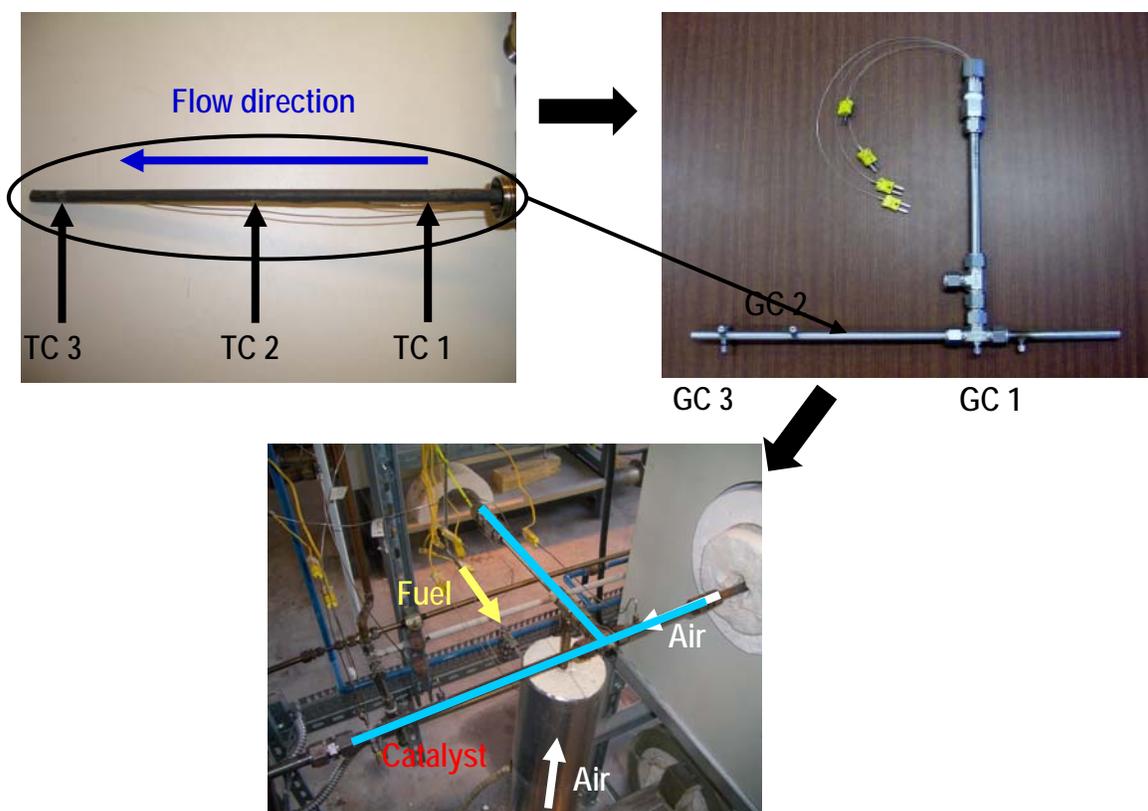


Figure 10 Single Tube Test Rig

Single tube testing begins with the air temperature reduced to below the expected lightoff temperature. The temperature of both the split air and cooling are gradually increase until lightoff is achieved. Lightoff can be clearly seen by a rapid increase in the catalyst surface temperatures. One the catalyst is lit it is brought to steady state conditions at an inlet temperature of 376 C. At this point GC data is obtained through all of the ports. For model comparison the data from the Engelhard COM 7 tube was used. Table 3 shows the measured temperatures for 2 different tubes.

Steady State	TC 1 [C]	TC 2 [C]	TC 3 [C]	T mixed [C]
Temperatures from COM 7 18	500	586	616	498
Temperatures from COM 7 12-8	562	721	753	554

Table 3 Measured Temperatures for the COM7 Catalyst

TEMPERATURE PROFILE COMPARISON-THREE LAYER MODEL

The calculated temperatures from the three layer model are compared with the experimental data in Figure 11. With the modified Dueschmann mechanism the model does a reasonable job of reproducing the available data.

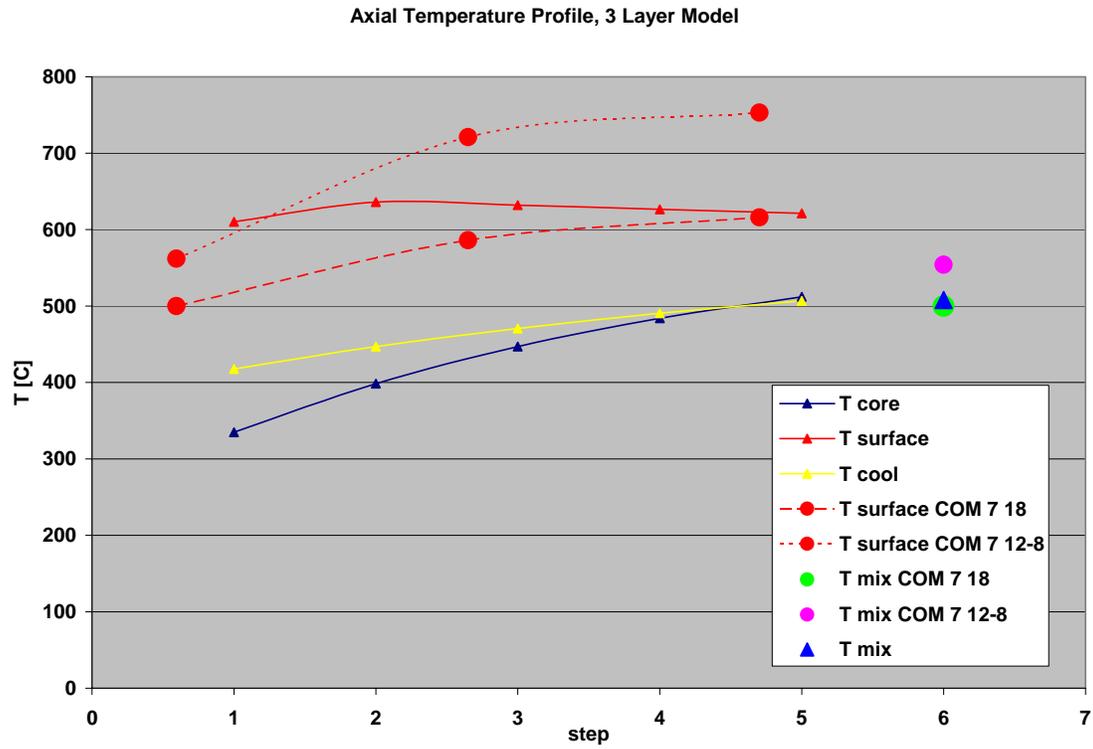


Figure 11 Three Layer Model Axial Temperature Profile

TEMPERATURE PROFILE COMPARISON-SHEAR FLOW MODEL

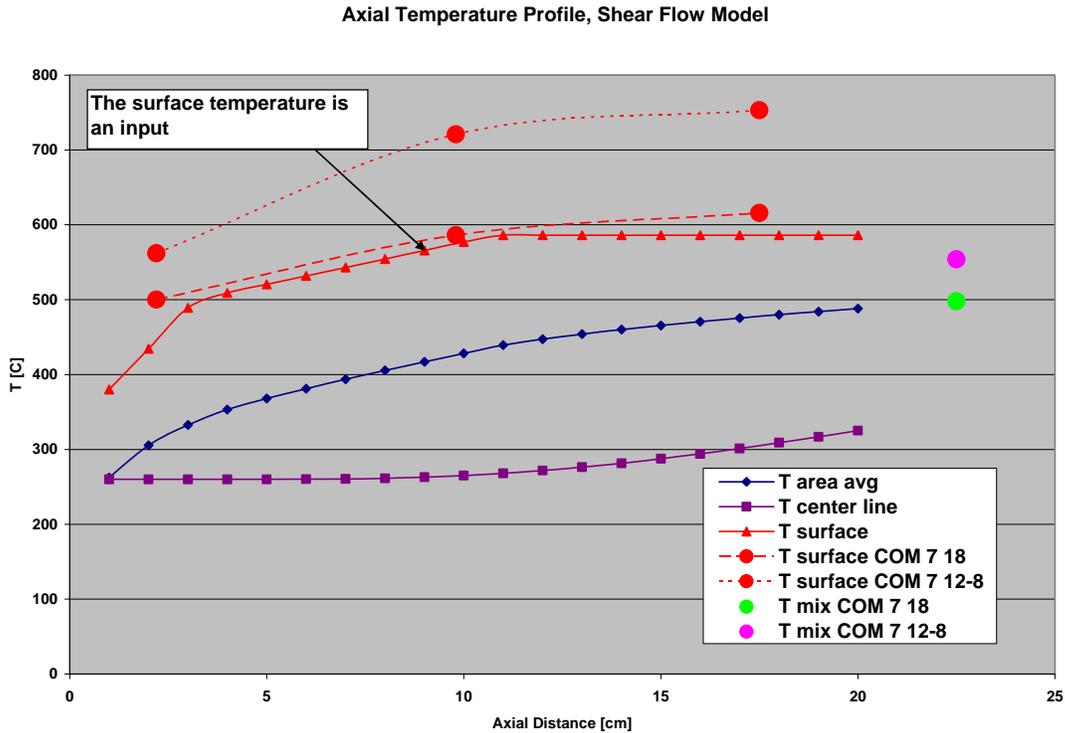


Figure 12 Shear Flow Model Axial Temperature Profile

Figure 12 shows the temperatures calculated with the shear flow model compared to the data. It is not possible to directly compare the temperatures from the shear flow model because the wall temperature is used as an input parameter to the model. The calculated reacting gas temperature at the exit is not directly comparable because only the mixed temperature is measured. Future experiments will be performed to get the gas temperature at the exit to the cooling channel.

CONCENTRATION MEASUREMENTS

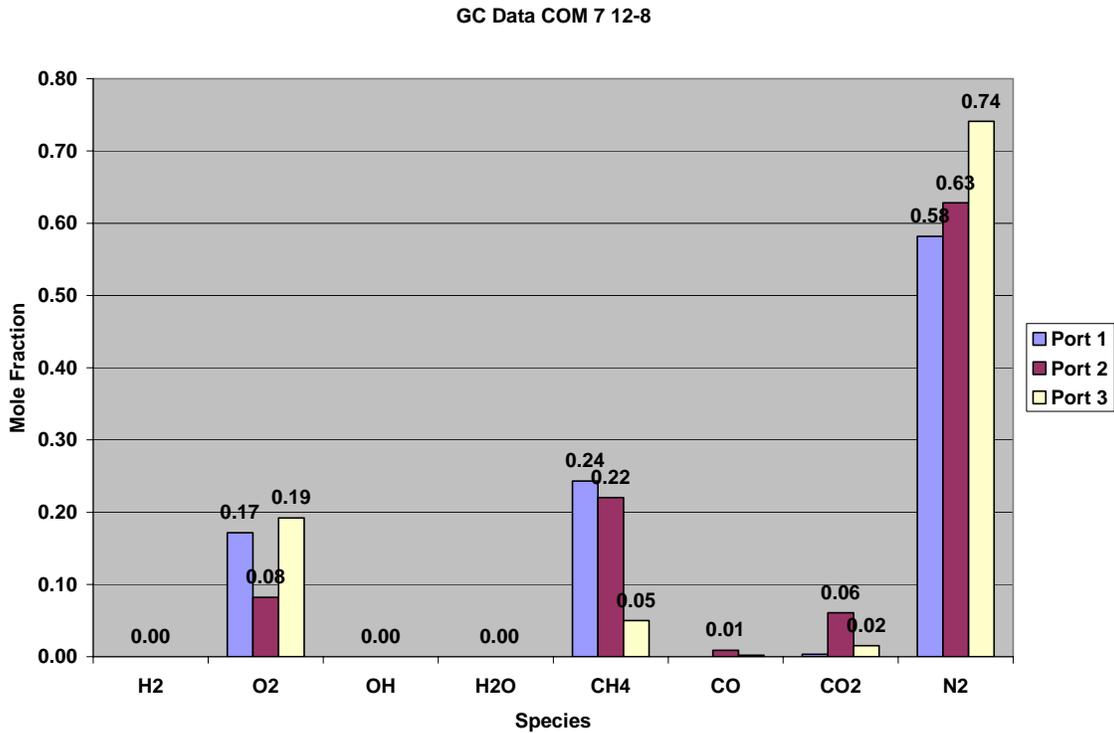


Figure 13 Single Tube Test GC Data for Catalyst COM 7 12 -8

The GC data are taken when the system reached steady state conditions at an inlet temperature of 376 C. Port 1 extracts a probe of the fuel and air mixture before it enters the catalytic region. Port 2 reads the mole fraction at the end of the catalytic coating and port 3 shows the mole fractions after the exhaust of the catalyst is mixed with the cooling air. The measured concentrations for the Engelhard COM7 tube are shown in Figure 13.

Dry Mole Fractions, 3 Layer Model

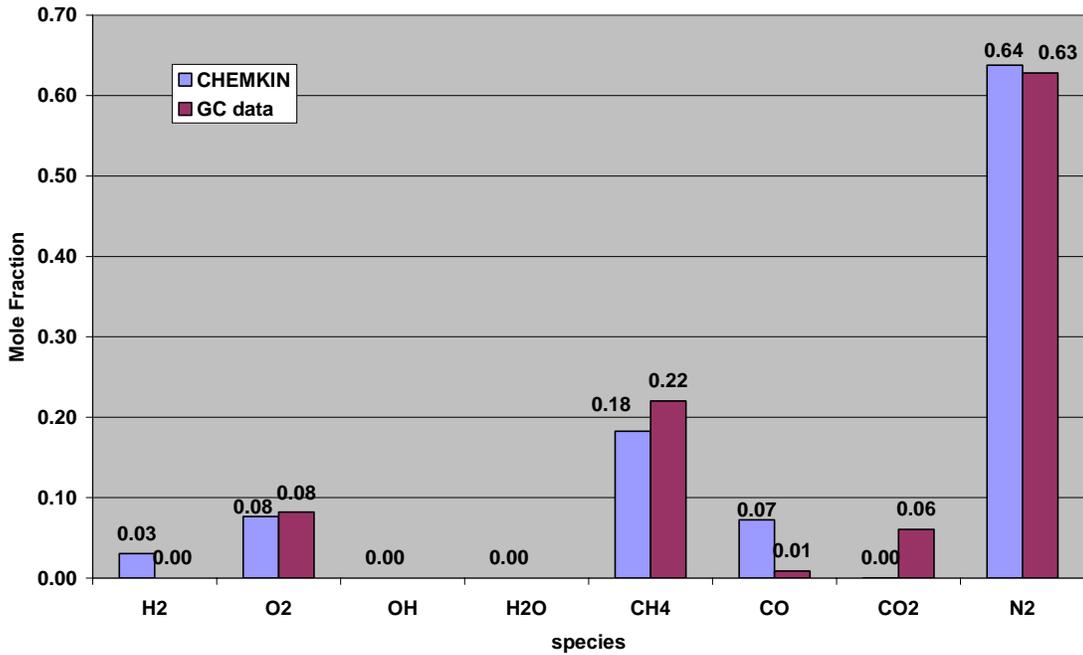


Figure 14 Three Layer Model Dry Mole Fraction Compared to GC Data

The dry mole fractions of the core flow calculated by the three layer model are compared to the GC data for COM 7 12-8 in Figure 14. The three layer model produces hydrogen, while no hydrogen was detected in the measurement. The oxygen mole fraction is in good agreement with the GC data. Water is not measured as it destroys the GC column. For comparison to the experiments the output from the CHEMKIN program was corrected to a dry basis. The mole fraction of Methane is under predicted. The model does not complete the oxidation of CO to CO₂ as can be seen from the diagram, because it over predicts CO and does not produce CO₂. The discrepancy of the H₂, CO and CO₂ mole fractions are due to a deficiency in the surface reaction mechanism. Improving the surface reaction mechanism will be a goal of the next phase of the project.

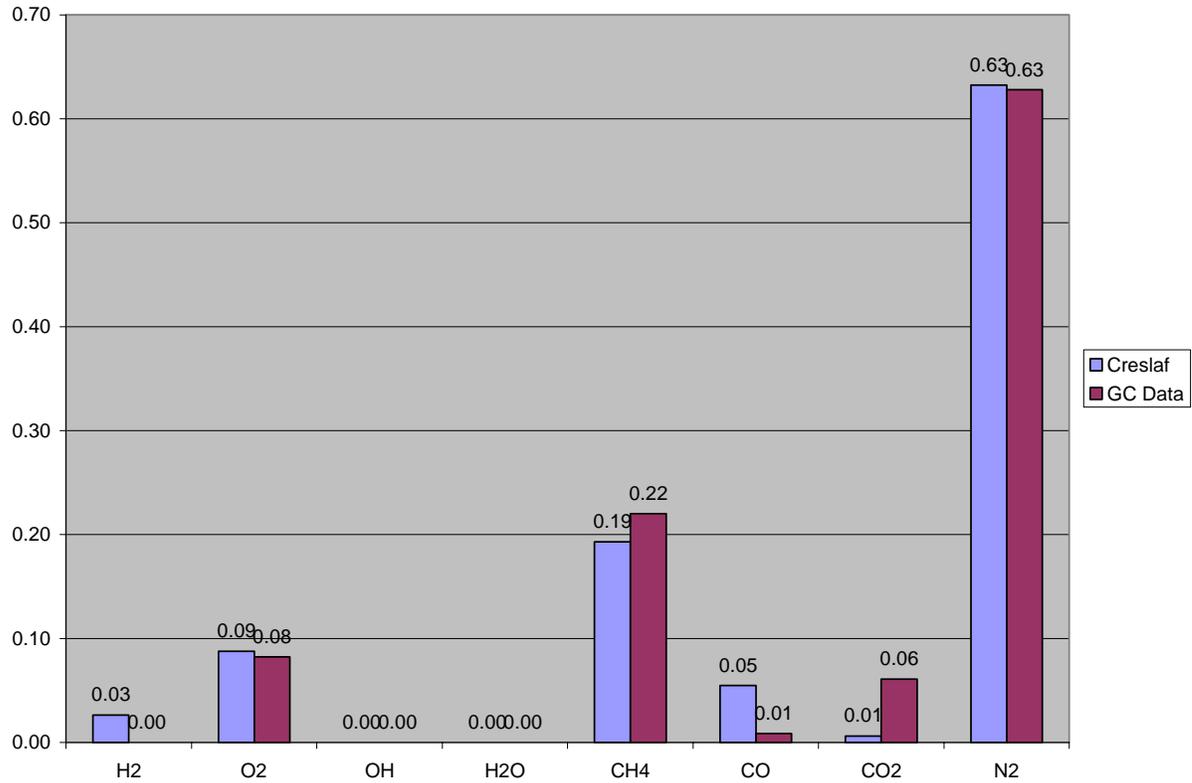


Figure 15 Shear Flow Model Dry Mole Fraction Compared to GC Data

Figure 15 shows the comparison of the calculate mole fractions at the reactor centerline to the measured data. The oxygen and fuel conversion results compare well with the measured data. Since the same mechanism is used for both models the problems with CO and hydrogen are common top both models.

Table 4 gives a comparison of the relative merits of each modeling technique,

Table 4 Comparison of Modeling Approaches

Parameter	3 Layer Model	Shear Flow Model
Heat Transfer	Heat transfer to cooling side solved, heat transfer to shell side included in exchange rate Input: heat transfer coefficient	Heat transfer to cooling side not solved, heat transfer to shell side solved reactor internally Input: surface temperature profile
Mass Transfer	Exchange rate between core and surface reactor Input: exchange rate	Molecular diffusion, can be addressed with Eddy viscosity, diffusivity, conductivity Input: turbulent factor

Mixing / Turbulence	Perfect Mixing in one step, limit for conversion is the exchange rate and reaction rate	Laminar velocity profile Can be enhanced by turbulent multiplication factor
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Parameter	3 Layer Model	Shear Flow Model
Data fit	Temperature: OK ? (Lack of Spatial Resolution) Composition: CO, CO2, H2O problem Conversion: over predicts	Temperature: OK ? (Cannot be Compared cooling air temperature is not calculated) Composition: CO, CO2, H2O problem Conversion: very good
Spatial Resolution	Poor Average over large area	very good Print distance can be chosen
Velocity	Residence time, no data for comparison available Gas phase temperature measurement at end of catalytic tube	Laminar velocity profile, no data for comparison available Gas phase temperature measurement at end of catalytic tube

Parameter	3 Layer Model	Shear Flow Model
Input parameter handling	poor Complex set of input parameter due to amount of reactors	OK
Convergence	Stiff Input composition on surface needs to be close to solution	More flexible
Cost	License 16,000\$	free

Both the CRESF and the 3 layer model provide a good representation of the data. Currently

work is underway to extend this modeling work to the corrugated plate geometry and to syngas and hydrogen fuel.

TASK II.4 – DEVELOPMENT OF CATALYTIC MODULE

Module Test Results

For phase II of the program the module testing was moved to the Siemens small industrial turbine facility in Lincoln, England. This facility has the capabilities to test a catalytic module at full SGT-6-5000F conditions on both natural gas and syngas fuels. Previous testing at Solar Turbines was limited to scaled FD conditions and natural gas. As part of this program a new module design, module 8 was created. Module 8 uses the basic flared tube design with the fuel injection manifold redesigned to include the capability for syngas operation. By using the flared tube design in these tests it is possible to obtain a good baseline comparison with the results obtained at the new facility to the previous testing at Solar Turbines.

The module design with the two fuel manifolds is shown in Figure 16. Two separate fuel feeds are required for natural gas and syngas. This is due to the fact that the flow rate of syngas to the module is significantly higher than natural gas because of its lower heating value. The injection hole pattern for each manifold was optimised using CFD analysis. It was not possible to obtain a single injection hole pattern that would work acceptably for both fuels. Figure 17 shows the final assembled module 8 on the cover plate ready for testing.

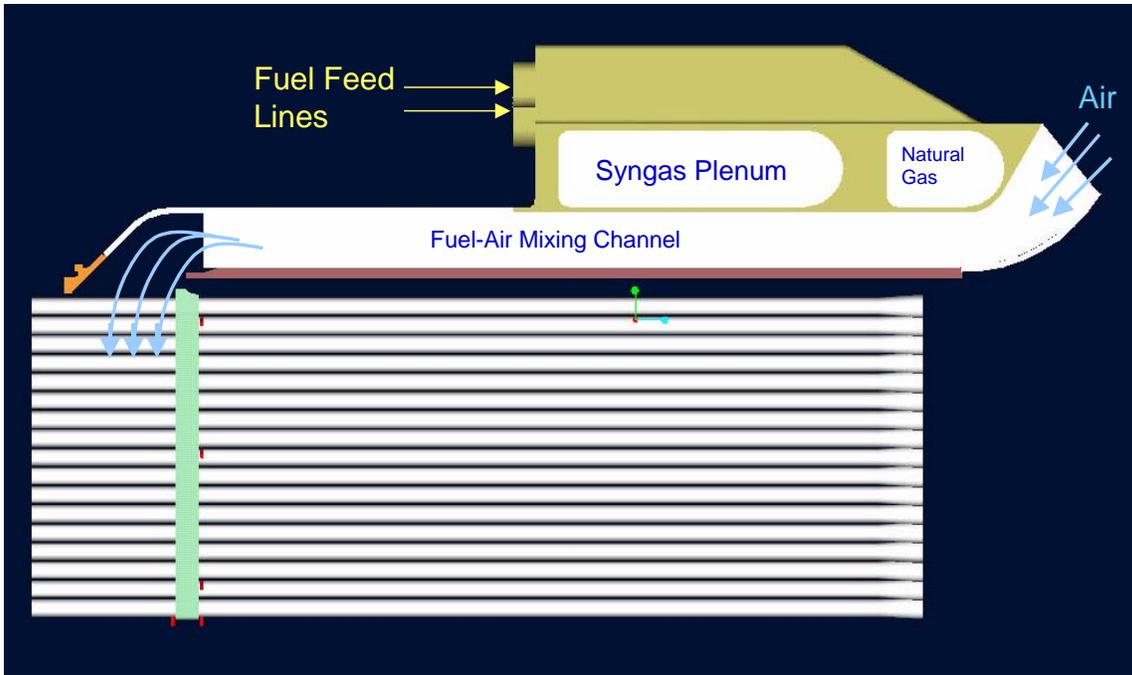


Figure 16 Module 8 with Dual Fuel Injection (Syngas and Natural Gas)

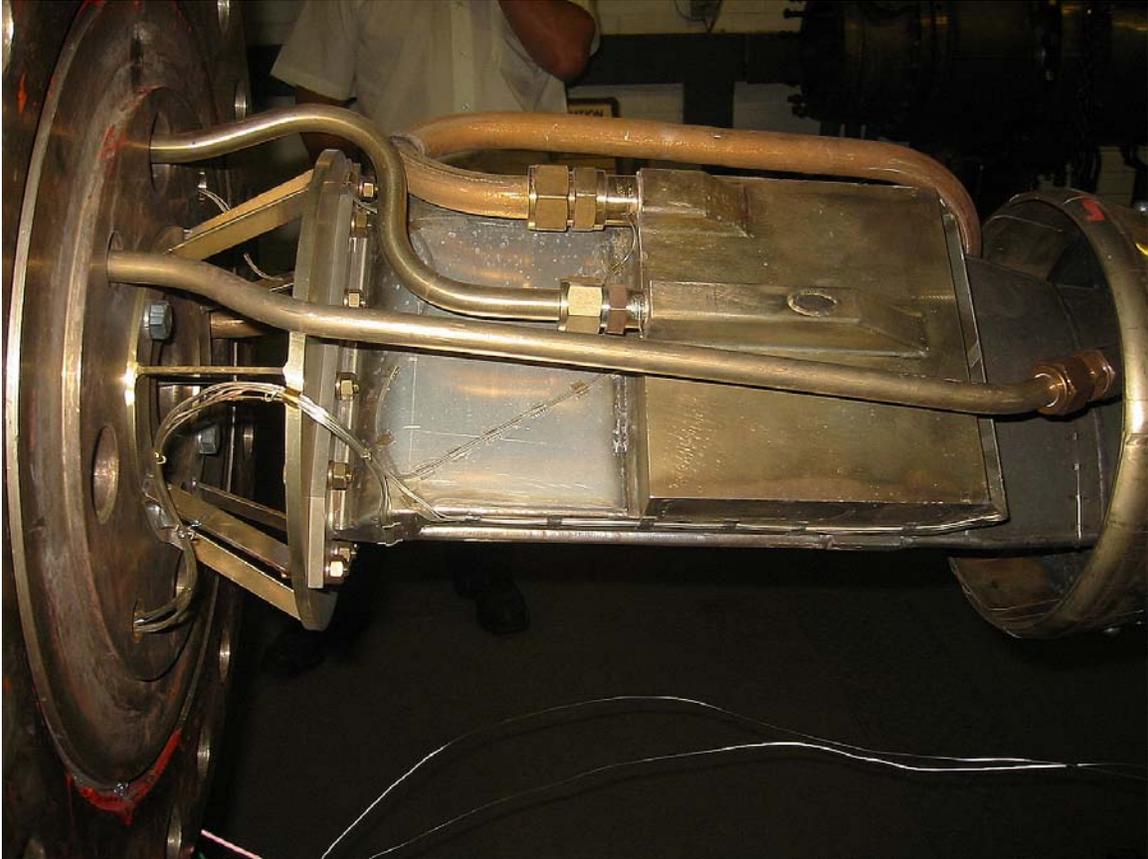


Figure 17 Module 8 Assembled to the Cover Plate

This module was tested in September 2005 on natural gas and the results compared well previous testing performed at the Solar Turbines test facility. Figure 17 shows the emissions results for this design as a function of firing temperature. This design easily meets the goals of the DOE program on natural gas. At F class firing temperatures the NO_x emissions are less than 2 ppm.

During this project period testing was performed on this module using syngas fuel. For these tests the module was ignited and brought to baseload on natural gas and then the fuel was transferred to syngas. The plan was to test two typical syngas compositions as listed in Table 5. The initial testing was performed on the petcoke composition. All testing was performed with undiluted syngas because the catalytic module is designed to produce low emissions without the need for dilution.

% vol (unless otherwise noted)		Petcoke	Coal
Ar		0.00%	0.00%
CH4		7.42%	3.34%
CO		59.83%	40.07%
CO2		7.89%	11.35%
H2		23.97%	27.35%
H2O		0.00%	0.00%
N2		0.89%	17.90%
Total		100.0%	100.0%
LHV(BTU/lb)		5565.00	3974.00
MW		22.15	22.32

Table 5 Syngas Composition

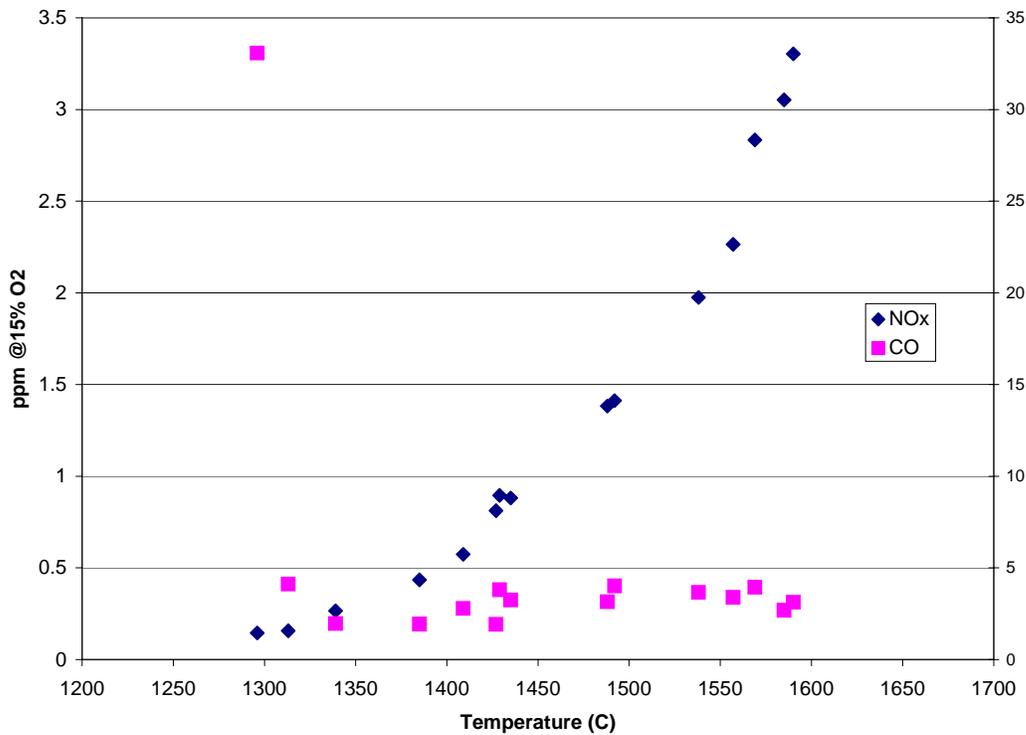


Figure 18 Module 8 Test Results as a Function of Firing Temperature

The emissions obtained from the syngas testing are compared to the previous natural gas tests in Figure 19. The data obtained on pure natural gas was higher than the previous values but this is not unexpected because for these tests the natural gas was injected through the syngas manifold. The fuel injection pattern in this manifold was optimized for the higher syngas flows and therefore the jet penetration and mixing on natural gas would be much less than optimum.

When the module was transferred to syngas the emissions did not improve. In this design high NOx emissions are generally caused by hot spots in the downstream flame. This would indicate inadequate mixing of the fuel and air in the catalyst region. Table 6 compares the

catalyst operating conditions between natural gas and syngas. The split and the oxygen conversion were calculated from GC data. As expected the increased fuel flow during syngas operation reduces the split causing the catalyst to operate more toward the rich region. This results in a drop in the oxygen conversion and results in a lower temperature rise across the catalyst surface. For the next phase of testing some of the syngas fuel will be diverted to the cooling air side of the tubes to increase the split. As expected the split and the conversion is reduced as the fuel flow is increased.

Fuel	AFR	T cat inlet	T cat outlet	T cat surface	Delta T cat	air split	Oxygen conversion
		Deg C	Deg C	Deg C	Deg C	%	%
Natural gas	37.8	417	544	705	127	12.7	55
Syngas	8.28	424	492	527	68	3.9	33
Syngas	8.58	425	485	541	60	3.7	24

Table 6 Catalyst Operation on Natrual Gas and Syngas

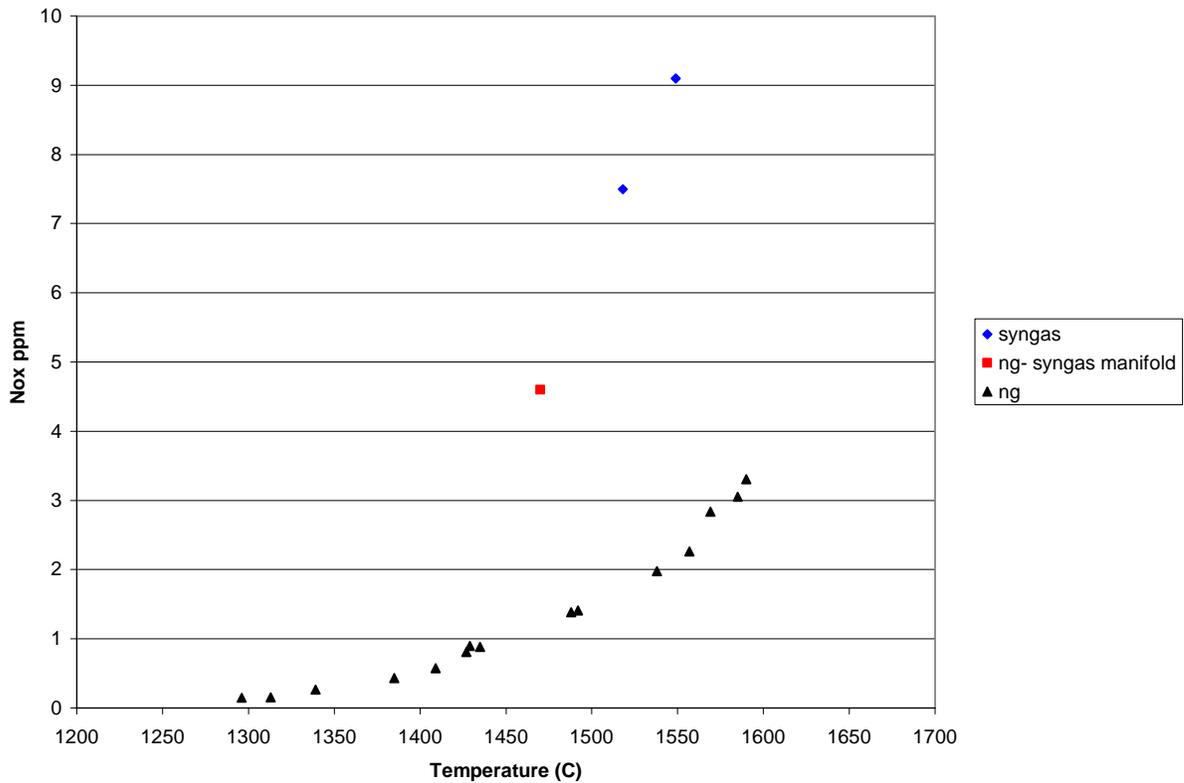


Figure 19 Syngas Testing Results

Testing began at F class temperatures and was increased to G class temperatures. At G class temperatures a flashback event occurred in the exit mixing section of the module. After this event the module was removed and damage was observed on the exit mouth of the module as can be seen in Figure 20. The flashback damage was only to the exit mouth of the module, no problems were discovered with any of the catalyst tubes.

The next step in this program is to redesign the exit mouth to obtain more margin for flashback. The main issue is that the velocity in this region must be increased. Also the fuel manifold and mixer will be redesigned to improve mixing. Two issues were discovered with the fuel manifold and fuel mixing region. The CFD analysis assumed that the pressure distribution at the syngas injection holes was uniform. Because the inlet pipe located to one side of the manifold, there is a possibility that the flow did not evenly feed all of the injection holes. Also the inlet area in the syngas pipe is only twice that of the natural gas line. Since the syngas flow is four times that of natural gas the velocity entering the manifold would be significantly larger. These issues will be addressed in the redesign of the syngas fuel injection manifold.

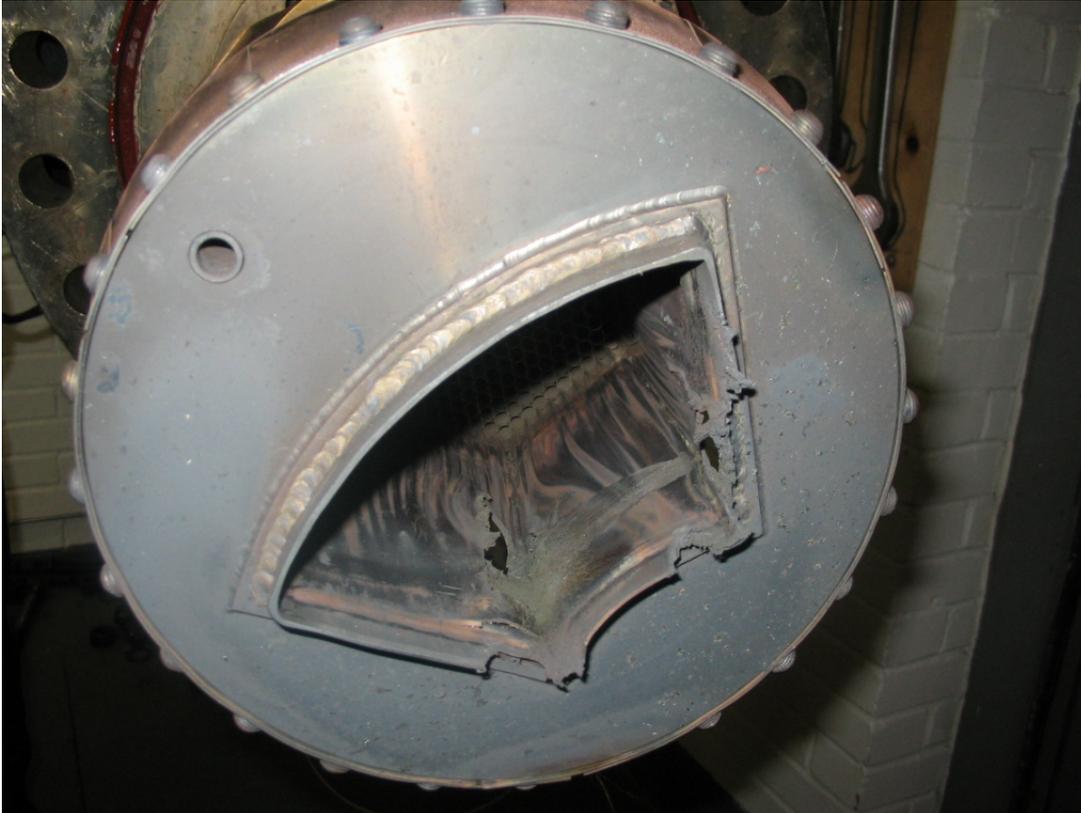


Figure 20 Mixing Section of the Module After Flashback

STATUS OF MILESTONES

First Quarter

10/1/05-12/31/05

Begin durability testing on coatings in the 60 tube rig.

Status: complete

Second Quarter

1/1/06-3/31/06

Down select alternative module designs for natural gas and syngas.

Status: complete

Third Quarter

4/1/06-6/30/06

Evaluate basket burnout region and down select best module designs for syngas.

Status: ongoing

7/1/06-9/30/06

Fabricate alternative module designs for testing.

Status: ongoing

CONCLUSIONS

The major accomplishments during this phase of the project are:

- Rainbow testing of 6 different coatings was initiated in the 60 tube rig. These coatings will be tested for 100 hr and then inspected.
- Engelhard COM7 down selected as the primary coating for the alternative reactor studies.
- Engelhard, Miratech, and Guild supplied coatings which met the natural gas light off requirements.
- Syngas durability studies initiated at EERC at the University of North Dakota.
- Two alternative module concepts were down selected for further testing, the revised capture plate design and the corrugated cylinder design. Design details are being finalized for both designs and manufacturing are scheduled to begin next month.
- Module tests were performed on syngas. The initial design demonstrated higher than anticipated NOx emissions at F class temperatures. When the firing temperature was

increased to G class temperatures flashback occurred. Redesign is underway to improve the mixing and flashback margin.

The expected activity during the next six months includes:

- Complete 100 hr rainbow durability testing on natural gas in the 60 tube rig.
- Complete syngas durability and sulphur poisoning tests at the EERC facility at the University of North Dakota.
- Map out the coating performance on syngas and hydrogen in the single tube rig as a function of the split air ratio. Determine optimum operating conditions for all cases.
- Redesign the syngas module to improve the mixing and flashback margin. Perform testing on the redesigned basket on syngas and diluted hydrogen.
- Complete CFD analysis of the burnout region on the SGT-6-5000F geometry. Down select the final basket concept for syngas and natural gas.
- Complete manufacturing of the scale modules of the alternative reactor concepts for testing at the Siemens PGI test facility. Perform testing at the Siemens PGI test facility.

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