

PRODUCTION OF HYDROGEN BY SUPERADIABATIC DECOMPOSITION OF HYDROGEN SULFIDE

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EXECUTIVE SUMMARY

Hydrogen sulfide (H₂S) is present in the industrial world chiefly as an undesirable by-product of fossil fuel processing, including natural gas, petroleum, and coal. In natural gas, H₂S is the primary sulfur component, along with lower levels of hydrocarbon sulfides (mercaptans). In petroleum, H₂S appears at various stages in the refining process, and it must be removed to facilitate the production of low-sulfur liquid fuels. H₂S also appears in coal gasification and is generally removed prior to fuel gas utilization.

Conventional technologies in use to decompose H₂S (Claus, Superclaus, and variations thereof) produce elemental sulfur as a by-product, which sells for about \$30/ton. However, the hydrogen present in the original H₂S leaves the process as water. At the same time, hydrogen is in demand at petroleum refineries and other facilities such as ammonia synthesis plants. The value of hydrogen in these applications exceeds its fuel value, and so it may be worthwhile to recover the hydrogen as H₂ from the H₂S, if an economical and reliable process can be found to do so.

In this program, the Institute of Gas Technology (IGT), UOP and BP Amoco in an advisory role, and the University of Illinois at Chicago (UIC) are developing a low-cost process for the thermal decomposition of H₂S in H₂S-rich waste streams to high-purity hydrogen and elemental sulfur, without generating any carbon dioxide. The novel feature of this process is the superadiabatic combustion (SAC) of part of the H₂S in the waste stream to provide the thermal energy required for the decomposition reaction, as indicated by the following two reactions:



Each molecule of H₂S reacting with oxygen can provide enough energy to dissociate up to 10 additional molecules of H₂S. While this chemistry offers an attractive way to decompose H₂S, it cannot be done using conventional burners because the adiabatic combustion temperature is not sufficient to support the reaction kinetics. However, the SAC reactor can support this reaction because the temperature obtained at rich conditions can be much higher with SAC than with conventional combustion.

Superadiabatic combustion (SAC), also known as filtration combustion, consists of combustion of a fuel gas-oxidant mixture in a porous ceramic medium with a high thermal capacity. The intense heat exchange between burning gas mixture and the porous medium permits the accumulation of combustion energy in the porous matrix. As a result, the flame temperatures developed can be much higher than the adiabatic temperature for the mixture in free air. Using an H₂S-rich stream as both the fuel and hydrogen source, the high SAC flame temperature promotes rapid thermal decomposition of most of the H₂S to hydrogen and elemental sulfur. This same concept is being developed for hydrogen production from natural gas and gasification of low-energy feedstocks.

This research program is divided into two phases. In Phase 1, a numerical model has been developed for rich and ultra-rich filtration combustion of H₂S/air mixtures within the one-dimensional approach, taking into account multi-step chemistry and separate energy equations for the gas and solid phases. Particular consideration is given to the optimization of H₂S decomposition into hydrogen. Preliminary numerical modeling of the SAC reactor has been performed and species and temperature profiles are predicted. The parameters considered in the modeling effort included fuel gas composition (i.e., H₂S-rich and H₂S-lean), oxidant composition (air/enriched air), equivalence ratio, superficial gas velocity, feed gas temperature (pre-heating effect), and product gas quenching.

Based on the developed numerical model, optimization studies of hydrogen production were conducted by varying the characteristics of the ultra-rich superadiabatic waves. **The major findings indicate that by optimizing the reactor configuration, equivalence ratio, and filtration velocity, the overall H₂S decomposition in a single pass can be as high as 30-50%, with a conversion of H₂S to the desirable product hydrogen (H₂) reaching a level of 30%.** This reactor performance can be obtained using equivalence ratios in the range of 10 to 15, while maintaining a filtration velocity greater than 100 cm/s. For these high values of equivalence ratio and filtration velocity, the resulting temperature is considerably higher than the adiabatic combustion temperature. Such high temperature promotes the decomposition of H₂S, the hydrogen (H₂)/water (H₂O) selectivity, and the elemental sulfur (S₂)/sulfur dioxide (SO₂) selectivity. Given that in a single pass the H₂S decomposition can reach 30-50%, the overall process performance can be substantially improved, with respect to hydrogen production, by membrane separation of product gases and recirculation of unreacted H₂S. It can be shown that in 4 to 5 passes nearly total hydrogen sulfide decomposition into sulfur can be realized, with 30-40% of the hydrogen component recovered as hydrogen (H₂).

The most optimum scenario in the results of the computer modeling to-date indicate that, with feed gases entering the reactor at ambient temperature, a maximum temperature of 1631 K (1394°C or 2541°F) can be achieved in the SAC reactor, resulting in an overall H₂S conversion of 50%, with a hydrogen (H₂)/water (H₂O) selectivity of 57/43 and an elemental sulfur (S₂)/sulfur dioxide (SO₂) selectivity of 99/1.

These predictions offered valuable guidelines for the preparation of a design and cost estimate package of a suitable bench-scale reactor testing system to be assembled and tested in Phase 2 of the program. Modeling efforts also made possible the identification of key SAC process parameters and the preparation of a parametric testing plan for Phase 2. The chemical kinetic mechanisms used in the formulation of this preliminary model will be updated based on direct comparison with the experimental data that will be obtained in Phase 2, further enhancing the reliability of the model.

To develop the necessary experimental data to demonstrate the technical and economical viability of the SAC reactor unit, **a bench-scale testing system has been designed for H₂ production from thermal decomposition of up to 1,400 standard cubic feet per**

hour (SCFH) of H₂S-oxidant gas mixture. This reactor system consists of a fuel gas/oxidant conditioning system to generate appropriate inlet gas mixtures, a packed-bed reactor, a sulfur condenser and recovery subsystem, an exit gas scrubbing subsystem, and equipment for sampling and analysis of H₂S decomposition products. Predetermined amounts of feed gas components are mixed and delivered to a packed-bed reactor where H₂S is converted to H₂ and S at high temperatures. Hot off-gas leaving the reactor is cooled with a cooling medium in a condenser where sulfur vapor (S(g)) is condensed and collected. Cooled gas is then scrubbed with a caustic solution where H₂S and sulfur dioxide (SO₂) are removed and the cleaned gas is discharged to the atmosphere. A design package has been prepared containing all information required for design, engineering, procurement and installation of this unit including system description, equipment design, and equipment specifications.

A preliminary market assessment shows that there are large and growing markets for hydrogen, and that the SAC-based decomposition process has the potential to offer cost savings to sulfur recovery and gas upgrading plant operators as a result of byproduct hydrogen sales or offset purchase cost. Because of the large amounts of H₂S handled, along with a large on-site demand for hydrogen, the petroleum refining industry may ultimately be the most lucrative market for this process. Natural gas producers who currently operate large Claus units might also benefit sufficiently from the sale of byproduct hydrogen to justify the expense of installing new technology if end users of the hydrogen are located sufficiently close to the treatment facilities. Cost savings for treatment of natural gas with high H₂S content, even with modest conversion yields and a capital cost equal to a Claus plant, are expected to be sufficiently high to favor this technology.

Successful development of SAC technology for acid gas treatment in refining, natural gas sweetening, and IGCC power generation applications can result in the recovery of significant quantities of hydrogen from acid gas waste streams that would otherwise be lost as water vapor in conventional sulfur recovery processes. Recovery of hydrogen as a byproduct of sulfur recovery offers the potential for hydrogen production at a very low cost, with no additional carbon dioxide emissions to the environment. Further benefits include the elimination of sulfur recovery catalyst and chemical costs, and the cost and environmental liability of spent catalyst and chemical disposal.

IGT, UIC, and industry advisors UOP and BP Amoco are ready to commence Phase 2 of the program. During Phase 2, the bench-scale unit will be constructed and parametric testing conducted to validate the SAC concept. The computer model developed in Phase 1 will be updated with the experimental data and used in future scale-up efforts. The process design will be refined and the cost estimate updated. Market survey and assessment will continue so that a commercial demonstration project can be identified.

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PROGRAM OBJECTIVE

The objective of this program is to develop an economical process for hydrogen production, with no additional carbon dioxide emission, through the thermal decomposition of hydrogen sulfide (H_2S) in H_2S -rich waste streams to high-purity hydrogen and elemental sulfur. The novel feature of the process being developed is the superadiabatic combustion (SAC) of part of the H_2S in the waste stream to provide the thermal energy required for the decomposition reaction such that no additional energy is required.

The program is divided into two phases. In Phase 1, detailed thermochemical and kinetic modeling of the SAC reactor with H_2S -rich fuel gas and air/enriched air feeds is undertaken to evaluate the effects of operating conditions on exit gas products and conversion efficiency, and to identify key process parameters. Preliminary modeling results are used as a basis to conduct a thorough evaluation of SAC process design options, including reactor configuration, operating conditions, and product/by-product separation schemes, with respect to potential product yields, thermal efficiency, capital and operating costs, and reliability, ultimately leading to the preparation of a design package and cost estimate for a bench-scale reactor testing system to be assembled and tested in Phase 2 of the program. A detailed parametric testing plan was also developed for process design optimization and model verification in Phase 2.

During Phase 2 of this program, IGT, UIC, and industry advisors UOP and BP Amoco will validate the SAC concept through construction of the bench-scale unit and parametric testing. The computer model developed in Phase 1 will be updated with the experimental data and used in future scale-up efforts. The process design will be refined and the cost estimate updated. Market survey and assessment will continue so that a commercial demonstration project can be identified.

BACKGROUND

Superadiabatic Combustion

Superadiabatic combustion (SAC), also known as filtration combustion (FC), consists of combustion of a fuel gas-oxidant mixture in a porous ceramic medium with a high thermal capacity.¹ Research interest in filtration combustion (FC) has been driven by numerous applications such as utilization of low calorific fuels,² low emission burners,³ and pollution control devices. Recent novel applications include fuel reforming and processing in the ultra-rich superadiabatic combustion waves.⁴ This topic has been under study by scientists at UIC's combustion lab since 1994.

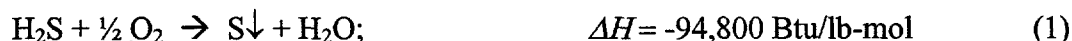
The intensive heat exchange between the filtrating and burning gas mixture and the porous medium through the highly developed internal surfaces permits the accumulation of combustion energy in the solid matrix. As a result, the flame temperatures can be much higher than the adiabatic temperature for the mixture in free air. Another unique effect of this situation in a cylindrical vessel is the linear propagation of a slow thermal oxidation wave, which can be periodically changed in direction by switching the flow of the fuel-oxidant mixture. This "reverse flow reactor" can be exploited for certain types of chemical processing.

Filtration combustion in a porous medium differs substantially from combustion in a homogeneous medium. The difference is the heat transfer between filtrated gas and the porous medium under conditions of active interfacial heat transfer. FC also differs from flames stabilized within a porous body in that FC is an inherently transient process. These differences lead to positive or negative enthalpy fluxes between the reacting gas and the solid carcass, resulting in combustion temperatures in excess of or below the adiabatic temperature for the supply mixture. Combustion waves in the porous body, including excess enthalpy (superadiabatic) flames, have been the focus of many recent experimental and theoretical studies.⁵ However, almost all of these studies were limited to very lean mixtures.

One of the most interesting aspects of this phenomenon is the possibility to combust very rich or very lean fuel mixtures that would not support a flame under normal conditions. This can be done in a linear cylindrical reactor, which is well insulated so that the heat loss in the radial direction (through the walls) is negligibly small. Some examples of lean-fuel combustion applications include destruction of methane-containing exhaust gases from coal mines and destruction of VOC emissions from industrial processes. On the other end of the spectrum, super-rich mixtures can be processed with very little oxygen. This is the type of application of interest to this program.

Hydrogen Sulfide Decomposition

One attractive application for SAC is the thermal decomposition of H₂S to produce elemental sulfur and hydrogen as a simpler alternative to the Claus process for processing H₂S from refinery streams, natural gas sweetening, or cold gas cleanup trains in gasification systems. The reactions of interest are as follows:



Each molecule of H₂S reacting with oxygen can provide enough energy to dissociate up to 10 additional molecules of H₂S. While this chemistry offers an attractive way to decompose H₂S, it cannot be done using conventional burners because the adiabatic combustion temperature is not sufficient to support the reaction kinetics. However, the SAC reactor can support this reaction because the temperature obtained at rich conditions is much higher with SAC than with conventional combustion.

Theoretical Considerations

Ultra-lean filtration combustion results in complete burnout of the hydrocarbon fuel with the formation of carbon dioxide and water. Thus, both the composition of the final products and the heat release are well defined. In contrast with the ultra-lean case, the combustion products of rich waves are not clearly defined. In this case, fuel is only partially oxidized in the filtration wave and the total heat release could be kinetically controlled by the degree of the partial combustion. As a result, chemical kinetics, heat release, and heat transfer are strongly coupled in the ultra-rich wave making it a more complicated and challenging phenomenon than the ultra-lean wave. Previous analyses⁵⁻¹⁰ of the FC waves were based upon a model in which the gas

phase chemical reactions were approximated by a single-step kinetic mechanism for combustion. These studies predict the general properties of filtration combustion waves, including direction and velocity of propagation, thermal structure, superadiabatic phenomena, etc. However, this approach cannot describe the complex chemical structure of the waves, nor predict the completeness of combustion and pollutant formation.

To fully exploit FC potential applications, numerical models need to be extended to the practically important limit of rich and ultra-rich filtration combustion of gases, addressing the issues of multi-step kinetics,¹⁰ heterogeneous reactions,¹¹ pore level mechanisms of combustion,¹² and adequate heat and mass transport phenomena in porous media.

Table 1 (adapted from Ref. 1) shows the calculated decomposition of H₂S as a function of the oxygen molar concentration and SAC reactor temperature, based on thermodynamics. The shaded region designates conditions under which the reaction cannot be self-sustained.

Table 1. Estimated Percent H₂S Conversion in SAC Reactor¹

O ₂ mol percent	Temperature (°F)					
	1700	1880	2060	2240	2420	2600
0.99	15.9	23.2	31.8	40.9	49.9	58.3
1.96	18.5	25.6	33.9	42.8	51.6	59.7
2.91	21.0	27.9	36.0	44.7	53.2	61.0
3.85	20.7	27.7	35.9	44.5	53.1	61.0
4.76	23.2	30.0	38.0	46.4	54.7	62.4

From Table 1, it can be seen that H₂S decomposition in excess of 60% can be achieved with only about 5% oxygen in the mixture, provided that an SAC flame temperature of 2600°F can be obtained. The percentage of available H₂ theoretically consumed to provide energy for decomposition is shown in Table 2.

Table 2. Estimated Percent of Available H₂ Consumed in SAC Reactor¹

O ₂ mol percent	Temperature (°F)					
	1700	1880	2060	2240	2420	2600
0.99	10.7	7.8	6.0	4.9	18.0	14.8
1.96	25.4	18.4	13.9	11.4	9.7	8.7
2.91	35.7	26.9	21.1	17.2	14.8	13.1
3.85	34.3	25.3	20.1	16.2	13.9	12.5
4.76	42.7	33.0	26.3	21.8	18.6	16.8

For example, at 4.76% oxygen and 2600°F, of the 62.4% H₂S decomposed (in a single pass), 16.8% of the available hydrogen will be consumed, leaving the remaining 83.2% (or 51.9% of the hydrogen contained in the original H₂S) available as product. Recycle of the unconverted product gas, after separation of H₂, could increase the H₂S conversion and allow the H₂ yield to approach the theoretical maximum implied in Table 3.

Table 3. Theoretical Maximum H₂ Yield from SAC Reactor with Recycle¹

O ₂ mol percent	Temperature (°F)					
	1700	1880	2060	2240	2420	2600
0.99	89.3	92.2	94.0	95.1	82.0	85.2
1.96	74.6	81.6	86.1	88.6	90.3	91.3
2.91	64.3	73.1	78.9	82.8	85.2	86.9
3.85	65.7	74.7	79.9	83.8	86.1	87.5
4.76	57.3	67.0	73.7	78.2	81.4	83.2

Previous Experimental Work

In 1998, IGT and UIC conducted an in-house research project to determine the potential viability of this application. The immediate objectives were:

- to determine whether a stable superadiabatic flame can be supported with only H₂S as fuel
- to determine whether significant quantities of elemental sulfur are produced
- to determine whether the behavior of the flame is consistent with UIC kinetic model predictions
- to make a preliminary market assessment of hydrogen and sulfur from H₂S
- to make a preliminary technical and economic comparison of SAC-based H₂S decomposition with commercial technology such as the Claus and SuperClaus[®] processes

A test unit was set up and operated by UIC personnel in an IGT laboratory equipped to safely handle H₂S-containing gases. A sketch of the atmospheric-pressure SAC test reactor, associated gas delivery and data system, and sulfur capture device is shown in Figure 1. The reactor is a 1.4-inch-ID quartz tube packed with 0.22-inch alumina beads and insulated with about 0.75 inches of high-temperature ceramic blanket. A thermowell in the center of the tube measures bed temperature at six axial locations. Mass flow controllers were used to blend the reactant gases which flow upward into the bed. The product gases exited to atmosphere at the top and were drawn into the lab ventilation system through a 4-inch duct containing a sulfur trap of Pyrex wool (rich mixture tests only).

The system was initially fired with methane and air to bring the reactor up to temperature and establish the combustion wave. The wave was then brought back to the bottom of the reactor and the methane gradually replaced by a H₂S:N₂ mixture. Methane was Matheson technical grade (98% CH₄), air was Matheson dry grade (99% air), and the H₂S mixture was Matheson analyzed gas mixture consisting of 20.33% H₂S in nitrogen.

Exhaust gases from the reactor were continuously drawn through a sulfur trap, which allowed elemental sulfur to condense and collect on the Pyrex wool. The exhaust air flow was estimated at 600 ft/min, or 52 scfm in a 4-inch duct. Following each test, the glass wool was removed for total sulfur assay. The sulfur assay was performed by grinding the wool with silica sand (sulfur content <0.01 wt%) and determining sulfur content with a LECO SC-132 sulfur analyzer. The sand was used both to homogenize the sample and reduce the sulfur content to within the working range of the analyzer.

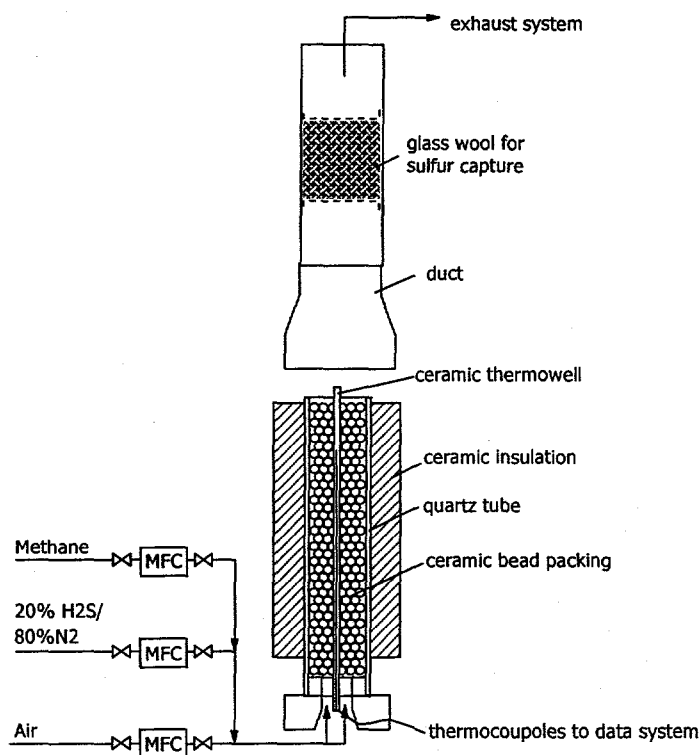


Figure 1. Experimental SAC Reactor System for H₂S Decomposition

A total of seven successful tests were performed, from which the test data are summarized in Table 4.

Tests LM-2, LM-3, and LM-4 were first performed with lean mixtures (equivalence ratio¹ $\phi < 1$) to determine whether a stable SAC wave could be obtained with H₂S as the only fuel. No sulfur collector was used in these tests, since it was not expected that any elemental sulfur would be produced under lean conditions. In these tests, a stable SAC wave was produced at a temperature of 1120-1130°F. The sulfur absorber was then installed, and tests RM-1 through RM-4 were then performed at rich conditions ($\phi > 1$). Again, a stable wave was established, and in these tests a measurable quantity of elemental sulfur was produced.

The data in Table 4 indicate that significant sulfur was produced in the stoichiometric range of $2.8 < \phi < 4.1$, but no sulfur was collected at the highest $\phi = 4.76$. Table 1 predicts a conversion in the range of 25-38% of H₂S at the temperatures and oxygen levels produced in these tests. While the amounts of sulfur collected was below predictions, it does not necessarily mean that the decomposition rate was lower than predicted. There are two possible causes of the lower collected sulfur amount: (1) inadequate collection efficiency of the glass wool trap, and (2) combustion of a portion of the elemental sulfur in a secondary diffusion flame at the exit of the reactor. Such a secondary flame was indeed observed by the operator at the end of the test series.

¹ Ratio of H₂S in the mixture to the H₂S required for stoichiometric combustion with oxygen to SO₂ and H₂O.

Table 4. SAC Experimental Test Data

Test #	LM-2	LM-3	LM-4	RM-1	RM-2	RM-3	RM-4
Temperature, °F	1121	1126	1130	1904	1931	1976	2012
Equivalence ratio	0.21	0.11	0.15	2.86	3.33	4.05	4.76
Time, h	2.77	1.58	1.62	1.97	1.62	1.19	0.99
Gas flows							
Air, sL/min	3.00	6.00	4.50	1.50	1.50	1.50	1.50
H ₂ S mixture, sL/min	0.50	0.50	0.50	3.00	3.50	4.25	5.00
H ₂ S, sL/min	0.10	0.10	0.10	0.61	0.71	0.86	1.02
H ₂ S, mol/h	0.26	0.26	0.26	1.55	1.80	2.19	2.58
O ₂ , mol%	18.0	19.3	18.9	7.0	6.3	5.5	4.8
Wave velocity, cm/h	12.9	24.0	18.5	16.6	18.5	21.2	24.0
Sulfur collected							
Appearance	nil	nil	nil	yellow fused solid	Yellow fused solid	yellow fused solid	brown stain
Quantity, g	nil	nil	nil	9.7	2.3	4.9	nil
Quantity, g mol	nil	nil	nil	0.31	0.07	0.16	nil
% of sulfur fed	nil	nil	nil	9.7	2.4	5.6	nil

Process Concept

The basic process concept encompasses the conversion of H₂S in an H₂S-rich waste stream to high-purity hydrogen and elemental sulfur. One concept for the application of SAC technology for this purpose is illustrated in Figure 2. H₂S-rich acid gas from an H₂S-selective amine system is mixed with a substoichiometric volume of air or enriched air before entering the SAC reactor. Gases exiting the reactor would include the H₂S decomposition products, hydrogen and sulfur vapor, as well as unreacted H₂S, water vapor, sulfur dioxide, and any contaminants. The exit stream would be cooled by heat exchange with recycled H₂S and possibly the acid gas feed. Sulfur vapor would be removed in a conventional sulfur condenser as a molten product, generating additional steam. The remaining H₂S, hydrogen, and nitrogen would be separated in a series of gas separation devices such as the separation membranes shown. Recycle of unconverted H₂S would be employed to maximize conversion, as discussed earlier.

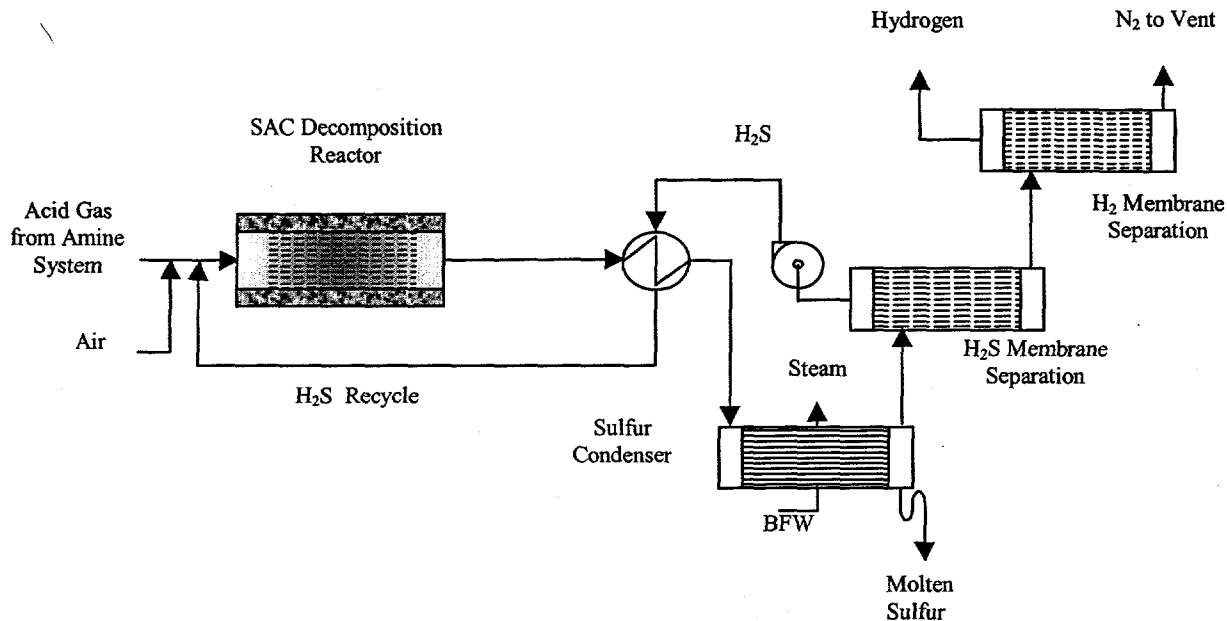


Figure 2. Conceptual Process Design for SAC-Based H₂S Decomposition/Hydrogen Recovery System

In addition to a practical SAC reactor design, an economical means for separation of unreacted H₂S and product hydrogen from residual water and other contaminants in the product gas stream is a critical consideration in the overall system design. Membrane technologies are under development for this purpose, although systems suitable for high-H₂S streams are not yet commercially available.¹³ Polyamide membranes yield good separation, but cannot currently handle more than 10% H₂S, and ceramic membranes operating via Knudsen diffusion have poor separation factors. A membrane based on surface diffusion is currently under development by Air Products and Chemicals, Inc. and offers some promise for this application.¹⁴ The membrane uses adsorption followed by permeation mechanisms, allowing significantly better separation factors than Knudsen diffusion membranes. Also, it is the H₂S, which preferentially permeates the membrane, meaning hydrogen is available with a minimum pressure drop.

Another decomposition system under development¹⁵ by Media & Process Technology employs a catalyst-impregnated membrane to enhance the decomposition of a high temperature H₂S stream while continuously removing hydrogen from the reaction products. A process scheme employing this high temperature hydrogen separation membrane, either with or without catalyst, might improve single-pass conversion and system economics by significantly reducing the H₂S recycle requirements and therefore the size of the front end components ahead of the recycle point.

The remaining system components would be either similar to those in the Claus plant (sulfur condensation and recovery) or consist of conventional equipment (blowers, heat exchangers, pumps, etc.). Depending on acid gas components and the membrane systems selected, additional equipment such as knockout drums, coalescing filters and guard beds may be required to protect the membranes.

One possible design concept for the SAC reactor for the decomposition of H_2S is shown in Figure 3. H_2S and oxidant are premixed and introduced at one end of the U-shaped reactor and pass into the reaction zone. Decomposition products exit the other end, giving up heat rapidly to the cooler ceramic packing. The flame front advances slowly to a control point, at which time the three-way valve positions are switched to reverse the flow, and the flame front begins to move in the other direction. A procedure is required to avoid contamination of the product stream with residual H_2S at the time of flow reversal. This can be done by purging the upstream zone with a fuel-air mixture (either natural gas-air or hydrogen-air from the products) for a short time just prior to flow reversal.

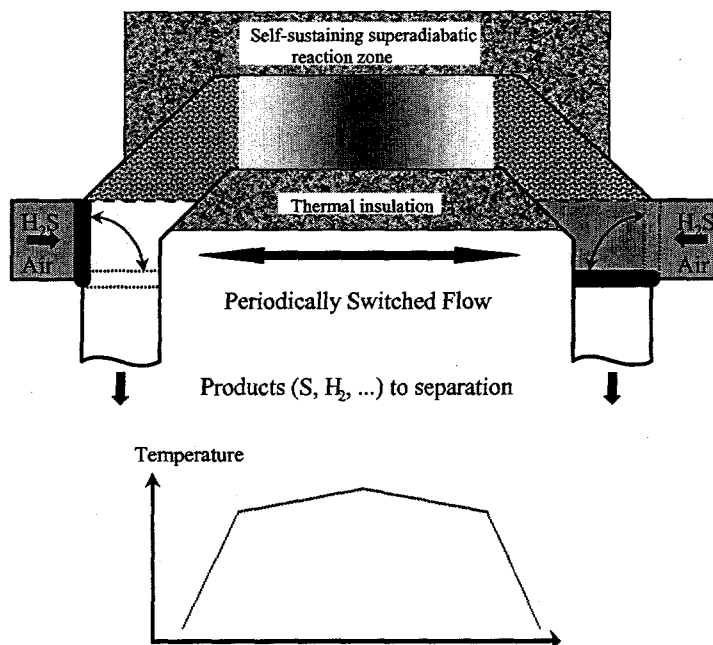


Figure 3. Conceptual Design for SAC-Based H_2S Decomposition Reactor

Integration of this switching-reactor concept into the process concept of Figure 2 would require a second recycle heater. A single sulfur condenser and membrane separation train would be used, with feed and reaction product streams switched from one end of the reactor to the other to maintain the moving flame front within the required control boundaries.

Another possible reactor design concept would employ a moving bed of ceramic beads to stabilize the combustion wave position and avoid the complications of the switching reactor configuration. While this approach introduces solids-handling issues into the design, they would involve relatively small amounts of solids transported for a short distance at manageable temperatures.

PHASE 1 ACTIVITIES

This research program is divided into two phases. In Phase 1, detailed thermochemical and kinetic modeling of the SAC H_2S decomposition reactor with H_2S -rich fuel gas and air/enriched

air feeds is undertaken to evaluate the effects of operating conditions on exit gas products and conversion efficiency, and to identify key process parameters. Preliminary modeling results are used as a basis to conduct a thorough evaluation of SAC process design options, including reactor configuration, operating conditions, and product/by-product separation schemes, with respect to potential product yields, thermal efficiency, capital and operating costs, and reliability, ultimately leading to the preparation of a design package and cost estimate for a bench-scale reactor testing system to be assembled and tested in Phase 2 of the program. A detailed parametric testing plan was also developed for process design optimization and model verification in Phase 2.

Phase 1 activities are described in detail below.

REACTOR MODELING

The objective of this task is to provide preliminary input information for the economic assessment of the process as well as the design of a bench-scale reactor system and the identification of key process variables.

This task was carried out, as a sub-contract to IGT, by the University of Illinois at Chicago (UIC) as a joint effort between the Energy Systems Laboratory and the High Temperature Laboratory. UIC led the modeling effort with input and review from IGT and the project's industrial partners (BP Amoco and UOP). Modeling of H_2S decomposition through superadiabatic combustion was undertaken by these two UIC research groups, which have extensive experience in physical and numerical modeling of non-reacting and reacting flows, combustion and pollutant chemistry, superadiabatic combustion, soot formation and plasma decomposition of H_2S . UIC researchers have, in fact, developed a kinetic mechanism of H_2S decomposition, which has been applied in this modeling effort.

Also, as cost-sharing for the sub-contract efforts, UIC researchers used their experimental facility, which is equipped to characterize combustion waves in porous media, to analyze comparatively filtration combustion waves in an inert porous medium for lean and rich H_2S -air mixtures. The purpose of this study was to qualitatively verify model predictions and the validity of hydrogen and elemental sulfur production through the superadiabatic combustion of H_2S -containing gases. Temperature, velocity, and chemical products of the combustion wave were studied experimentally in the range of equivalence ratios from 0.1 to 5.5. This range of reacting concentrations from ultra-lean to ultra-rich was used to explore applicability of the superadiabatic combustion concept to practical applications, such as utilization of low calorific fuels, low emission burners, pollution control devices, and fuel reforming and processing.

The model is based on computational models of filtration combustion waves developed for filtration combustion of ultra-rich methane-air mixtures. These include numerical programs for unsteady simulation of ultra-rich combustion waves with multi-step chemical mechanisms. Detailed mechanisms that were developed for H_2S combustion are used and then improved in constant comparison with complimentary experimental data on ultra-rich H_2S combustion. Superadiabatic combustion of ultra-rich H_2S /air mixtures is represented within a one-

dimensional, non-steady model, taking into account multi-step chemistry and separate energy equations for the gas and porous medium. The combustion wave propagation in an inert packed-bed is described by a system of conservation equations for gas energy, solid medium energy, mass fractions of gas species, and mass flow rates. The boundary conditions for the gas are imposed at the inlet and the exit of the reactor. A numerical model was developed to describe combustion wave characteristics in a coordinate system moving together with the wave front. Standard reaction flux/pathway and gradient sensitivity analysis technique will be applied at each step to identify important reaction pathways. The model is updated with kinetic mechanism of H₂S combustion compiled at UIC.

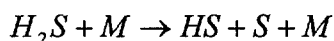
The combustion wave properties are strongly influenced by the superadiabatic reactor characteristics, in particular the effective heat conductivity of porous media or interfacial heat exchange, heat exchange rate between gas and solid material, and heat loss intensity, all of which should be accurately specified. The major factors controlling the combustion wave behavior under filtration in an inert porous medium are: (i) heat deposition in the gas phase due to fuel oxidation; (ii) forced convection of fuel/air mixture; (iii) longitudinal effective heat conductivity of the porous medium; (iv) intense interfacial heat exchange between gas and the solid frame; and (v) heat exchange between the porous medium and surroundings. The factors (i)-(iii) are accurately represented within the one-dimensional approach adopted in this investigation due to the high degree of radial uniformity of the combustion wave front found in the measurements for the reactor arrangement under consideration.¹⁶ The substantial radial non-uniformity can appear due to various instabilities. Superadiabatic wave propagation under the conditions where no instabilities occur is addressed in this work, and only axial profiles of temperatures, gas velocities, and species concentrations are of importance. The factors (iv)-(v) can be taken into account only parametrically, via the heat exchange in solid state energy equation, within a one-dimensional approach due to their explicit multi-dimensional nature.

The model developed in this work can provide a more accurate combustion wave description than models based on local volume-averaged treatment and well-mixed pore approximations. A H₂S/air mixture flows through a porous medium in a thermally insulated packed-bed and exits after reacting. The boundary conditions for the gas are posed at the inlet and exit of the reactor. The radiative transfer in the porous medium is described implicitly via the appropriate contribution into the effective thermal conductivity of the porous medium. The flame is assumed to be laminar, stable, and one-dimensional. Therefore, various instabilities, such as the thermo-diffusive instability,¹⁷ which forms multi-dimensional cellular structures, do not occur under the conditions considered in this study.

The numerical solution procedure is based on the finite difference formulation combined with the stiff equation integration subroutine DVODE. The one-dimensional laminar flame code PREMIX was used following various modifications, as deemed necessary for the task being undertaken. Accurate description of the very narrow combustion zone requires adaptive, non-uniform computational grids. In this computational model, a constant number of grid points are used, but their distribution over the axial coordinate is changed after a specified number of time steps. It was determined that 70-100 grid points provided sufficiently accurate solutions. The adaptive placement of the grid points (except two outmost points) is done to resolve accurately the gradient and the curvature of the gas temperature profiles, which undergo much sharper

changes in time and space than the solid profiles. The numerical algorithm implemented in the PREMIX code was used to find the combustion wave velocity.

The Chemkin subroutines were used to implement the chemical kinetics description¹⁸ and the Transport subroutine¹⁹ was used to calculate gas properties. Two chemical kinetic mechanisms were used. The first mechanism, developed by the Frenklach's group,²⁰ includes 17 species and 47 reactions, and is considered more appropriate under combustion conditions (i.e., moderately high equivalence ratios). The second kinetic mechanism was developed at UIC to describe more accurately the partial oxidation of H₂S (i.e., ultra-high equivalence ratios). In the second kinetic mechanism the thermal decomposition of H₂S according to the following reaction



is described with a rate constant of $1.76 \cdot 10^{16} \exp(-66210/RT)$, while the corresponding rate constant in the first mechanism is $4.63 \cdot 10^{14} \exp(-82469/RT)$, which is considerably smaller than the previous one.

Detailed information about initial and boundary conditions and model and solid-phase properties are provided in UIC's report, attached in Appendix A. Inasmuch as possible, all simulation parameters were selected to correspond to the conditions of previous experimental work at UIC,¹⁶ where characteristics of combustion waves, concurrent with filtration flow through a packed-bed column of porous alumina, were studied.

Simulations of ultra-rich combustion of H₂S/air mixtures were carried out over a range of equivalence ratios (1 to 5), flow rates, and other packed-bed parameters. Particular consideration is given to the optimization of hydrogen production via the ultra-rich superadiabatic combustion of hydrogen sulfide, where the overall process could be characterized as combustion-based fuel modification. Other considerations include:

- Development of numerical models for prediction of output hydrogen concentrations in linear and reverse-flow superadiabatic combustors;
- Production of preliminary database to assist in the design of the SAC H₂S decomposition process; and
- Optimization of hydrogen production, by-product composition, and energy consumption based on results of numerical simulations.

Preliminary numerical modeling of the SAC reactor has been performed. The parameters considered in the modeling effort included fuel gas composition (i.e., H₂S-rich and H₂S-lean), oxidant composition (air/enriched air), equivalence ratio, superficial gas velocity, feed gas temperature (pre-heating effect), and product gas quenching. The products of partial H₂S oxidation, hydrogen (H₂) and elemental sulfur (S₂), are dominant for ultra-rich superadiabatic combustion, which is essentially a fuel reforming reaction. The chemistry in the combustion wave is modeled and species and temperature profiles are predicted. A database of H₂S conversion is generated in a wide range of equivalence ratios and other process parameters.

The major conclusions from the modeling predictions obtained are:

- In oxygen-enriched air (i.e., 30% O₂-N₂ gas mixture), conversions of H₂S to hydrogen and elemental sulfur are better than when pure oxygen is used as the oxidant.
- Product gas quenching can substantially increase the selectivity of H₂S conversion to H₂; however, the selectivity of H₂S conversion to elemental sulfur decreases. For example, at typical filtration velocities ranging from 20 to 30 cm/s, equivalence ratios of about 2-3, and oxygen-enriched air containing about 20-40% O₂, H₂S conversion to hydrogen is about 20% and H₂S conversion to elemental sulfur is about 60%. With quenching of product gas, H₂S conversion to hydrogen and elemental sulfur is about 35% and 25%, respectively.
- Water addition to the initial mixture does not improve the reactor performance with respect to hydrogen and elemental sulfur production.
- When air is used as the oxidant, conversion of H₂S to H₂ decreases as filtration velocity increases. In contrast, when pure oxygen is used as the oxidant, increasing the filtration velocity plays a positive role.
- SAC reactor performance can be significantly improved by separating and recirculating unreacted H₂S in the product gas.

Based on the developed numerical model, optimization studies of hydrogen production were conducted by varying the characteristics of ultra-rich superadiabatic waves. The major findings appear to indicate that by optimizing the porous body reactor configuration, equivalence ratio, and filtration velocity, the overall H₂S decomposition in a single pass can be as high as 30-50%, with a conversion of H₂S to the desirable product hydrogen (H₂) reaching a level of 30%. This reactor performance can be obtained using equivalence ratios in the range of 10 to 15, while maintaining a filtration velocity greater than 100 cm/s. For these high values of equivalence ratio and filtration velocity, the combustion temperature is considerably higher than the adiabatic combustion temperature, which is in fact too low for combustion to take place in the gas phase. Such high temperature promotes the decomposition of H₂S, the hydrogen (H₂)/water (H₂O) selectivity, and the elemental sulfur (S₂)/sulfur dioxide (SO₂) selectivity. Given that in a single pass the H₂S decomposition can reach 30-50%, the overall process performance can be substantially improved, with respect to hydrogen production, by membrane separation of product gases and recirculation of unreacted H₂S. It can be shown that in 4 to 5 passes nearly total hydrogen sulfide decomposition into sulfur can be realized, with recovery of 30-40% of the hydrogen component.

The most optimum scenario in the results of the numerical modeling indicates that, with feed gases entering the reactor at ambient temperature, a maximum temperature of 1631 K can be achieved in the SAC reactor, resulting in an overall H₂S conversion of 50%, with a hydrogen (H₂)/water (H₂O) selectivity of 57/43 and an elemental sulfur (S₂)/sulfur dioxide (SO₂) selectivity of 99/1.

The results of the experimental investigation undertaken at UIC indicate that certain products,

oxygen, sulfur dioxide, and sulfur, correlate fairly well with model predictions. Others, notably hydrogen, diverge over the whole range of rich mixtures. Hydrogen in the products is present after stoichiometry and maximizes at $\phi=2$ to achieve a maximum conversion rate of 20% based on the hydrogen sulfide input. Its production fell rather gently thereafter to where nothing is gained by equivalence ratio of 5.5. The concentration of unreacted hydrogen sulfide rises linearly with equivalence ratio at post-stoichiometry. Some sulfur based products peaked at the extremities: sulfur dioxide at stoichiometry (100% conversion), and elemental sulfur (50% conversion) at $\phi=4$. Finally, the formation of sulfuric acid in ultra-lean combustion was qualitatively verified. Detailed modeling results were presented in a final report submitted to IGT (see Appendix A).

These predictions have offered valuable guidelines for the preparation of a design and cost estimate of a suitable bench-scale reactor testing system to be assembled and tested in Phase 2 of the program. Modeling efforts also made possible the identification of key SAC process parameters and the preparation of a parametric testing plan for Phase 2. The chemical kinetic mechanisms used in the formulation of this preliminary model will be updated based on direct comparison with the experimental data that will be obtained in Phase 2, further enhancing the reliability of the model and its capabilities to explore conditions not explored experimentally.

LAB-SCALE TESTING SYSTEM DESIGN

To develop the necessary experimental data to demonstrate the technical and economical viability of the SAC H_2S decomposition process, a bench-scale testing system has been designed for H_2 production from thermal decomposition of up to 1,400 standard cubic feet per hour (SCFH) of H_2S -oxidant gas mixture. The schematic diagram of the overall process is shown in Figure 4. In the proposed testing system, predetermined amounts of feed gas components are mixed and delivered to a packed-bed reactor where H_2S is converted to H_2 and S at high temperatures. Hot off-gas leaving the reactor is cooled with a cooling medium in a condenser where sulfur vapor ($S(g)$) is condensed and collected. Cooled gas is then scrubbed with a caustic solution where H_2S and sulfur dioxide (SO_2) are removed and the cleaned gas is discharged to the atmosphere.

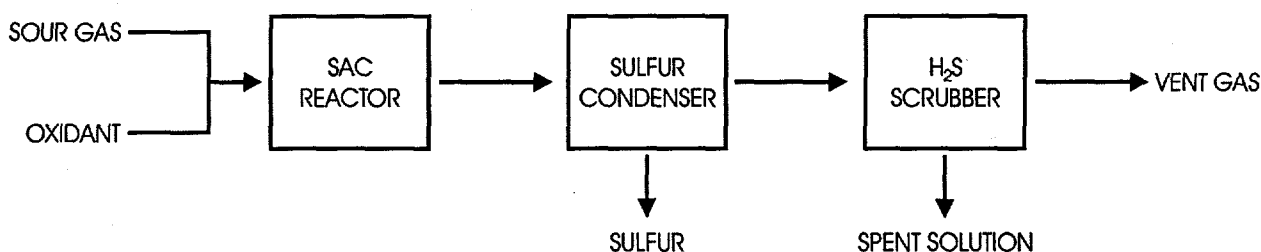


Figure 4. Process Schematic Diagram for a Bench-Scale Testing System

The major equipment for the proposed bench-scale testing system includes: a gas mixing chamber, a reactor, a thermal fluid cooler, a thermal fluid pump, a sulfur condenser, a gas

scrubber, a caustic tank, a recirculating caustic pump, and a makeup caustic pump. The information required for design, engineering, procurement and installation of this system including the system description, equipment design, and equipment specifications is presented in a design package attached in Appendix B. The total purchased equipment cost is estimated at \$94,300 and the estimated total installed cost (TIC) for the bench-scale testing system, based on vendor quotations and engineering estimates, is \$292,000. A brief description of the system is given below.

H₂S, oxygen (O₂) and nitrogen (N₂) feed gases, supplied from individual compressed gas cylinders, are de-pressurized and delivered at ambient temperature at pre-determined flow rates (i.e., equivalence ratios) to a mixing chamber where the feed gases are thoroughly mixed. The pre-mixed gas mixture is then fed to a reactor. Three-way valves and by-pass pipings are used to allow the feed gas mixture to be fed to the reactor in an upflow or a downflow mode.

The reactor is a vertical, cylindrical tube packed with ¼-inch diameter alumina pellets where H₂ is produced by superadiabatic decomposition of H₂S at high temperatures. The decomposition reaction of H₂S is endothermic and requires high temperatures to proceed. In the reactor, a portion of H₂S is combusted with O₂ to provide the thermal energy required for the decomposition reaction. The intense heat exchange between the hot gas mixture and the porous medium allows the accumulation of energy in the solid matrix and consequently results in reactor flame temperatures that are much higher than the adiabatic flame temperatures of the feed gas mixture. The high reactor temperatures promote the progression of the decomposition reaction.

A schematic diagram describing reactor details is presented in Figure 5. The reactor consists of a vertical, cylindrical carbon steel shell (21-inch ID x 21.5-inch OD x 72-inch H) lined with 6-inch thick rigid fibrous (low thermal conductivity) ceramic insulation. An impervious ceramic tube (6-inch ID x 7-inch OD x 72-inch H) containing 99+% alumina is used as the inner reactor tube to contain the alumina packing and reactor gases. A 3-zone, silicon carbide or molybdenum disilicide electric heater is located in the space between the ceramic tube and the insulation to provide auxiliary heat for cold startup and temperature control (total heat duty: 30 kW; maximum temperature: 2800°F; 3 16-inch long heating zones). Support and hold-down plates are used to support and contain the alumina packing and ceramic insulation (packing height: 60 inches; packing weight: 130 lbs). High-temperature gaskets are used in the ceramic-metal joints and the flanged connections to prevent any leakage of reactor gases.

All insulation materials with low thermal conductivity are porous. The porosity of castable refractory may vary from 20 to 50% depending on the compositions, densities, and installation and curing methods. The porosity of rigid ceramic fiber insulation, which has much lower thermal conductivity than castable refractory, can be as high as 85%. The porosity of the fixed bed packed with alumina pellets is about 40%. Therefore, an impervious ceramic tube is needed as the inner reactor tube such that all feed and reactor gases flow through the packed bed and no gas will by-pass or channel through the porous insulation layers. Furthermore, the reactor gases containing H₂ may attack the high temperature silicon carbide or molybdenum disilicide heating elements, which reduces the efficiency of heating elements. The ceramic tube prevents any direct contact of heating elements with reactor gases.

A carbon steel shell is placed outside of the inner reactor tube to prevent reactor gases from leaking to the atmosphere, should there be a rupture or a crack in the inner reactor tube. The outer metal shell is lined with layers of rigid fibrous ceramic insulation such as Zircar AL-30AAH and ALC. These low-density (less than 30 lb/ft³) insulation materials have lower thermal conductivity and provide better thermal insulation than castable refractory at high temperatures.

A vertical fixed-bed reactor packed with ¼-inch diameter alumina pellets is used to facilitate the thermal decomposition of H₂S via superadiabatic combustion. A reactor diameter of 6 inches (15 cm) is used so that the data generated from the bench-scale reactor can be used for future scale-up design. The maximum superficial and interstitial gas velocities of 2 ft/s (60 cm/s) and 5 ft/s (150 cm/s), respectively, are used based on modeling and experimental studies conducted at the University of Illinois at Chicago (UIC). The superficial gas velocity is defined based on the feed gas flow rate in an empty reactor column at ambient conditions; the interstitial gas velocity is also defined based on the feed gas flow rate in the interstitial space of the alumina packing at ambient conditions. A minimum gas residence time of 2 seconds in the packed-bed of the reactor based on the maximum superficial gas velocity is used to ensure complete conversion of decomposition reaction. This results in a packing height of 48 inches. Based on these conditions, the proposed reactor is capable of processing about 1,400 SCFH of total feed gas mixture containing H₂S and oxidant. The estimated pressure drop across the packed-bed at maximum gas throughput ranges from 0.7 to 1.6 psi at average gas temperatures ranging from 1000 to 2500°F (538 to 1371°C). The reactor is designed for a maximum pressure of 3 psig.

The alumina pellets are randomly packed and supported by a perforated grid plate. A hold-down plate is used at the top of the reactor to prevent the packing pellets from being blown out of the reactor. A thin layer of high-temperature insulation blanket is used to cover the inner wall of the reactor tube to minimize the effect of differential thermal expansion between the ceramic tube wall and alumina pellets. The instrumentation for the reactor includes thermocouples placed inside a thermowell located along the axis of the reactor, a pressure indicator, a differential pressure transmitter for pressure drop across the packing, and a pressure relief valve. A set of three-way valves located at the inlet and outlet of the reactor and by-pass pipings is used to allow the feed gas mixture to be fed to the reactor in an upflow or a downflow mode.

Off-gas leaving the reactor (containing H₂, elemental sulfur, H₂S, SO₂, N₂, and water vapor) is maintained at temperatures above the dew point of S_(g) to prevent any condensation of S_(g) in the reactor (at a minimum temperature of 800°F). Hot off-gas is fed to a sulfur condenser where the gas is cooled and sulfur vapor is condensed and collected. The sulfur condenser is a vertical, tube-and-shell heat exchanger where the off-gas flows downward in the tube side and the cooling medium flows counter-currently in the shell side. Liquid sulfur (S_(l)) is drained by gravity and collected in an electrically traced sulfur drum. Temperatures of the liquid sulfur are controlled at about 300°F (149°C) to maintain a low viscosity for the liquid sulfur. Cooled gas is then scrubbed with caustic solution in a countercurrent, multiple-spray type of gas scrubber where SO₂ and unreacted H₂S are removed. The cleaned gas is then discharged to the atmosphere.

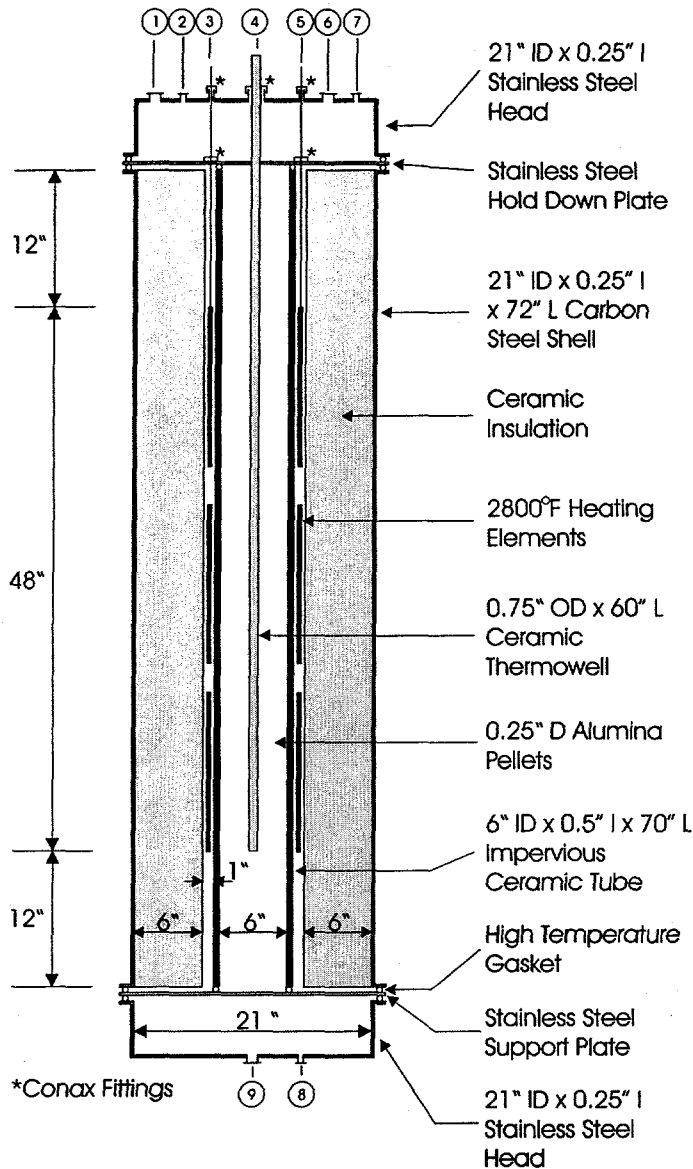


Figure 5. SAC H₂S Decomposition Reactor Details

One concern of using cooling water as the cooling medium for the sulfur condenser is that the water inlet temperature is much lower than the temperatures of the condenser off-gas and liquid sulfur. This large temperature difference may cause some temperature control problems such as over cooling the gas and S_(l), which can result in potential plugging due to increased viscosity of S_(l) at lower temperatures. This problem can be overcome by using a waste heat boiler type of sulfur condenser, which is the conventional design for most commercial-scale units, or a thermal fluid system such as Dowtherm with the inlet and outlet temperatures of the thermal fluid maintained close to the temperature of S_(l). Both systems are complicated and expensive due to the need of additional equipment, instrumentation, and control. The use of a thermal fluid system also requires a much larger sulfur condenser due to the decreased driving force for heat transfer, i.e., the log mean temperature difference.

Thermal fluid is used as the cooling medium in the condenser. Returned hot thermal fluid leaving the condenser is cooled with city water in a cooler. Cooled thermal fluid leaving the cooler is then pumped by the thermal fluid pump and returned to the condenser.

Process gas stream leaving the sulfur condenser is scrubbed with caustic solution in a countercurrent spray column where unreacted H_2S and SO_2 are removed. The condenser off-gas contains trace amount (less than 0.1 vol %) of $\text{S}_{(\text{g})}$ which may be condensed in the scrubber when the gas is cooled. This precludes the use of a packed or a tray column due to the potential plugging from sulfur condensation. A spray column is used because of its low capital cost, easy maintenance, operational flexibility, and low pressure drop. Multiple spray nozzles are used to improve the removal efficiency. A recirculating caustic pump provides caustic solution to the spray nozzles. Fresh caustic solution is pumped from a storage tank using a makeup caustic pump to a gas scrubber for maintaining a constant liquid level in the scrubber. Caustic solution (aqueous alkaline solution) is selected as the scrubbing liquid because of its high removal efficiency and low liquid-to-gas loading requirement which is about 6 times lower than that for potassium carbonate solution. This would simplify the handling and disposal of spent scrubbing liquid. The diameter of the gas scrubber is determined from the flooding velocity calculations for a spray column. The height of the scrubber is determined by calculations of transfer height and numbers of transfer unit based on liquid droplet size and an empirical correlation for mass transfer coefficient for a spray column. Clean gas leaving the top of the scrubber and is discharged to the atmosphere.

PHASE 2 DEVELOPMENT PLAN

The objective of Phase 2 is to develop the necessary experimental data to demonstrate the technical and economical viability of the SAC H_2S decomposition process. Also in Phase 2, industrial partnership for market evaluation and future commercial demonstration will be finalized. Phase 2 consists of the following 6 tasks:

- Task 1. Bench-Scale SAC Reactor Unit Construction
- Task 2. Reactor Modeling Studies
- Task 3. Bench-Scale Unit Operation
- Task 4. Technical Feasibility Verification
- Task 5. Economic Validation
- Task 6. Management and Reporting

Task 1. Bench-Scale SAC Reactor Unit Construction

The bench-scale SAC H₂S decomposition reactor will be installed (by a suitable vendor) in a separate and totally enclosed laboratory space to be provided in IGT's Emerging Energy Technology Campus (EETC). This newly constructed applied research facility is situated within walking distance from IGT's Headquarters in Des Plaines, IL. This facility houses several test furnaces, including 10- and 3-MMBtu/h boiler simulators; a 1.2-MMBtu/h heat treat furnace complete with a quench tank, a loading cart, and an endothermic gas generator; a 5-MMBtu/h modular test furnace; a 3-MMBtu/h submerged combustion melter; a 1.3-MMBtu/h low inertia furnace which utilizes flat radiant panels; and a 1-MMBtu/h high-temperature test furnace. Also in the facility are a wide variety of prototype and industrial burners, modular gas and air control skids, air heating skids, portable data acquisition rigs, and 4 complete sets of continuous emissions monitors (NO_x, CO, THC, O₂, and CO₂) available for laboratory and field use.

The bench-scale SAC reactor unit will consist of the following:

- A fuel gas/oxidant conditioning system to generate appropriate inlet gas mixtures
- A packed-bed reactor system
- A sulfur condenser and recovery subsystem
- An exit gas scrubbing subsystem
- Equipment for sampling and analysis of H₂S decomposition products

A bench-scale testing system is designed for hydrogen (and elemental sulfur) production from thermal decomposition of up to 1,400 standard cubic feet per hour (SCFH) of H₂S-oxidant gas mixtures. In the proposed testing system, predetermined amounts of feed gas components are mixed and delivered to a reactor packed with inert pellets where H₂S is converted to hydrogen and elemental sulfur at high temperatures. Hot off-gas leaving the reactor is cooled with a cooling medium in a condenser where sulfur vapor (S(g)) is condensed and collected. Cooled gas is then scrubbed with a caustic solution where sulfur dioxide (SO₂) and unreacted H₂S are removed and the cleaned gas is discharged to the atmosphere.

A design package for the bench-scale testing system being proposed for Phase 2 is provided as an attachment (see Appendix B). The information required for design, engineering, procurement, and installation of this system including the system description, equipment design, and equipment specifications is presented in the attached report. The estimated total installed cost (TIC) for the bench-scale testing system, based on vendor quotations and engineering estimates, is \$292,000.

Important features of the designed bench-scale SAC reactor system include:

- A reactor diameter of 6 inches (15 cm) is used so that the data generated from the bench-scale testing can be used for future scale-up design.
- A minimum gas residence time of 2 seconds in the packed-bed of the reactor (based on the maximum superficial gas velocity) is used to ensure complete conversion of the H₂S decomposition reaction.
- The designed reactor is capable of processing up to 1,400 SCFH of total feed gas mixture containing H₂S and oxidant.
- The estimated pressure drop across the packed-bed at maximum gas throughput ranges from 0.7 to 1.6 psi at average gas temperatures ranging from 1000 to 2500°F (538 to 1371°C).
- The reactor consists of a vertical, cylindrical carbon steel shell (21-inch ID x 21.5-inch OD x 72-inch H) lined with 6-inch thick rigid fibrous ceramic insulation. An impervious ceramic tube (6-inch ID x 7-inch OD x 72-inch H) containing 99+% alumina is used as the inner reactor tube to contain the inert pellets and reactor gases.
- A 30 kW 3-zone, silicon carbide or molybdenum disilicide electric heater is located in the space between the ceramic tube and the insulation to provide auxiliary heat for cold startup and temperature control.
- Support and hold-down plates are used to support and contain the inert pellets and ceramic insulation.
- High-temperature gaskets are used in the ceramic-metal joints and the flanged connections to prevent any leakage of reactor gases.

Following installation of the bench-scale SAC reactor unit, the operability of the individual system components will be verified. Shakedown runs will then be performed to confirm the integrated system operability and the control, instrumentation, and sampling system reliability. Equipment and instrument inspections, sample analysis, and data evaluations will be performed after each shakedown run, and equipment and system modifications made as necessary.

Task 2. Reactor Modeling Studies

The objective of this task is to provide guidelines for the operation of the bench-scale reactor unit according to a prepared test plan. As a sub-contractor to IGT, UIC will utilize the numerical model that was developed in Phase 1 of this program to predict process performance (i.e., overall H₂S conversion, H₂/H₂O selectivity, S₂/SO₂ selectivity, etc) over a range of operating conditions, including equivalence ratios, flow rates, and other packed-bed reactor parameters. Each set of conditions for the numerical simulations will be carefully selected by IGT. The previously developed numerical model of rich and ultra-rich filtration combustion (FC) of H₂S-containing

fuel/oxidant gas mixtures will be modified as necessary to best simulate the designed bench-scale reactor configuration and its operating conditions. The results obtained will help in the selection of suitable sets of operating conditions for the installed reactor system, within the ranges of operating parameters specified in the test plan (see Task 3 below). As before, particular consideration will be given to the hydrogen production via ultra-rich superadiabatic combustion of H₂S, where the overall process could be characterized as combustion-based fuel modification. These numerical studies are expected to:

1. Define the structure and properties of filtration combustion waves including reaction and chemical product information,
2. Improve raw numerical models for prediction of output hydrogen concentrations in superadiabatic combustors,
3. Optimize the hydrogen production, by-product composition, and energy consumption based on results of numerical simulations

Modeling studies of H₂S decomposition through SAC have been conducted based upon computational models of filtration combustion waves in a porous media developed for ultra-rich filtration combustion of methane/air mixtures. These include numerical programs for unsteady simulation of ultra-rich combustion waves with multi-step chemical mechanisms. Superadiabatic combustion of ultra-rich H₂S/air mixtures is represented within a one-dimensional, non-steady model, including separate energy equations for the gas and porous medium. The boundary conditions for the gas are imposed at the inlet and the exit of the reactor. Standard reaction flux/pathway and gradient sensitivity analysis techniques are applied at each step to identify important reaction pathways.

UIC will lead the modeling effort with review and process/mechanical design input from IGT and UOP.

Task 3. Bench-Scale Unit Operation

The objective of this task is to determine the optimum operating conditions to maximize the SAC reactor temperature, thereby optimizing the overall H₂S conversion, the hydrogen/water selectivity, and the elemental sulfur/sulfur dioxide selectivity. The scope of work in this task is estimated to comprise about 40 tests and extend over a period of 9 months. Tests are designed to assess the effect of key operating variables that have been identified for the operation of the process based on numerical modeling results during Phase 1. These key process parameters are listed below along with a summary in Table 5 of the ranges recommended for experimental exploration. Suitable values of each process parameter will be selected based on the detailed modeling efforts to be conducted in Task 2.

- Inlet fuel gas composition (H₂S-rich, H₂S-lean, simulated gas composition from a typical refinery, etc.)

- Inlet oxidant gas composition (oxygen/nitrogen ratio: air, enriched air)
- Equivalence ratio (defined as the ratio of the amount of O₂ that is stoichiometrically required to combust all H₂S in the fuel gas to the amount of O₂ available)
- Type of inert pellets (pellet heat capacity)
- Pellet porosity (for optimum type of pellet)
- Diameter of inert pellets (0.3 cm has been used by UIC previously; they recommend decreasing this size by 3-10 times)
- Interstitial or filtration gas velocity (defined based on the feed gas flow rate in the interstitial space of the alumina packing at ambient conditions)
- SAC reactor temperature (this will be determined by the operating conditions, but can also be artificially maintained at a certain level through external heat input to further promote H₂S decomposition reaction)

Table 5. Ranges of Key Process Parameters

Key Process Parameter	Recommended Range
H ₂ S Fuel Gas Content, vol%	10 - 50
O ₂ Oxidant Content, Vol%	21 - 100
Equivalence Ratio	5 - 20
Type of Inert Pellets	2 - 4
Pellet Porosity, %	20 - 60
Inert Pellet Diameter, mm	1 - 5
Filtration Velocity, cm/s	75 - 150
SAC Reactor Temperature, °C	1300 - 1500

The following major process measurements will be made:

- Inlet gas flow rate, temperature, and pressure
- Inlet gas composition (major constituents)
- Inlet gas H₂S and O₂ content
- SAC reactor temperature and pressure
- Pressure drop across the packed-bed
- Exit gas flow rate, temperature, and pressure

- Exit gas composition
- Amount of elemental sulfur collected
- Amount of water collected

Task 4. Technical Feasibility Verification

In this task, the data developed in Task 3 will be thoroughly analyzed to assess the performance of the SAC H₂S decomposition reactor. Under each set of operating conditions, the extent of H₂S conversion will be determined and its distribution between the desirable hydrogen product and water will be quantified. Sulfur distribution among the desirable elemental sulfur product, sulfur dioxide, water, and unreacted H₂S will also be quantified. Optimum operating conditions will be identified and the technical feasibility of the process under these conditions will be evaluated. The original conceptual layout of the SAC process (shown in Figure 2) will be revised according to the results obtained.

The project team will develop a process design for the integrated H₂S to hydrogen and sulfur process. The system will consist of 5 subsystems: Acid-Gas Preconditioning, SAC Reactor, Sulfur Recovery, Gas Separation and Recycle, and Hydrogen Delivery. The required unit operations will be determined for each subsystem, based on the SAC reactor operation and performance as determined in Task 3. The various parameters that will be specified include SAC reactor feed requirements (H₂S concentration, oxygen or enriched air), gas velocities, operating temperature and pressure ranges, reactor configuration (continuous or switching, internal and/or external product gas cooling), purge requirements, porous media characteristics, H₂S decomposition conversion and recycle requirements, side reactions, sulfur condensation, availability and performance of suitable gas separation devices, product hydrogen and sulfur purity, hydrogen delivery pressure, and system control requirements.

In addition to technical issues, other factors will be considered in the development of an integrated SAC H₂S decomposition reactor, including:

- Feedstocks: availability of acid gas waste streams, proximity to hydrogen end-users, composition including H₂S concentration, CO₂, N₂, moisture, and trace hydrocarbon contaminants;
- Product Markets: Hydrogen and sulfur market size, price fluctuation, required hydrogen delivery conditions.

IGT will conduct the process design study with input from UIC, UOP, and BP Amoco.

Task 5. Economic and Market Validation

Economic benefit from the technology may be realized both by improvement in sulfur recovery

efficiencies as well as by-product hydrogen production. Evaluation of potential markets will therefore include analysis of both the sulfur recovery markets as well as hydrogen and sulfur end-user markets. Factors considered in the analysis will include:

- Current and projected hydrogen and sulfur prices
- Current hydrogen sulfide sour gas treatment processes
- Status of competing hydrogen production and combined hydrogen and sulfur recovery processes under development
- Current size and demand projections for the various hydrogen market sectors, including petroleum refining, ammonia, methanol, and fuels
- Current size and demand projections for sulfur market sectors, including sulfuric acid, fertilizers, etc.

Information on the sulfur recovery, hydrogen and sulfur markets will be used to determine the most favorable potential settings for deployment of the SAC hydrogen sulfide decomposition technology.

IGT will conduct the market and economic study with industry input from UOP and BP Amoco.

Task 6. Management and Reporting

IGT will manage the project and be responsible for all project activities and coordination with project team members. An industrial advisory group will be formed to provide guidance for the successful development of a commercially viable hydrogen production process. In addition, IGT will communicate technical progress and financial status to DOE throughout the duration of the project. Two detailed Technical Progress Reports and a Final Report will be submitted during the course of the proposed program. The first Technical Progress Report will be submitted at the end of Task 1 and will contain complete documentation of the installed SAC H₂S decomposition reactor and the results of the shakedown tests. The second Technical Progress Report will address the technical feasibility of the SAC H₂S decomposition process, based on thorough analyses of all experimental data collected in Tasks 2 and 3. Viability of the process within economic and market constraints will be discussed in the Final Report along with plans for commercial demonstration at an industrial site.

Project Schedule

The schedule for the proposed Phase 2 process development effort is illustrated in Figure 6. The project will begin with the construction and shakedown of the bench-scale reactor unit. In parallel with these efforts, UIC will conduct a detailed modeling study. IGT and UOP will monitor and review the modeling effort on a regular basis to direct it as necessary toward the

information required for the final selection of most suitable operating parameters, within the ranges specified in the test plan. The SAC H₂S decomposition bench-scale unit will then be operated according to the test plan, to address the effect of key variables on process performance. Technical feasibility of the process will then be verified as data are generated. Commercialization potential for the process will be assessed, with input and assistance from industrial advisors, taking into consideration market and economic constraints. When sufficient process performance data and market information become available to confirm the technical and economic parameters governing a successful development, process commercialization activities will be initiated. It is estimated that the above activities will require 24 months to complete.

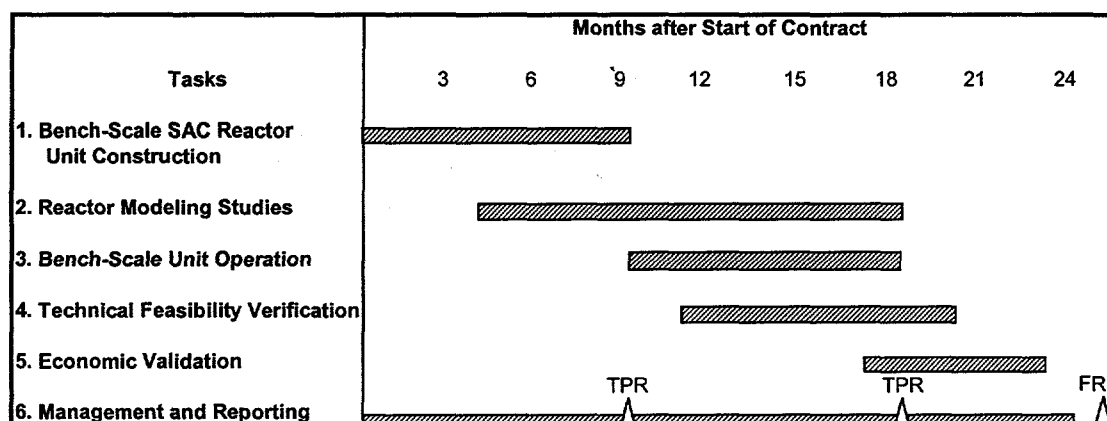


Figure 6. Project Schedule

Project Deliverables

The Phase 2 project deliverables will include the following:

- Complete documentation of installed bench-scale SAC H₂S decomposition reactor system
- Results of shakedown tests
- Results of detailed numerical modeling studies
- Results of the planned tests and evaluation of process technical feasibility and economic viability
- Plan for integrated demonstration of the SAC process at an industrial site

MARKET AND ECONOMIC STUDY

Hydrogen sulfide (H₂S) is present in the industrial world chiefly as an undesirable by-product of fossil fuel processing, including natural gas, petroleum, and coal. In natural gas, H₂S is the primary sulfur component, along with lower levels of hydrocarbon sulfides (mercaptans). In petroleum, H₂S appears at various stages in the refining process, and it must be removed to facilitate the production of low-sulfur liquid fuels. H₂S also appears in coal gasification and is generally removed prior to fuel gas utilization.

Conventional technologies in use to decompose H₂S (Claus, Superclaus, and variations thereof) produce elemental sulfur as a by-product, which sells for about \$30/ton. However, the hydrogen present in the original H₂S leaves the process as water. At the same time, hydrogen is in demand at petroleum refineries and other facilities such as ammonia synthesis plants. The value of hydrogen in these applications exceeds its fuel value, and so it may be worthwhile to recover the hydrogen as H₂ from the H₂S, if an economical and reliable process can be found to do so.

Worldwide installed sulfur recovery capacity is estimated at 128,000 ton/day,²¹ which is about evenly divided between petroleum and natural gas, with some dual-purpose facilities and a small fraction (less than 2%) associated with chemical processing, coal gasification, etc. Twenty-eight percent (28%) of the total sulfur recovery capacity exists in the U.S., of which 29% is accounted for by natural gas and 70% by refinery gases. 128,000 ton/day of sulfur recovery capacity corresponds to approximately 136,000 ton/day of hydrogen sulfide processing capacity worldwide. With sulfur recovery units operating at an average of 50% capacity, and assuming that 75% of the available hydrogen can be recovered, the potential recovery of hydrogen gas is about 3,000 ton/day (5×10^7 scfh), of which the U.S. portion is 870 ton/day (1.37×10^7 scfh).

Total hydrogen consumption in the U.S. totaled 3.1×10^{12} scf in 1997 or 354×10^6 scfh.^{22,23} Ammonia manufacture consumes 40% of this amount, followed by petroleum refining at 39.5%, methanol production at 10%, and all other users consuming the remaining 10.5%. About 95% of the hydrogen used in the U.S. market is produced by steam methane reforming. The next most common method of hydrogen recovery is extraction from gaseous byproducts of other industrial processes, followed by electrolysis.

Petroleum

In the petroleum industry, hydrogen is used for hydrocracking and hydrotreating to produce fuels with low sulfur and aromatics content. Hydrotreatment, in turn, is the main source of H₂S requiring destruction. The estimated²² in-house hydrogen usage by the U.S. petroleum industry for 1997 was 141×10^6 scfh. Based on the sulfur recovery data,²¹ about 13% of this could be supplied from H₂S decomposition units.

Natural Gas

Based on recent surveys, about 15-25% of natural gas has H₂S levels high enough (> 5 ppm) to require treatment.²⁴ The natural gas industry does not use hydrogen *per se* like the oil industry does, but since much of the natural gas is located in the same areas as the oil deposits and the associated refineries, there are nearby markets for hydrogen obtained from natural gas sweetening as well. Ammonia synthesis plants also tend to be near natural gas supply since most of the hydrogen used by those plants is produced by natural gas reforming. It is believed that the H₂S associated with natural gas upgrading in the U.S. alone (5300 ton/day at 50% capacity) could produce 4.6×10^6 scfh of hydrogen gas, which is about 3 percent of the estimated hydrogen usage by U.S. ammonia plants.

Gasification

Gasification technologies have been commercialized by Texaco, Shell, and others, including IGT. Current and near-term applications of gasification technology are primarily in refinery settings, such as the Texaco refinery in El Dorado, Kansas, and a number of plants in Europe. Gasifiers accept a wide range of fuels, including high-sulfur coal and wastes. When employed in an IGCC configuration, gasification products can include a flexible mix of synthesis gas, steam, and electric power. A major environmental advantage of gasification is that sulfur in the fuel is reduced to H_2S , which is readily removed from the synthesis gas by commercially-available cold gas cleanup methods. As more IGCC systems are deployed, a significant amount of hydrogen can be recovered from the concentrated H_2S streams produced by these systems.

The current annual growth in gasification is about 3000 MW_{th} of synthesis gas, or about 7% of the total operating worldwide capacity. The cumulative worldwide gasification capacity of 61000 MW_{th} of synthesis gas is shown in Figure 7, indicating a clear and sustained growth in gasification. The current growth in gasification is mostly in electric power generation. As with fuels, the electric power generation market is orders of magnitude larger than the chemicals market. Other cogeneration and coproduction markets for gasification include the pulp and paper industry, where gasification can be used for chemical recovery and power from black liquor; steel manufacturing, for power and direct reduction of iron; and in the chemicals industry, which requires power and synthesis gas. In the longer-term, domestic utility deregulation, increased electricity demands, and stricter air quality standards will spur the deployment of IGCC for greenfield and retrofit baseload electric power generation after 2010.²⁵

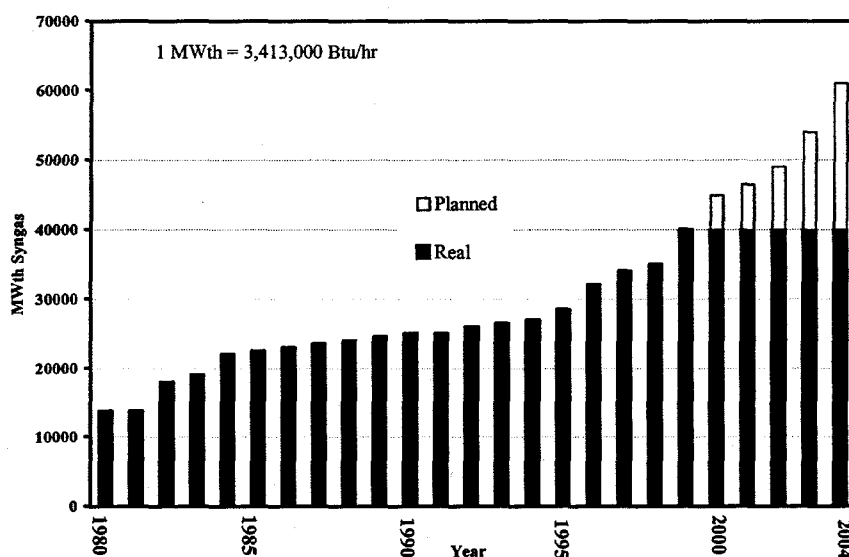


Figure 7. Cumulative Worldwide Gasification Capacity and Growth

Refining:

The economics of gasification are favorable in refineries due to the availability of low-cost fuels such as petroleum coke and refinery residues, and the opportunity to take maximum economic advantage of a flexible product slate including hydrogen, steam, syngas fuel, and power. The worldwide refining market for gasification is estimated at 4GW (2.5 GW power and the balance as syngas) through 2005.²⁶ Assuming an average of 4 wt% sulfur in the wastes gasified, an additional 61 ton/day (950,000 scfh) of hydrogen could be produced through SAC decomposition of H₂S.

Pulp and Paper:

Black liquor gasification is being developed as a replacement for energy and pulping chemicals recovery in conventional Tomlinson recovery furnaces. Black liquor IGCC systems offer the potential to increase overall plant efficiencies by as much as 10% while increasing electric power production by as much as 300%. The success of IGCC in this market will depend on the development of highly efficient systems to recover sodium- and sulfur-based pulping chemicals present in black liquor. Depending on the gasification conditions, a significant portion of the sulfur leaves the gasifier as H₂S with the product gas. Recovery of sulfur as sodium sulfite by scrubbing with NaOH allows for recycle directly back to the Kraft process. Residual H₂S escaping the scrubbers must be removed prior to the combustion gas turbine, and the SAC decomposition route would increase overall sulfur recovery as well as recover hydrogen for increased overall energy efficiency.

Chemicals:

Gasification synthesis gas can be used to produce chemicals, intermediates, and electric power for the chemical industry from a variety of fuels, offering significant protection against market and regulatory risk. Synthesis gas for chemicals continues to be the dominant application or product of gasification, as shown in Figure 8. Assuming a 4.5% per year growth rate for synthesis gas production from current gasification capacity, the gasification market²⁷ is projected to be 1000 × 10⁶ scf/day of synthesis gas and 2 GW power by 2005. This corresponds to about 38 ton/day (560,000 scfh) of hydrogen recoverable through SAC decomposition of H₂S, assuming 4 wt% sulfur in the gasification fuel.

Steel:

Direct reduction of iron is used by integrated mills and mini-mills to replace coke ovens and relieve scrap steel supply requirements. The synthesis gas for the direct reduced iron (DRI) process is primarily obtained through reforming natural gas, but gasification is an alternative for areas where cheap natural gas is not available. The projected market²⁷ for gasification in iron making is equivalent to 1.5 GW. Up to 21 ton/day (330,000 scfh) of hydrogen could be recovered from H₂S decomposition assuming similar low-cost, high-sulfur fuels are gasified.

Electric Power Generation:

The Energy Information Agency (EIA) projects that 300 GW of new power generating capacity will be needed by 2020 to meet increasing U.S. electricity demand and replace retired fossil-

fueled generating capacity²⁸. An additional 280 GW of baseload capacity will be added by 2020 to repower or life-extend existing fossil plants and replace retired nuclear plants. Due to low costs and short construction times, natural gas combined-cycle is expected to capture about 75-85% of the total market, with IGCC plants not expected to be built until after 2010. Short-term power generation by gasification in the U.S. is projected to be about 3800 MW_{th}. Between 2010 and 2020, coal's share of new baseload capacity additions is projected at about 30 GW. Assuming that about 20% of repowering is also coal based, the total IGCC market, including new capacity, would be about 80-90 GW. With 3 wt% sulfur coal at 12,500 Btu/lb and 75% hydrogen recovery from SAC decomposition of H₂S, up to 800 ton/day (12.6×10⁶ scfh) of hydrogen could be recovered.

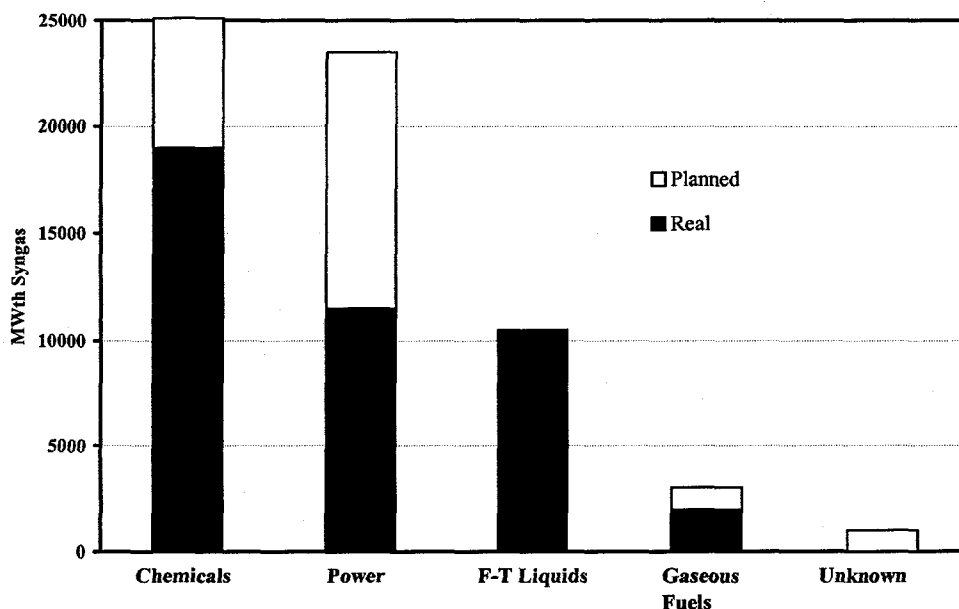


Figure 8. Gasification by Application

Competing Technologies

The most widely used methods of sulfur removal from fuels (other than coal combustion followed by SO₂ scrubbing) involve the reduction of sulfur species to H₂S followed by ad/absorption and subsequent regeneration as a concentrated H₂S stream. In some cases (natural gas sweetening), most of the sulfur is already present as H₂S, so no reduction step is required. A number of technologies are used for H₂S sorption, using either chemical solvents (*e.g.*, amines) or physical solvents (*e.g.*, methanol) to scrub out the H₂S from the waste gas. In either instance, the H₂S is regenerated as a concentrated stream, with the balance of the gas stream consisting mainly of N₂ and/or CO₂. The H₂S must then be converted to elemental sulfur, which has an economic value of around \$30/ton.

Table 6. Summary of Potential Hydrogen Recovery Using SAC Decomposition of H₂S

H ₂ S Source	Hydrogen Recovery	
	ton/day	10 ⁶ scfh
Existing Sulfur Recovery Capacity at 50% Utilization	870	13.7
IGCC for refining, chemicals and steel making	120	1.9
IGCC for baseload power	800	12.6
Total	1790	28.3

The best-known H₂S conversion process is the Claus process,²⁹ which operates in two steps: the thermal stage represented by Equation 3, and the catalytic stage represented by Equation 4.



These two reactions combine to yield the equivalent of reaction (1). Most Claus plants also incorporate a sulfur polishing step that removes residual H₂S from the tail gas irreversibly (*i.e.*, ZnO, Fe₂O₃), although variations (*i.e.*, Superclaus, Parson's Hi-Activity) replace the polishing stage with a selective catalytic oxidation reactor in which reaction 1 takes place, converting residual H₂S to elemental sulfur and delivering an overall sulfur recovery up to 99.2%. Other configurations (*i.e.*, Shell's SCOT, Beavon) treat the tail gas with a reducing agent, converting all sulfur species to H₂S which is then absorbed in an amine solution and recycled back to the Claus unit.

Claus plants require the waste stream to have an H₂S concentration of at least 25 mol%. Concentrations lower than 55-60 mol% require preheating of the feed stream and/or combustion air or a split-flow configuration, while more concentrated H₂S streams can be fed directly to the first-stage furnace.²⁹ These concentration-based limitations may also present an opportunity for an alternative technology, if such a technology can process low-concentration H₂S streams without difficulty.

Other competing available technologies²⁹ for H₂S removal and destruction include: the Stretford process, which uses a liquid-phase vanadium-based redox system, but today is mainly used in limited applications as a Claus tail gas treatment step; the Lo-Cat and SulFerox processes, which are similar to the Stretford but for the replacement of vanadium with iron; and NKK's Bio-SR process, which also uses an iron-based redox system but uses a sulfur-metabolizing microbe to regenerate the reactant solution. These processes are limited to relatively low capacities and pressures.

Another liquid redox process is CrystaSulf,SM originated by Radian L.L.C. under GRI funding.³⁰ This method uses non-aqueous solvents that maintain the elemental sulfur in solution until a final step, eliminating various handling problems reported by users of other liquid-phase processes, and producing a high-purity elemental sulfur. This technology is still in the development stage. Processes designed to obtain both elemental sulfur and hydrogen are also under development. These include Marathon's Hysulf process, which uses an organic solvent, and Idemitsu Kosan's process using ferric chloride solution and a low-voltage electrolyzer to produce hydrogen during regeneration. Alberta Sulfur Research is developing a thermal cracking technology using conventional indirect heating, and a microwave-based cracking process is being studied by Argonne National Labs and the Russian Kurchatov Institute. None of these processes have yet reached commercial status.

Economics

The economics of sulfur removal/recovery depend on the throughput. Leppin²⁴ estimates that the typical, rough, order of magnitude treatment costs for sulfur removal/recovery are > \$10,000/ton for scavenging processes, < \$1000/ton for liquid redox approaches, and \$100/ton for large-scale modified Claus units with Tail Gas Treatment. None of these processes produces byproduct hydrogen. Figure 9 shows some 1997 cost estimates for five types of sulfur cleanup technology applied to natural gas at 1000 psig and 100×10^6 scfd.³⁰

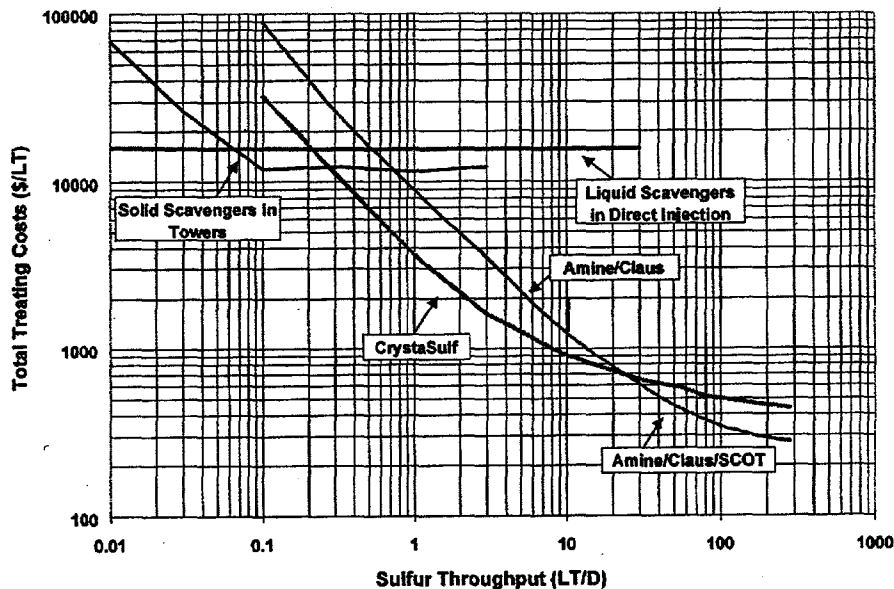


Figure 9. Treating Costs versus Sulfur Throughput

These estimates do not break out the costs between the absorption and conversion steps, but this is necessary to make a comparison with the SAC process being developed, which only converts H₂S after it has been removed from the gas stream. This was done for natural gas sweetening in

a paper by Tannehill, Echterhoff, and Leppin.³¹ Costs for H₂S absorption and sulfur conversion were presented separately, with gas treatment costs broken down to capital and operating costs per volume of natural gas treated. The raw gas, produced at 10 MMscfd, was assumed to contain 3% CO₂ and 3% H₂S. A selective amine unit was specified to scrub the gas, yielding a regeneration gas stream with 60% H₂S. The total net treatment cost for the amine unit was \$0.159/Mscf, including \$0.088/Mscf capital cost and \$0.045/Mscf operating cost. Elemental sulfur was recovered via an Amoco CBA unit – an extension of the Claus process – at 98.5%, resulting in 11.3 long tons/day of sulfur. The sulfur recovery cost was \$0.268/Mscf raw gas, consisting of \$0.200/Mscf capital cost and \$0.068/Mscf operating cost. The total net treatment cost was \$0.465/Mscf, consisting of \$0.159/Mscf for acid gas removal, \$0.039/Mscf for dehydration, and \$0.268 for sulfur recovery.

No economic estimates were previously made for SAC-based H₂S decomposition, because the concept is so new. However, a Canadian study³² was made of the comparative economics of hydrogen production by thermal H₂S decomposition using conventional combustion technology compared to H₂S treatment by the Claus process and steam reforming of natural gas to produce an equivalent amount of hydrogen. In this scheme, H₂S decomposition is driven by indirect heating in a reformer-type furnace fueled by natural gas. The cost of producing hydrogen in this manner (at 20×10⁹ scfd H₂ scale) was cited at \$1160/ton (\$3.08/Mscf), compared to \$670/ton (\$1.78/Mscf) for a comparably sized Claus plant plus steam reformer. However, the portion of the hydrogen cost attributable to natural gas fuel for the decomposition reactor was \$727/ton, or 63% of the total. The SAC-based decomposition reactor being developed in this program, on the other hand, does not use natural gas under normal operation, obtaining all of the necessary heat from H₂S partial oxidation. This is possible because of the higher thermal efficiency of the process. Essentially, the necessary process heat is obtained by oxidation of a portion of the potential hydrogen in the form of H₂S.

An estimate of the comparative economics of the conceptual SAC-based process with a Claus-based process for H₂S removal from natural gas was derived from reference 29, as follows.

- Annual operating costs for the SAC unit were assumed to be similar to those of the CBA (Claus) unit. These costs amounted to \$0.068/Mscf raw gas, which is 25.4% of the total treatment cost.
- Sensitivity to capital cost for the SAC unit was determined over a range of 80% to 120% of the capital cost of the CBA unit (both units assumed to have a lifetime of 10 years). The CBA unit capital cost was \$1.85 million, accounting for \$0.200/Mscf raw gas.
- Sensitivity to H₂ yield from the H₂S exiting the amine unit was determined over the range of 30% to 80% yield.
- Economics were determined for three hydrogen selling prices: \$5, \$6, and \$7/million Btu. These are reasonable numbers for hydrogen produced by a steam reforming plant at a user's site.

The results of this comparison are presented in Figure 10. The family of curves represent capital cost ratio relative to a CBA (Claus) unit. Depending on the capital cost, hydrogen yield, and hydrogen selling price, there is a potential for significant reductions in gas treatment cost. For example, as shown in Figure 10a, for an SAC unit equal in capital cost to the Claus unit, and a relatively low hydrogen selling price of \$6/MMBtu, treatment cost savings of 5-14% can be projected, depending on hydrogen yield. If the capital cost can be reduced 20% compared to the CBA unit, these savings would increase to 20-29%. At higher hydrogen prices or credits (Figure 10b and 10c), the savings are even more impressive. With a hydrogen price of \$7/MMBtu, an SAC plant with a 20% lower capital cost than the Claus plant and an H₂S-to-H₂ yield of 75% would be 34% cheaper than the Claus plant on a raw gas volume basis. Note that in all cases where SAC gas treatment costs are equal to or less than Claus in the above examples, hydrogen is produced at zero or negative cost to the gas treatment plant operator.

Economics for oil refinery applications should be similarly favorable, if not better. These applications also use Claus-based sulfur conversion technologies extensively. The presence of on-site hydrogen requirements would tend to make this technology more attractive, and the trends in the refining industry toward more extensively reformed fuels coupled with the gradually decreasing availability of lighter crudes will continue to spur the installation of additional hydrogen producing capacity. This means that a new technology for hydrogen generation from waste streams, such as the SAC process being developed in this program, would have market entry opportunities not only for retrofits but for new units as well.

Comparative Economics of a SAC-Based Process with a Claus-Based Process

Summary:

To compare the economics of a SAC-based process with a Claus-based process, a commercial-scale plant producing 2,610,000 SCFD of hydrogen and 200 LTPD of sulfur by thermal decomposition of H₂S-rich waste gas stream using superadiabatic combustion (SAC) process was designed. Major equipment was sized and costed. The capital cost was estimated to be about \$16,000,000. This capital cost is about 6% higher than that of a Claus plant producing 200 LTPD of sulfur, estimated at about \$15,000,000. Details of this cost comparison are provided below.

Plant Design and Cost Estimate:

In the commercial-scale superadiabatic H₂S decomposition plant designed, H₂S-rich waste gas is mixed with air and fed to the SAC Reactor (R-1) operated at 40 psia. The reactor consists of fixed-beds packed with alumina pellets where hydrogen sulfide is thermally decomposed to hydrogen and sulfur. Off-gas leaving the SAC reactor is cooled in the Sulfur Condenser (E-3) where sulfur vapors are condensed and low-pressure steam is generated. Liquid sulfur is drained and collected in the Sulfur Storage Tank (T-1). Off-gas from the Sulfur Condenser is cooled in the Feed Gas Heater (E-1) by heating the feed gas stream to the SAC Reactor. Cooled off-gas from the Sulfur Condenser is compressed to 300 psia by the Gas Compressor (C-2) and then fed to the H₂S Separator (S-1) where unconverted H₂S is removed from the gas stream and recycled

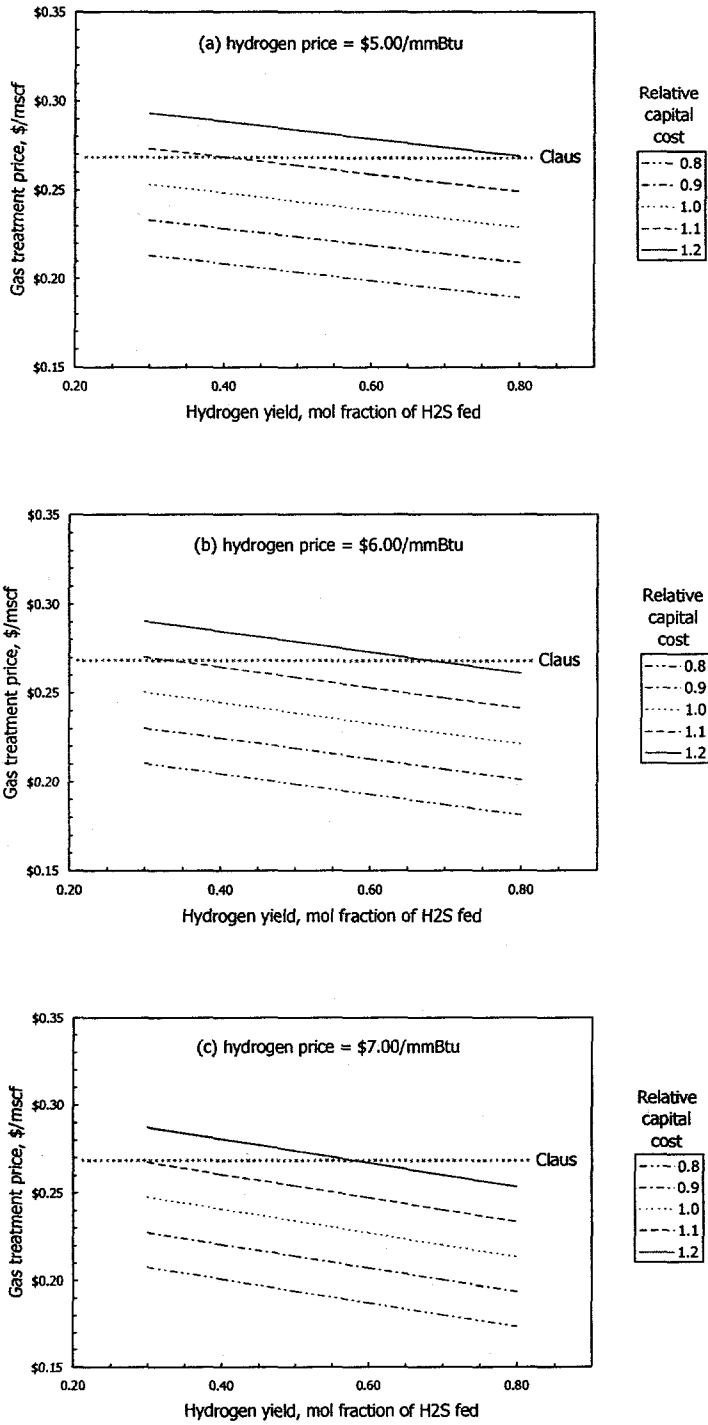


Figure 10. Economic Comparison of SAC with Claus Plant for Treatment of Natural Gas

to the SAC Reactor. Off-gas leaving the H₂S Separator is then fed to the H₂ Separator (S-2) where hydrogen is recovered and the off-gas is discharged to the atmosphere.

Major equipment is sized and summarized in Table 7. Purchased equipment costs are estimated based on estimating charts and previous cost information, and are given in Table 8. Capital cost is estimated based on conventional cost estimating factors and is shown in Table 9.

Table 7. Equipment Summary for a Superadiabatic H₂S Decomposition Plant

<u>Equip. No.</u>	<u>Equipment Name</u>	<u>Qty</u>	<u>Description</u>
C-1	Air Compressor	1	Centrifugal compressor designed to compress 3,790 lb-mol/h air from 14.7 psia to 40 psia. Equipped with control system and 2,230 hp motor drive.
C-2	Gas Compressor	1	Multi-stage centrifugal compressor designed to compress 4,440 lb-mol/h flue gas from 30 psia and 100°F to 300 psia. Equipped with intercoolers, control system, and 6,630 hp motor drive
E-1	Feed Gas Heater	1	Tube-and-shell heat exchanger designed to cool 4,440 lb-mol/h flue gas from 300°F to 100°F by preheating 4 590 lb-mol/h of feed gas from 70°F to 260°F. Carbon steel construction with 8x10 ⁶ Btu/h heat duty and 23,000 ft ² heat transfer area.
E-2	Sulfur Condenser	1	Tube-and-shell condenser designed to cool 5,010 lb-mol/h flue gas from 700°F to 300°F and condense 570 lb-mol/h sulfur vapor by generating 19,000 lb/h low-pressure steam.
R-1	SAC Reactor	1	Fixed-bed reactor packed with ¼" alumina designed to process 4,590 lb-mol/h mixture of H ₂ S-rich waste gas and air. Carbon steel shell @ 19' diameter and 28' height, and lined with 18" thick 3,000°F castable refractory
S-1	H ₂ S Separator	1	Pressure swing adsorption or membrane separation system designed to remove 60 lb-mol/h H ₂ S from 4,440 lb-mol/h flue gas @ 300 psia and 100°F. H ₂ S free effluent gas leaves separator at 290 psia.
S-2	H ₂ Separator	1	Pressure swing adsorption or membrane separation system designed to remove 290 lb-mol/h H ₂ from 4,380 lb-mol/h flue gas @ 290 psia and 100°F.
T-1	Sulfur Storage Tank	1	300,000 gal liquid sulfur storage tank equipped with internal steam coils and steam-jacked sulfur pipes.

Table 8. Purchased Equipment Costs for a Superadiabatic H₂S Decomposition Plant

Equip. No.	Equipment Description	Purchased Costs, \$
C-1	Air compressor	710,000
C-2	Gas Compressor	1,700,000
<u>E-1</u>	<u>Feed Gas Heater</u>	<u>290,000</u>
E-2	Sulfur Condenser	110,000
R-1	SAC Reactor	290,000
S-1	H ₂ S Separator	1,600,000
S-2	H ₂ Separator	1,600,000
T-1	Sulfur Storage Tank	100,000
	Total	6,400,000

Table 9. Capital Cost for a Superadiabatic H₂S Decomposition Plant

<u>Description</u>	<u>Dollars</u>
Direct Costs ¹	12,480,000
Indirect Costs ²	<u>3,740,000</u>
Capital Cost	16,220,000

1. Direct Costs include Installed Equipment, Foundations/Concrete, Structural Steels, Installed Instrumentation & Control, Installed Piping, Installed Electrical, Site Preparation, Buildings, and Insulation/Painting/Safety.
2. Indirect Costs include Home Office and Field. The Home Office includes the costs of design, engineering, supervision, and contractor's overhead and fees. The Field includes all costs associated with construction or field management.

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APPENDIX A

MODELING OF HYDROGEN PRODUCTION BY SUPERADIABATIC COMBUSTION OF HYDROGEN SULFIDE

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ABSTRACT

In this work filtration combustion waves in hydrogen sulfide (H_2S)/air mixtures are modeled within the one-dimensional approach, taking into account multi-step chemistry and separate energy equations for the gas and solid phases. The superadiabatic wave propagation is a complex phenomenon, and many factors that influence wave properties, in particular the heat loss rate and the interfacial heat exchange or effective heat conductivity of the porous medium, must be accurately specified. A numerical model was developed to describe combustion wave characteristics in a coordinate system moving together with the wave front. Two chemical kinetic mechanisms have been used. The first mechanism was developed by Frenklach's group and is applicable under combustion conditions (i.e., moderately high equivalence ratios); the second kinetic mechanism has been developed at UIC to describe more accurately the partial oxidation of H_2S (i.e., ultra-high equivalence ratios). The products of partial H_2S oxidation, hydrogen (H_2) and elemental sulfur (S_2), are dominant for ultra-rich superadiabatic combustion, which is essentially a fuel reforming reaction. The chemistry in the combustion wave is modeled and species and temperature profiles are predicted. A database of H_2S conversion is generated in a wide range of equivalence ratios and other process parameters.

NOMENCLATURE

c	specific heat (J/kg K)
h_i	specific enthalpy of i^{th} species (J/kg)
Nu	Nusselt number
T	temperature (K)
u	filtration velocity (m/s)
u_w	combustion wave velocity (m/s)
V_i	diffusional velocity of i^{th} species (m/s)
W_i	molecular weight of i^{th} species
x	coordinate (m)
Y_i	mass fraction of i^{th} species

Greek Symbols:

α	interfacial heat transfer coefficient ($W/m^3 K$)
β	effective coefficient for heat exchange with surroundings $W/(m^3 K)$
ϵ	porosity (void fraction of porous medium)
ϕ	equivalence ratio
λ	heat conductivity (J/m K)
ρ	density (kg/m^3)
$\dot{\omega}_i$	molar rate of production of i^{th} species

Subscripts:

g	gas
s	solid material
p	pressure
i	chemical species

e	effective
o	ambient
rad	radiative

INTRODUCTION

Filtration combustion of gases draws constant interest of researchers due to numerous applications such as pollution control, low emission burners, fuel reforming and processing.¹ Combustion waves in a porous body, including excess enthalpy superadiabatic flames, have been under intensive study in recent experimental and theoretical works.¹⁻⁷ Developed analytical and numerical one-dimensional single-step reaction treatments include: models in one-temperature approximation for solid and gas,²⁻³ two-temperature models,^{4,5} and two-temperature models with discrete solid phase.⁶ However, advanced description of filtration combustion waves faces the necessity to account for the same important parameters as detailed kinetics models of flames stabilized within inert porous media. Important issues of multi-step kinetics,⁷ including heterogeneous reactions,⁸ pore-level mechanisms of combustion,^{9,10} and adequate heat and mass transport phenomena in porous media, should be addressed in the modeling of advanced filtration combustion.

Filtration combustion is a transient process, where a fuel is burned within a porous medium, which can be inert or part of the reaction process (i.e., cigarette smoldering). The great majority of filtration combustion studies hinge on the inert type of porous matrices. Fuels used in porous combustion systems are basically in gaseous form due to their ease of flow, although liquid fuels and solid fuel type reactors have been developed and utilized to a smaller extent. Porous matrices vary from metallic to sand particles and their selection depends on utilization criteria. Due to their non-catalytic properties and ability to withstand very high temperature loads without much deformation, ceramic materials have become the pre-eminent material used in filtration combustion studies by Kennedy et al.¹ and Howell et al.¹¹ Alumina, both as pellets and in reticulated form, has been particularly preferred because of cost and availability considerations.

As an internally self-organized process of heat recuperation, filtration combustion of gaseous mixtures in porous media differs significantly from homogeneous flames. This difference is mainly attributed to two factors. First, the highly developed inner surface of the porous medium results in efficient heat transfer between gas and solid. Second, the turbulent structure of the gas flow through porous media increases effective diffusion and heat exchange in the gas phase. As a gas mixture is ignited inside the media, the heat release from this intense reaction is absorbed by the solid matrix, which transfers the energy to the next layer of solid immediately above or below the combustion zone. This process facilitates combustion in a wide range of filtration velocities, equivalence ratios, and power loads.

Stationary and transient systems are the two major design approaches commonly employed in porous burners. The first approach is widely used in radiant burners and surface combustor-heaters. Here, the combustion zone is stabilized in the finite element of porous matrix by the imposed boundary conditions. In the porous radiant burner, the strong emission of thermal radiation from the solid matrix provides energy sink from the combustion zone. In the surface

combustor-heater system, the heat is transferred from the hot combustion gases and the porous matrix to a system of cooling tubes embedded directly in the porous combustion zone.

In unrestricted uniform porous media, the combustion zone is usually unsteady and can freely propagate as a wave in the downstream or upstream direction. Strong interstitial heat transfer results in a low degree of thermal non-equilibrium between gas and solid. These conditions correspond to the low-velocity regime of filtration gas combustion, according to a classification given by Babkin.² The relative displacement of the combustion zone results in positive or negative enthalpy fluxes between the reacting gas and solid carcass. As a result, observed combustion temperatures can be significantly different from the adiabatic predictions; they are controlled primarily by the reaction chemistry and the heat transfer mechanism. The upstream wave propagation, countercurrent to filtration velocity, results in the underadiabatic combustion temperatures as observed by Laevskii et al.,⁵ while the downstream propagation of the wave leads to the combustion in superadiabatic regime with temperatures much in excess of the adiabatic temperature in studies done by Zhdanok et al.³ Superadiabatic combustion significantly extends conventional flammability limits to the region of ultra-low heat content mixtures. The principles of transient filtration combustion are practically realized in several burner configurations, including linear reactors, moving-bed reactors, and reciprocal-flow burners. The modern applications of transient porous burners include combustion of low-calorific fuels, VOC emissions control with possible waste-to-heat recovery,¹² and fuel reforming in the ultra-rich superadiabatic flames.^{1,13} The latter application constitutes the subject of the present work.

Hydrogen sulfide (H_2S), a toxic pollutant, is produced as a byproduct of crude oil and natural gas production. Corrosive by nature, H_2S must be removed prior to hydrocarbon processing. Since environmental regulations prevent the venting of H_2S in the atmosphere, it is now burned with oxygen to form water and sulfur in a process known as the Claus Process. Previous studies on H_2S have been restricted to its homogeneous combustion. Since H_2S is a hydrogen-containing species, it is possible to produce H_2 by combustion of H_2S in a porous burner taking advantage of its ability to extend the flammability limits. In the present study, H_2S is burned in an inert packed-bed of alumina particles. Certain of its properties, i.e. flammability limits, are redefined in the porous media concept.

Results from numerical investigations of rich H_2S /air filtration combustion in packed-beds are presented and discussed in this report. One of the main purposes is to develop a numerical model including multi-step chemical kinetics of a superadiabatic combustion wave, which will be used for a detailed investigation of hydrogen formation due to hydrogen sulfide decomposition. The combustion wave properties are strongly influenced by the superadiabatic reactor characteristics, in particular the effective heat conductivity of porous media, heat exchange rate between gas and solid material, and heat loss intensity, all of which should be accurately specified.

NUMERICAL MODEL FORMULATION

Superadiabatic combustion wave propagation is represented with a one-dimensional model, which includes separate energy equations for the gas and porous medium, and multi-step

chemistry. Such a model can provide a more accurate combustion wave description than models based on local volume-averaged treatment and well-mixed pore approximations. A H₂S/air mixture flows through a porous medium in a thermally insulated packed-bed and exits after reacting. The boundary conditions for the gas are posed at the inlet and exit of the reactor. The radiative transfer in the porous medium is described implicitly via the appropriate contribution into the effective thermal conductivity of the porous medium. The flame is assumed to be laminar, stable, and one-dimensional. Therefore, various instabilities, such as the thermo-diffusive instability,⁹ which forms multi-dimensional cellular structures, do not occur under the conditions considered in the present study.

Governing Equations

The combustion wave propagation in an inert packed-bed is described by a system of conservation equations for gas energy, solid medium energy, mass fractions of gas species, and mass flow rate. More details are provided in reference 5.

Gas Energy Balance

$$(c_p \rho)_g (v-u) \frac{\partial T_g}{\partial x} = \frac{\partial}{\partial x} \left((\lambda_g + (c_p \rho)_g D_{ax}) \frac{\partial T_g}{\partial x} \right) - \frac{\alpha}{\varepsilon} (T_g - T_s) + \sum_i \dot{\omega}_i h_i W_i, \quad (1)$$

Solid Energy Balance

$$-(c_p \rho)_s u \frac{\partial T_s}{\partial x} = \frac{\partial}{\partial x} \left(\lambda_e \frac{\partial T_s}{\partial x} \right) + \frac{\alpha}{1-\varepsilon} (T_g - T_s) - \frac{\beta}{1-\varepsilon} (T_s - T_o), \quad (2)$$

Particle Balance Equation

$$\rho_g (v-u) \frac{\partial Y_i}{\partial x} + \frac{\partial}{\partial x} \left(\rho_g \sum_i Y_i V_i \right) = \sum_i \dot{\omega}_i W_i, \quad (3)$$

Continuity Equation

$$\varepsilon \rho_g (v-u) = \text{const}. \quad (4)$$

The equations are shown in a coordinate system that is moving together with the combustion wave front. In these equations, α is the coefficient describing volumetric heat transfer between porous medium and gas; β is the effective coefficient for heat losses from the system; T_o is the ambient temperature; λ_e is the effective thermal conductivity, which includes both the heat conductivity of the porous medium and radiation transfer; V_i is the diffusion velocity of the i^{th} species, and u is the combustion wave velocity, which is unknown. The diffusion velocity is taken within the mixture-averaged approach,¹⁴ based on the use of the binary diffusion coefficients.

Conservation Equation (4) is used for the mass flow rate instead of the continuity equation for gas density. The continuity equation for gas density usually is invoked if a fast (compared with

the local sound speed velocity) flow of compressible fluid occurs. In describing combustion waves, which have a velocity many orders of magnitude smaller than the filtration velocity, the use of Equation (4) is reasonable.

The major factors controlling the combustion wave behavior under filtration in an inert porous medium are: (i) heat deposition in the gas phase due to fuel oxidation; (ii) forced convection of fuel/air mixture; (iii) longitudinal effective heat conductivity of the porous medium; (iv) intense interfacial heat exchange between gas and the solid frame; and (v) heat exchange between the porous medium and surroundings. The factors (i)-(iii) are accurately represented within the one-dimensional approach adopted in this investigation due to the high degree of radial uniformity of the combustion wave front found in the measurements for the reactor arrangement under consideration.¹⁵ The substantial radial non-uniformity can appear due to various instabilities. Superadiabatic wave propagation under the conditions where no instabilities occur is addressed in this work, and only axial profiles of temperatures, gas velocities, and species concentrations are of importance. The factors (iv)-(v) can be taken into account only parametrically, via the coefficients α and β in Eqs. (1) and (2), within a one-dimensional approach due to their explicit multi-dimensional nature.

Boundary and Initial Conditions

In the numerical model, the flame position was not fixed beforehand as it is usually done in the pre-mixed adiabatic flame code.¹⁴ The boundary conditions specified are:

$$\text{Inlet:} \quad T_g = T_s = T_o, \quad Y_i = Y_i^o, \quad (5)$$

$$\text{Exit:} \quad \partial T_g / \partial x = \partial T_s / \partial x = \partial Y_i / \partial x = 0. \quad (6)$$

Y_i^o denotes the initial mixture composition. Typically, the narrow combustion zone is situated at more than 5 cm from the downstream edge of the reactor, and the residence time for molecules after they leave the combustion zone is greater than approximately 0.1-0.2 s. Such a time period is assumed to be sufficient to complete the chemistry, and thus the boundary conditions (6) are reasonable.

Computational Model

The one-dimensional laminar flame code PREMIX was used following various modifications, as deemed necessary for the task being undertaken. The adaptive placement of the grid points was done to accurately resolve the gradient and the curvature of the gas temperature and species profile. It was determined that 70-100 grid points provided sufficiently accurate solutions. The numerical algorithm implemented in the PREMIX code was used to find the combustion wave velocity u .

The Chemkin subroutines were used to implement the chemical kinetics description¹⁶ and the Transport subroutine¹⁷ was used to calculate gas properties.

Model and Solid-Phase Properties

All calculation parameters were selected to correspond to the conditions of the experimental work,¹⁵ where characteristics of combustion waves, concurrent with filtration flow through a packed-bed column of porous alumina, were studied. In this study the following solid properties

were used: $\varepsilon = 0.4$; $\rho_s = 3.9 \cdot 10^3 \text{ kg/m}^3$. The specific heat capacity and heat conductivity for the pure solid material were approximated as follows:

$$c_s \approx 0.92 + 3.0 \cdot 10^{-4} \cdot T_s, \text{ kJ/kg K}$$

and

$$\lambda_s \approx 1.4 \cdot 10^4 \cdot T_s^{-1.07}, \text{ W/m K.}$$

These approximations are accurate in the temperature range of 300-2000 K. The effective heat conductivity of the porous medium can be taken as $\lambda_e = \lambda_{cond} + \lambda_{rad}$,¹⁸ where the first term is the effective thermal conductivity in the porous medium when heat transfer occurs only by conduction. It is approximated as:¹⁸

$$\lambda_{cond} = 0.005 \lambda_s.$$

Radiation is treated with a radiant conductivity model

$$\lambda_{rad} = 4F\sigma T_s^3,$$

where F is the radiation exchange factor. In the conditions considered, F depends upon the value of the conductivity of the solid state (alumina). Values of F ranging from 0.3 to 0.6 were used. The coefficient α for interfacial heat exchange is specified as

$$\alpha = \frac{6\varepsilon}{d^2} N_u \lambda_g,$$

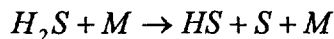
where d denotes the diameter of a spherical particle. The correlation for the Nu number is given by Wakao and Kagueli¹⁸ as

$$N_u = 2 + 1.1 \text{Re}^{0.6} \text{Pr}^{1/3}.$$

The coefficient β for heat losses controls the reactor-cooling rate. In the calculations the following value was used: $\beta = (1-5) \cdot 10^3 \text{ W/m}^3 \text{ K}$. The contribution of turbulent flow to the effective mass diffusion was described by the axial gas dispersion coefficient D_{ax} , based on unit void area. It is given by $D_{ax} = 0.5 dv$.¹⁹ According to a heat-mass transfer analogy the dispersive thermal diffusivity is the same as the mass diffusivity and the respective dispersion coefficients are equal. Similar to Howell et al.,¹¹ effective diffusion was represented as a sum of molecular diffusion and dispersion.

Kinetic mechanism

Two chemical kinetic mechanisms were used. The first mechanism, developed by the Frenklach's group, includes 17 species and 47 reactions, and is considered more appropriate under combustion conditions (i.e., moderately high equivalence ratios). The second kinetic mechanism was developed at UIC to describe more accurately the partial oxidation of H_2S (i.e., ultra-high equivalence ratios). In the second kinetic mechanism the thermal decomposition of H_2S



is described with a rate constant of $1.76 \cdot 10^{16} \exp(-66210/\text{RT})$,²⁰ while the corresponding rate constant in the first mechanism is $4.63 \cdot 10^{14} \exp(-82469/\text{RT})$,²¹ which is considerably smaller than the previous one.

RESULTS AND DISCUSSION

Gas and Solid Temperatures

The predicted gas and solid temperatures and concentration profiles of major species, as a function of reactor length at near-stoichiometric conditions, are shown in Figures 1 and 2. The dashed line represents the solid temperature profile. As indicated, except for a narrow wave front zone, gas and solid temperatures are close to each other due to the small value of the filtration velocity and the intense interfacial heat exchange rate under the specified conditions. The gas preheating by the radiative longitudinal heat conductivity in the porous medium results in a peak temperature that decreases afterwards because of fast interfacial heat exchange. The increase of the gas temperature has an important influence on H₂S reforming chemistry, that cannot be accurately modeled otherwise. The major products for these mixture compositions are SO₂ and H₂. Downstream (superadiabatic) wave propagation is observed for ultra-rich ($\phi \geq 1.7$) mixtures. Upstream (underadiabatic) propagation corresponds to the range of equivalence ratios < 1.7 . It should be kept in mind that this is valid for mixtures shown in Figures 1 and 2, when H₂S is strongly diluted by N₂. The Figures show also the predicted solid temperature profiles. With a decrease of the equivalence ratio ϕ of the initial methane-air mixture, the combustion wave slows down, and the wave velocity can change sign for $\phi < 1.7$. Virtually all reactions occur within the narrow zone of the combustion wave front. The species concentration profiles are stabilized shortly downstream of the combustion wave front.

Figure 3 shows the combustion wave calculated for two different values of heat loss intensity factor. The parameters are given in the figure caption. It can be seen that heat loss can significantly influence the exit temperature and product yield in the porous combustion reactor. In practice, this effect can be controlled with reactor heat insulation.

Wave propagation

The combustion velocity is correlated for with a formula by Zhdanok et al.^{3,4} This formula relates the rate of combustion propagation (u), the thermal wave velocity (v_t), adiabatic temperature (T_a), and combustion temperature (T_c) according to the following equation:

$$u/v_t = 1 - \Delta T_a / \Delta T_c, \quad (7)$$

where the thermal wave velocity ($v_t = v(c_g \rho_g) / c_s \rho_s$) is a function of the filtration velocity (v) and densities of the gas and solid.

To describe rich and ultra-rich filtration combustion, Kennedy et al.¹ suggested an energy balance for the wave inside the solid media with a negligible heat loss to the surrounding:

$$\rho_g v \Delta H_g - \rho_s u \Delta H_s = 0 \quad (8)$$

This leads to the following relationship:

$$u/v_t = (\Delta H_g / c_g) / (\Delta H_s / c_s) \quad (9)$$

This equation can be employed for qualitative analysis of the wave velocity in conjunction with T_a and T_c .

Product yield

Depending on the mixture composition, i.e. heat content, the major products, such S_2 , H_2 , H_2O , and SO_2 , can be in different proportions. For example, in lean mixtures, SO_2 is one of the dominant species due to the availability of O_2 to the extent that no H_2S remains unreacted. In rich mixtures, H_2S can be of the dominant species in the output, depending on its initial concentration in the feedstock. Gaseous product compositions and H_2 and S_2 conversions are given in Figures 4 through 10 and also in Tables 1-3. It must be noted that the degree of conversion was calculated differently in the Figures than in the Tables. In the figures, the amount of H_2 in H_2S was taken into account, while in the Tables the amount of H_2 in unconverted fuel was not considered. Specifically, Figure 4 shows the H_2 conversion as a function of equivalence ratio with the other parameters as for the previous figures and the heat loss intensity = $500 \text{ W/m}^3 \text{ K}$. Figure 5 gives the variation of H_2 and S_2 conversions as a function of the equivalence ratio in H_2S/O_2 mixture. The bottom figure corresponds to higher intensity of heat loss. The corresponding calculations in $H_2S/30\%O_2$ mixture are shown in Figure 6. The bottom figure corresponds to higher intensity of heat loss. In Figure 7 the major product composition in $H_2S/30\%O_2$ as a function of equivalence ratio is given. Figure 8 shows the effect of water addition to the initial mixture on hydrogen and sulfur conversions. The effect of water addition is studied in relation with a possible recirculation of combustion products to improve the overall conversion degree. One can conclude that water admixture does not influence the product yield significantly, and then the following recirculation is quite possible. Figure 9 shows the variation of H_2 conversion as a function of the filtration velocity, while the corresponding effect on product yield is given on the next figure.

The effect of initial mixture preheating was also investigated. The results are shown on Figure 11 for the case of 43.7% N_2 , 37.5% H_2S , and 18.7% O_2 ; this composition corresponds to an equivalence ratio of 3. In superadiabatic combustion the preheating is not so important as in regular combustion schemes. It was further confirmed that porous media combustion has more contrasts than similarities with homogeneous combustion.

To summarize, it can be concluded that by optimizing the porous body reactor configuration, equivalence ratio, and filtration velocity, the single-pass H_2S decomposition can be as high as 30-50%, while H_2 conversion can reach a level of 30%. These values can be obtained for the following conditions: equivalence ratio is around 10-15 and filtration velocity is higher than 100 cm/s. At such high values of the equivalence ratio and filtration velocity, the combustion temperature is considerably higher than the adiabatic one (which is too low for the combustion to be organized in a gas phase only), and the product composition is shifted towards S_2 instead of SO_2 . Taking into account that for a single pass run the H_2S decomposition can reach 30 %, the overall process performance can be substantially improved by product recirculation. In such a case, one can obtain nearly total hydrogen sulfide decomposition into sulfur, and additionally 30-40% of hydrogen.

Conclusions

Preliminary numerical modeling of the SAC reactor has been performed. The parameters considered in the modeling effort included fuel gas composition (i.e., H₂S-rich and H₂S-lean), oxidant composition (air/enriched air), equivalence ratio, superficial gas velocity, feed gas temperature (pre-heating effect), and product gas quenching. The major conclusions from the modeling predictions obtained are:

- In oxygen-enriched air (i.e., 30% O₂-N₂ gas mixture), conversions of H₂S to hydrogen and elemental sulfur are better than when pure oxygen is used as the oxidant.
- Product gas quenching can substantially increase the selectivity of H₂S conversion to H₂; however, the selectivity of H₂S conversion to elemental sulfur decreases. For example, at typical filtration velocities ranging from 20 to 30 cm/s, equivalence ratios of about 2-3, and oxygen-enriched air containing about 20-40% O₂, H₂S conversion to hydrogen is about 20% and H₂S conversion to elemental sulfur is about 60%. With quenching of product gas, H₂S conversion to hydrogen and elemental sulfur is about 35% and 25%, respectively.
- Water addition to the initial mixture does not improve the reactor performance with respect to hydrogen and elemental sulfur production.
- When air is used as the oxidant, conversion of H₂S to H₂ decreases as filtration velocity increases. In contrast, when pure oxygen is used as the oxidant, increasing the filtration velocity plays a positive role.
- SAC reactor performance can be significantly improved by separating and recirculating unreacted H₂S in the product gas.

Based on the developed numerical model, optimization studies of hydrogen production were conducted by varying the characteristics of the ultra-rich superadiabatic waves. The major findings appear to indicate that by optimizing the porous body reactor configuration, equivalence ratio, and filtration velocity, the overall H₂S decomposition in a single pass can be as high as 30-50%, with a conversion of H₂S to the desirable product hydrogen (H₂) reaching a level of 30%. This reactor performance can be obtained using equivalence ratios in the range of 10 to 15, while maintaining a filtration velocity greater than 100 cm/s. For these high values of equivalence ratio and filtration velocity, the combustion temperature is considerably higher than the adiabatic temperature, which is in fact too low for combustion to take place in the gas phase. Such high temperature promotes the decomposition of H₂S, the hydrogen (H₂)/water (H₂O) selectivity, and the elemental sulfur (S₂)/sulfur dioxide (SO₂) selectivity. Given that in a single pass the H₂S decomposition can reach 30-50%, the overall process performance can be substantially improved, with respect to hydrogen production, by membrane separation of product gases and recirculation of unreacted H₂S. It can be shown that in 4 to 5 passes nearly total hydrogen sulfide decomposition into sulfur can be realized, with recovery of 30-40% of the hydrogen component.

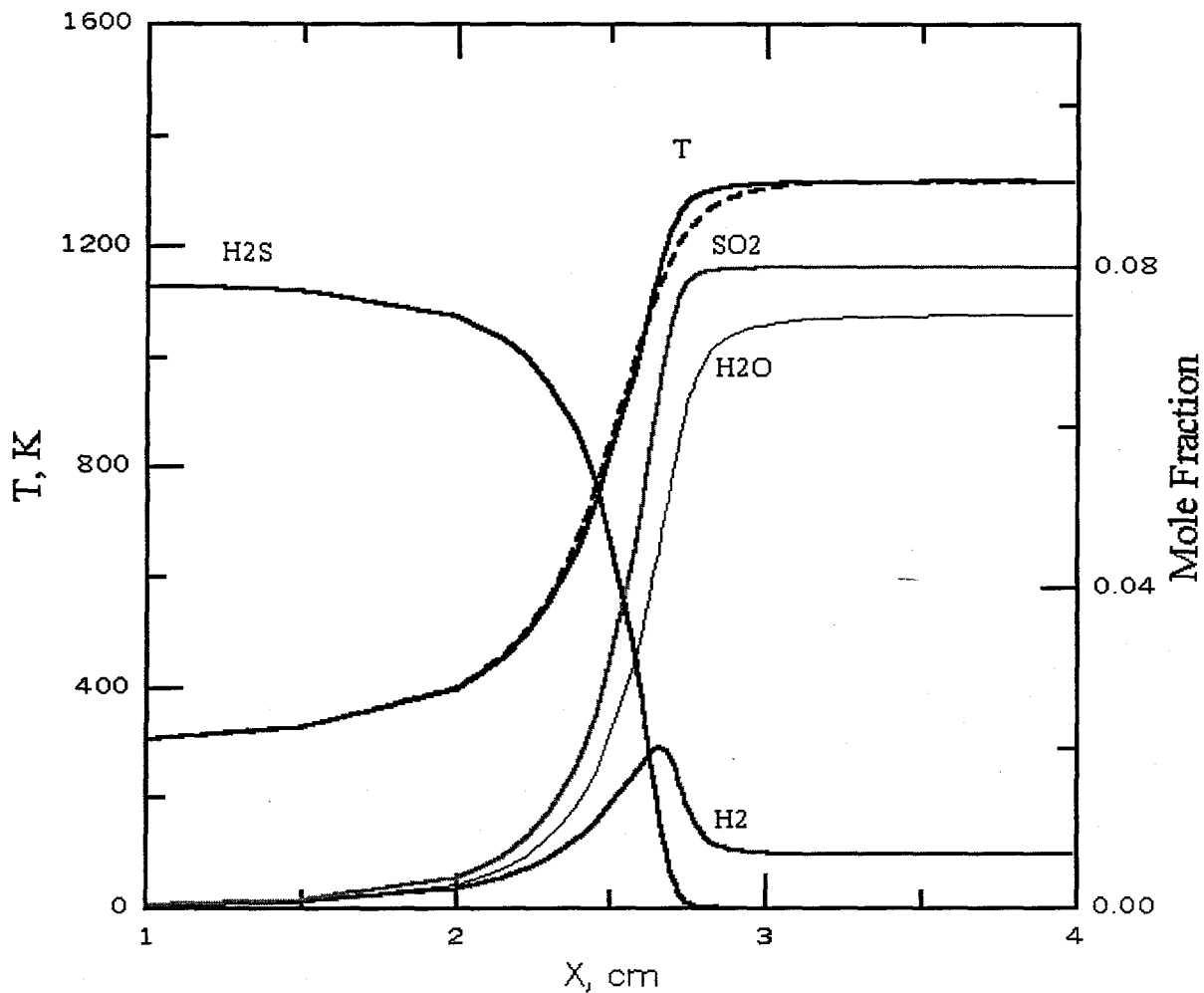
The most optimum scenario in the results of the computer modeling to-date indicate that, with feed gases entering the reactor at ambient temperature, a maximum temperature of 1631 K (1394°C or 2541°F) can be achieved in the SAC reactor, resulting in an overall H₂S conversion of 50%, with a hydrogen (H₂)/water (H₂O) selectivity of 57/43 and an elemental sulfur (S₂)/sulfur dioxide (SO₂) selectivity of 99/1.

These predictions have offered valuable guidelines for the preparation of a design and cost estimate of a suitable bench-scale reactor testing system to be assembled and tested in Phase 2 of the program. Modeling efforts also made possible the identification of key SAC process parameters and the preparation of a parametric testing plan for Phase 2. The chemical kinetic mechanisms used in the formulation of this preliminary model will be updated based on direct comparison with the experimental data that will be obtained in Phase 2, further enhancing the reliability of the model.

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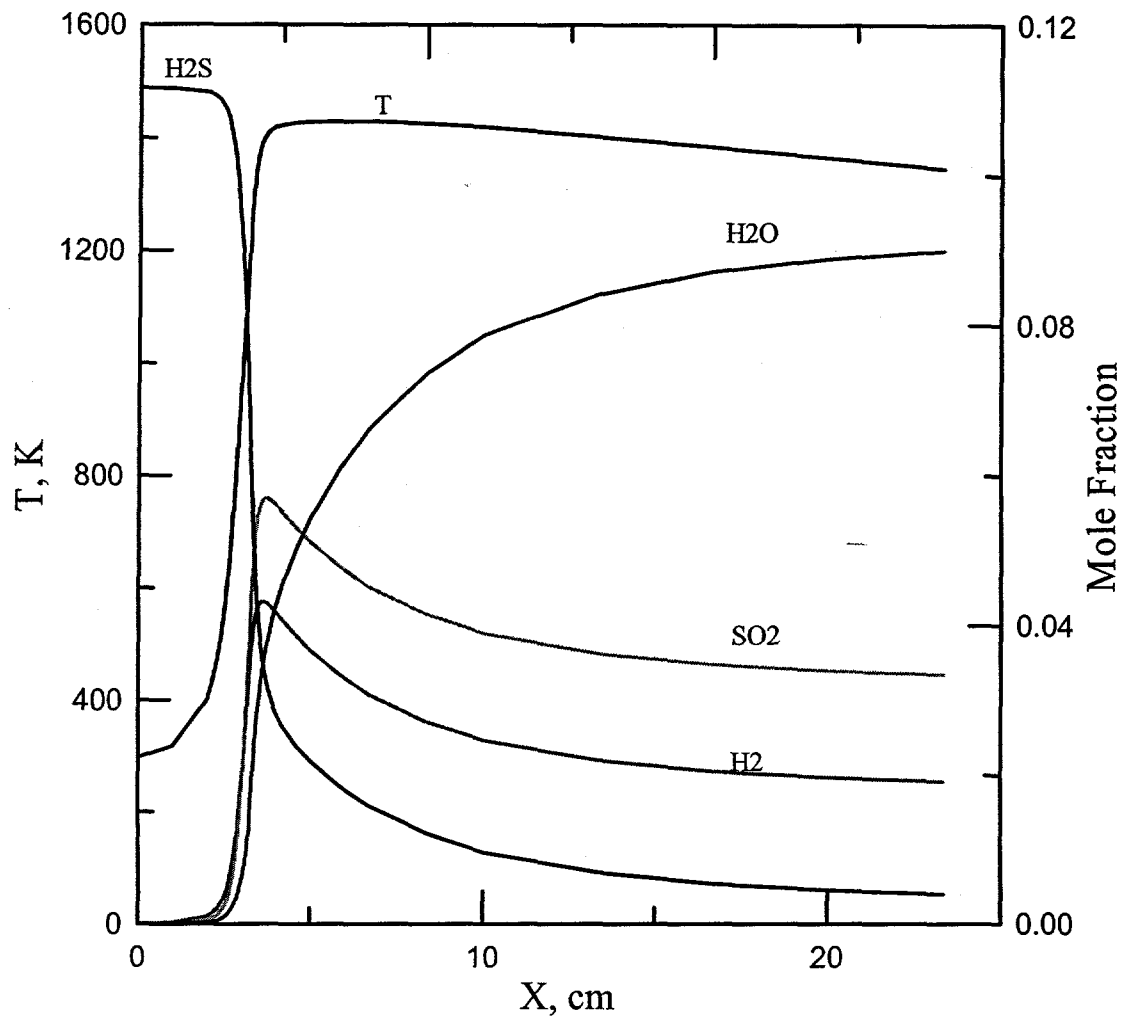


$[N_2]=80.65\%$, $[O_2]=11.32\%$, $[H_2S]=7.79\%$,
 $V=22$ cm/s, Loss=500 W/m³ K,

wave= $7.5E-4$ cm/s

$[H_2]=0.67\%$, $[H_2O]=7.4\%$, $[SO_2]=8\%$, $[N_2]=83.8\%$
 Conversion = 6%

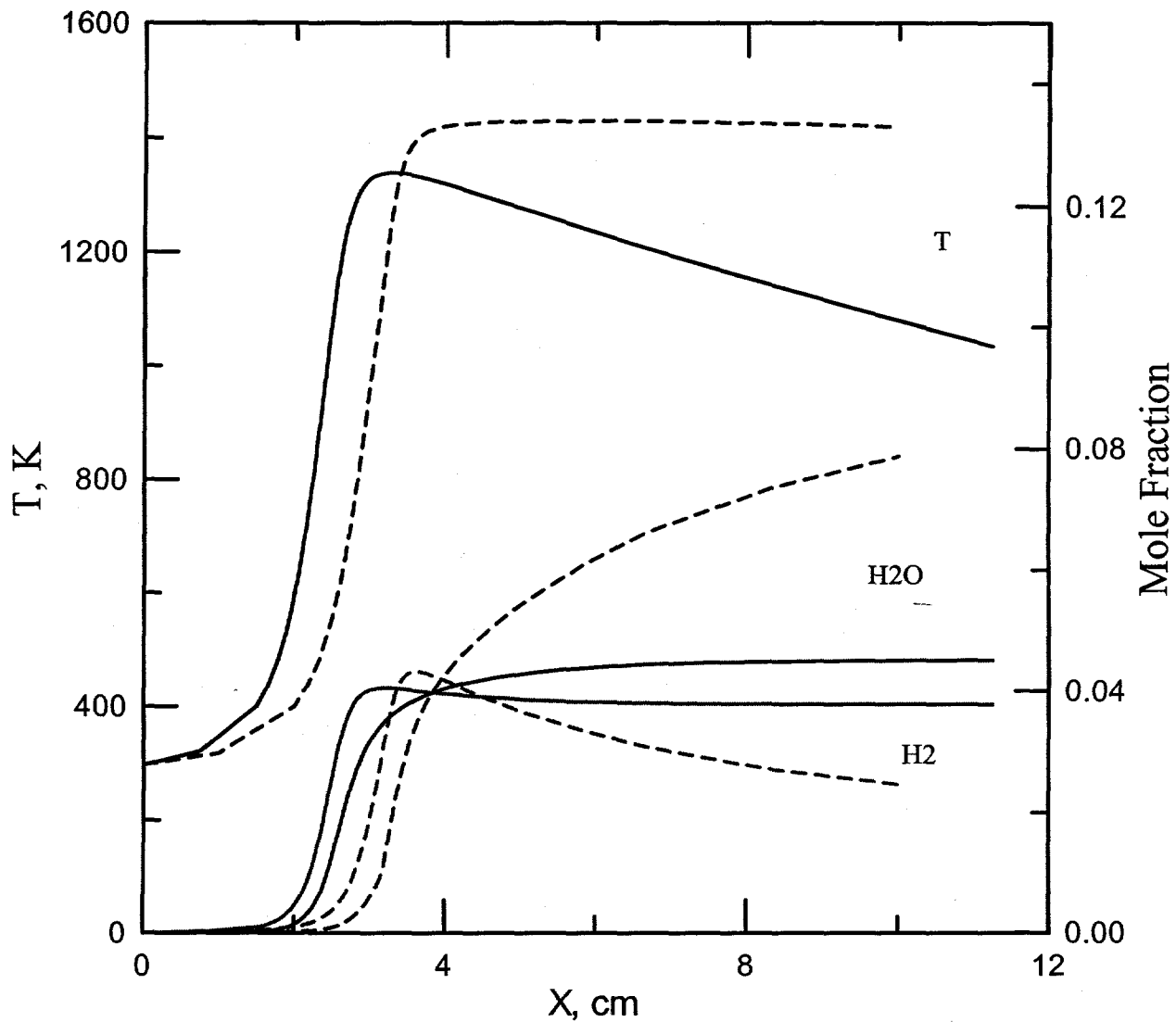
Figure 1. Calculated Temperature and Major Species Concentration Profiles as a Function of Reactor Length in near Stoichiometric Conditions. The Solid Temperature Profile is Shown by the Dashed Line.



$\Phi = 2$, $[N_2]=80.52\%$, $[O_2]=7.78\%$, $[H_2S]=11.09\%$,
 $V=40$ cm/s, $Loss=500$ W/m³ K,

$[H_2]=1.7\%$, $[H_2O]=9.1\%$, $[SO_2]=3.3\%$, $[N_2]=81.6\%$, $[H_2S]=0.43\%$
 Conversion = 15%

Figure 2. Calculated Temperature and Major Species Profiles as a Function of Reactor Length in Rich Conditions.



Phi = 2: [N2]=81.3%, [O2]=5.9%, [H2S]=12.75%
V=22 cm/s,

DASHED (Loss=500 W/m³ K),
wave=1.3E-3cm/s, [H2] = 1.8%,
Conversion=16%

SOLID (Loss=4000 W/m³ K)
wave=1.5E-3cm/s
[H2]=3.8%, Conversion = 35%

Figure 3. Influence of Heat Loss Intensity in the Reactor on Combustion Wave Characteristics

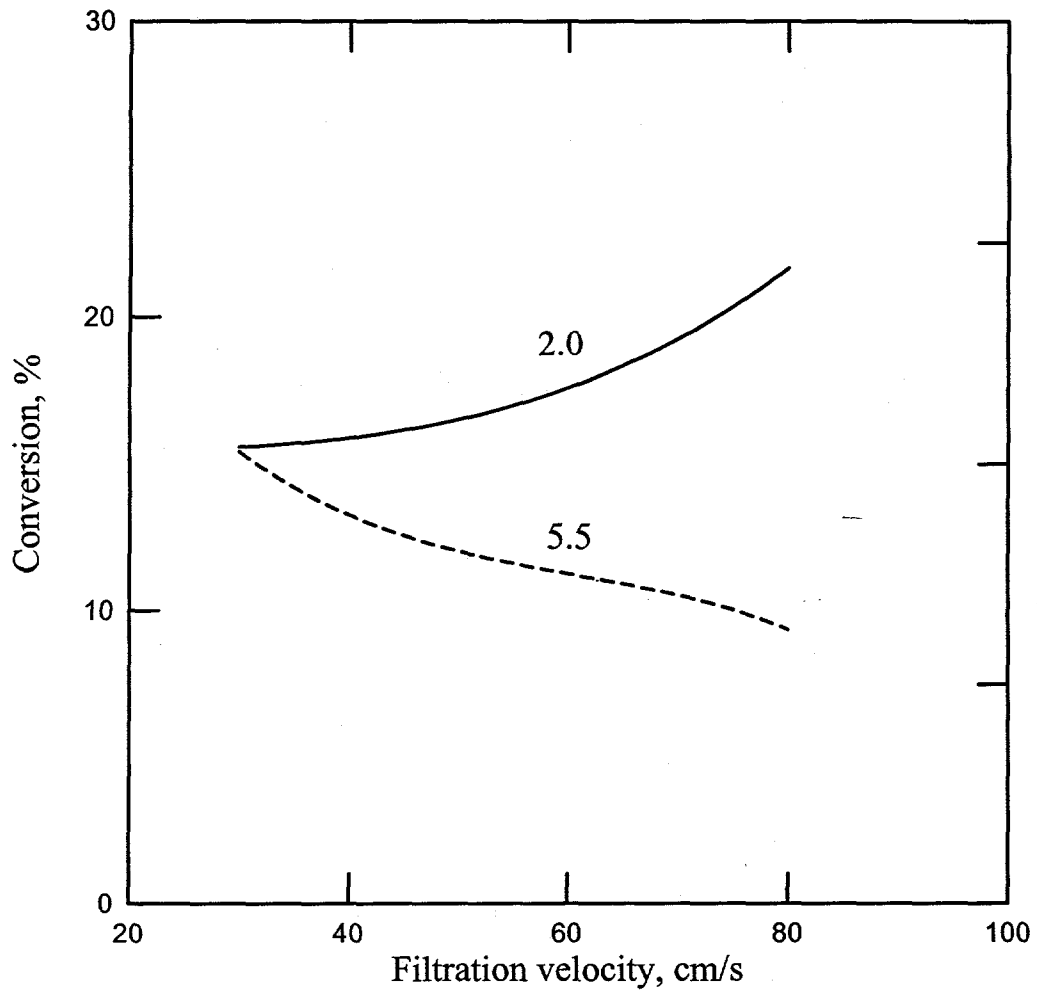


Figure 4. H₂ Conversion as a Function of Equivalence Ratio. Heat Loss Intensity = 500 W/m³ K

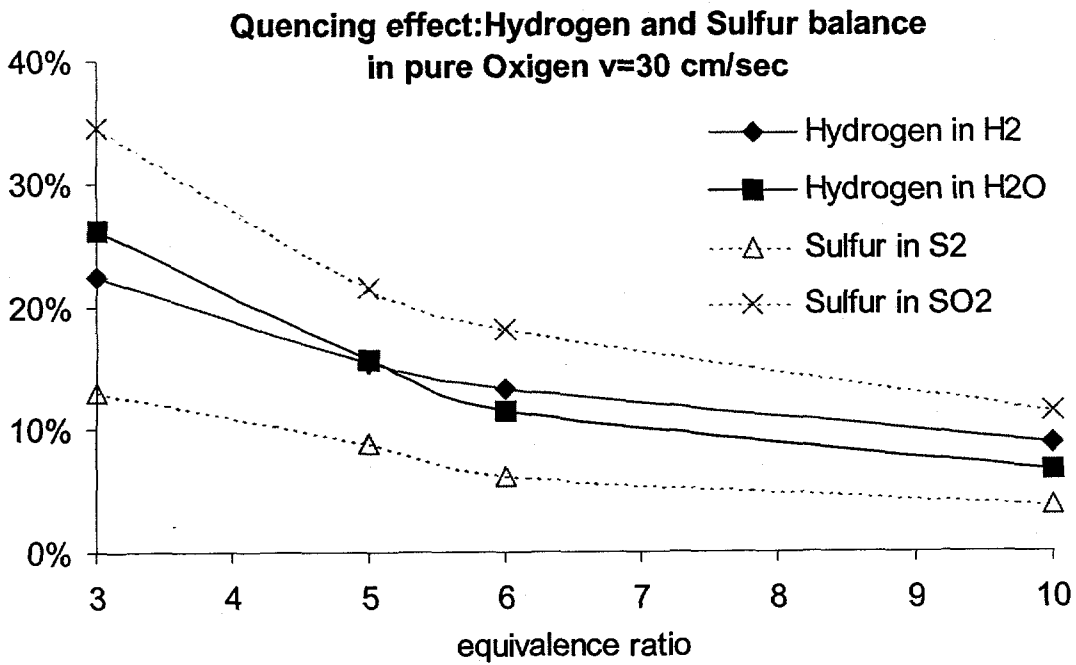
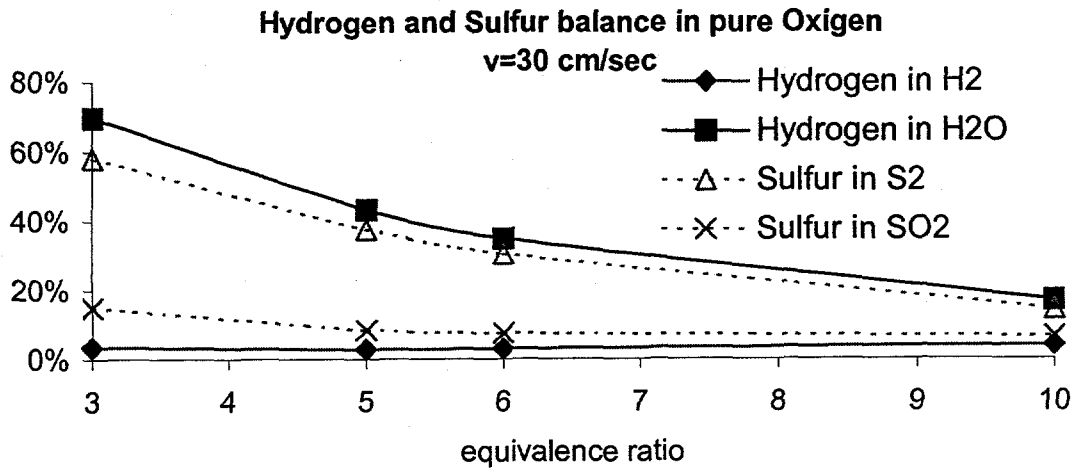


Figure 5. Variation of H₂S Conversion to H₂ and S₂ as a Function of Equivalence Ratio. Bottom Figure Corresponds to High Intensity of Heat Loss.

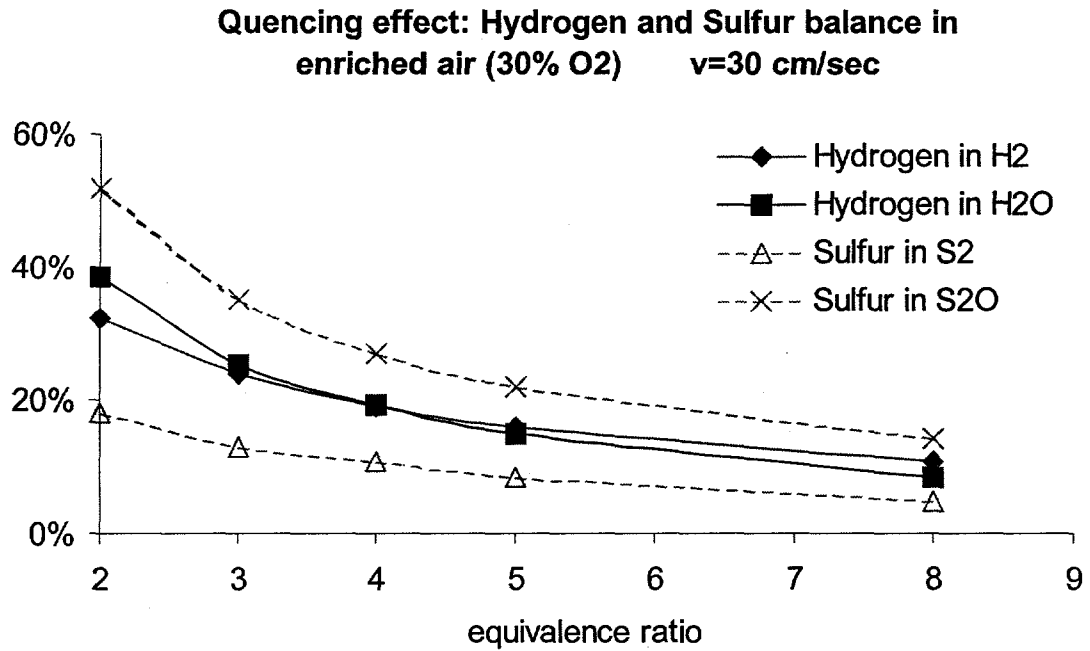
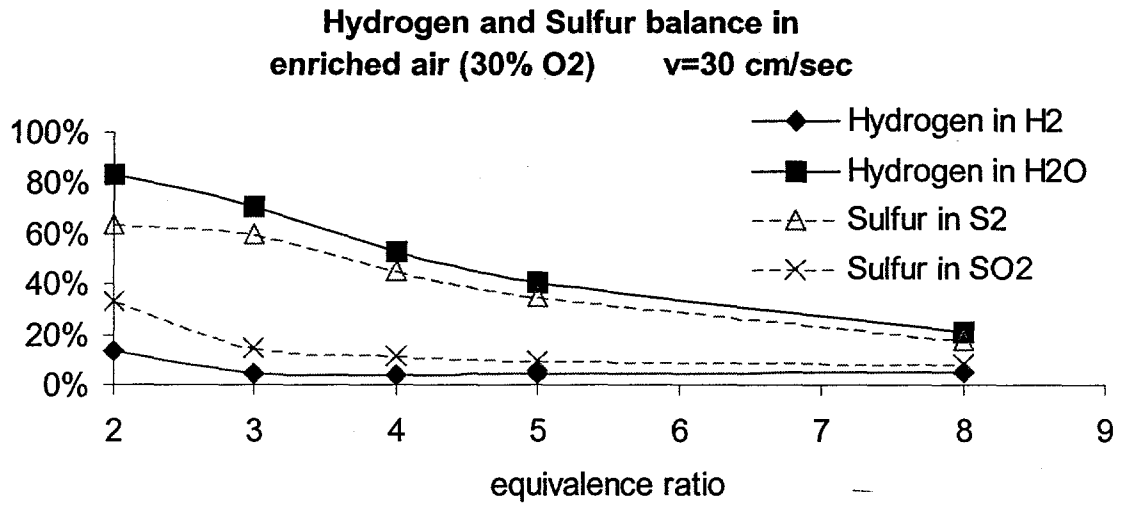


Figure 6. Variation of H₂S Conversion to H₂ and S₂ as a Function of Equivalence Ratio. Bottom Figure Corresponds to High Intensity of Heat Loss.

Product composition in enriched air 30%

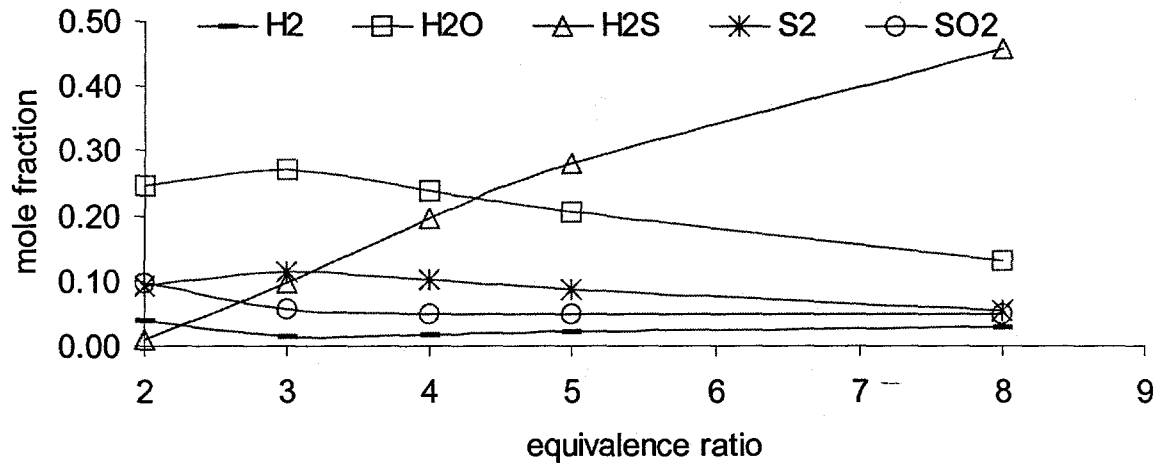


Figure 7. Major Product Composition as a Function of Equivalence Ratio. (Conditions are same as previous figure)

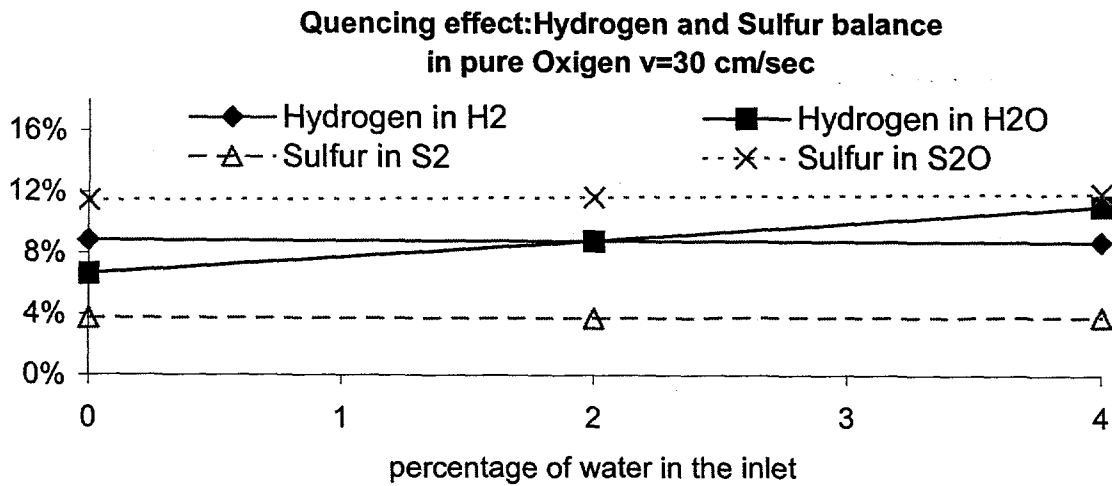
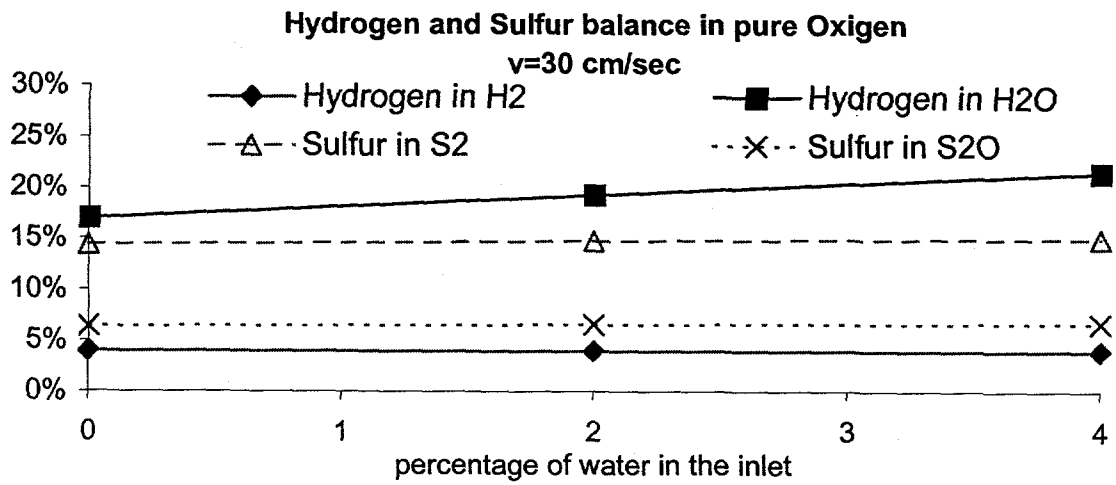


Figure 8. Effect of Water Addition to the Initial Mixture on H₂S Conversion to H₂S and S₂. (Conditions are same as in previous calculations)

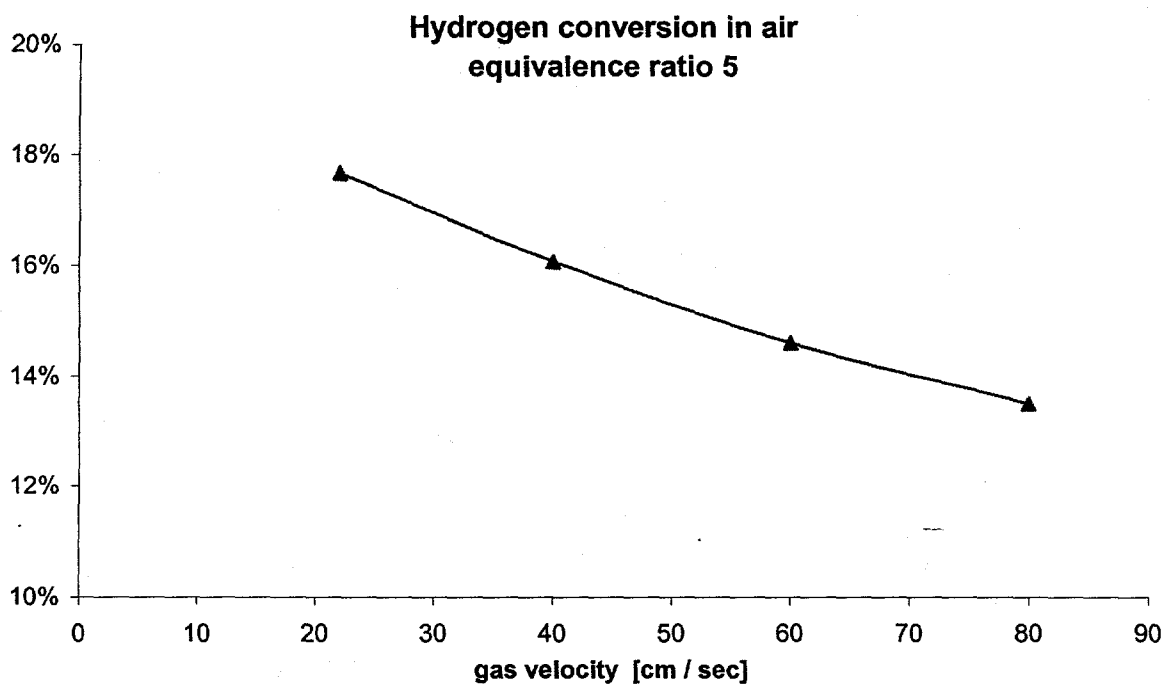


Figure 9. Variation of H₂S Conversion to H₂ as a Function of Filtration Velocity.

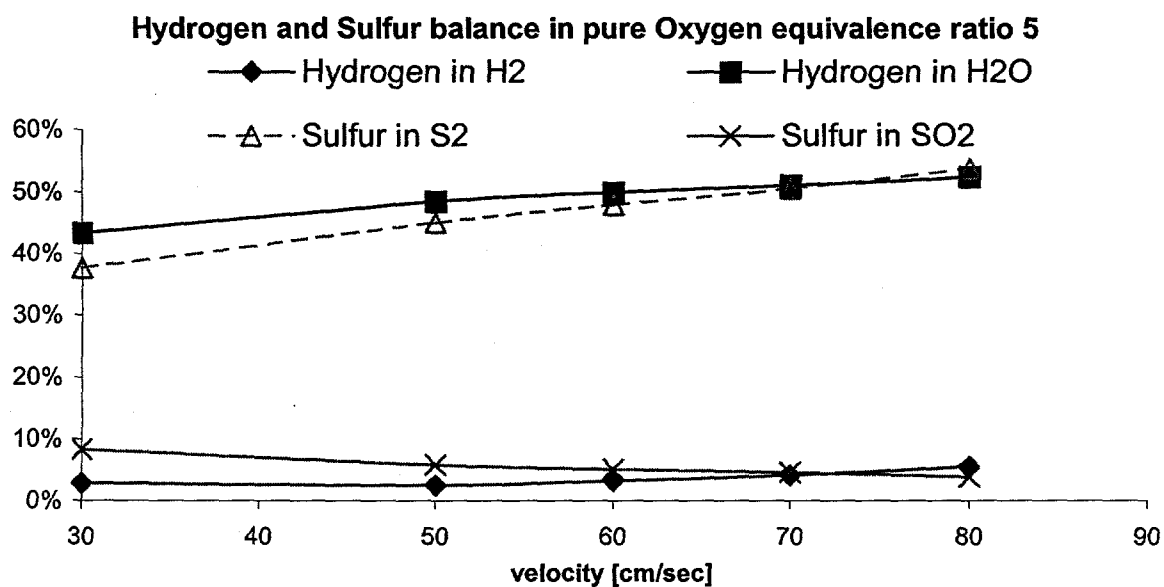


Figure 10. Effect of Filtration Velocity on Product Yield

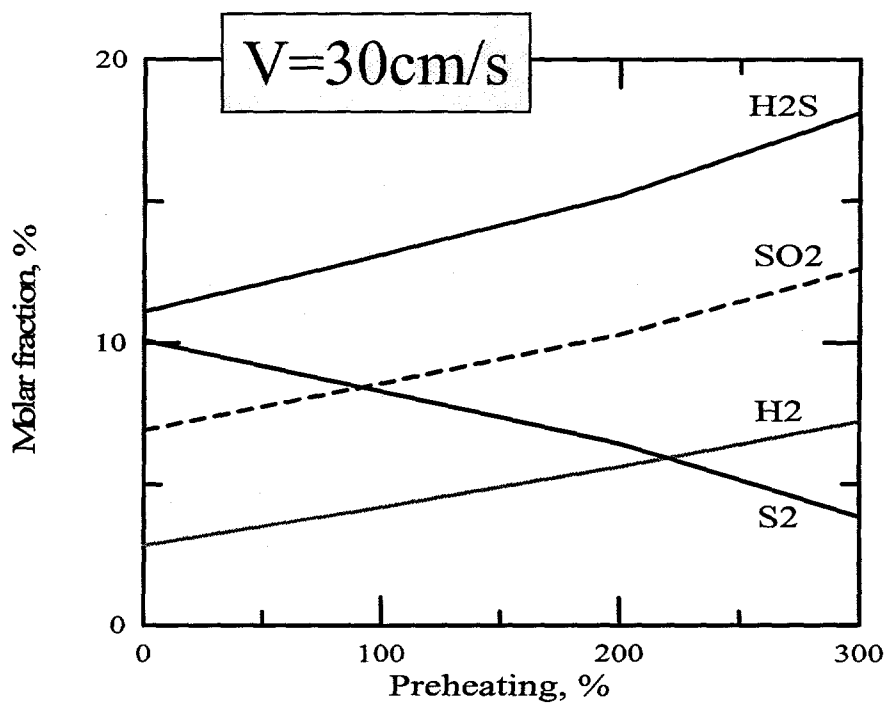
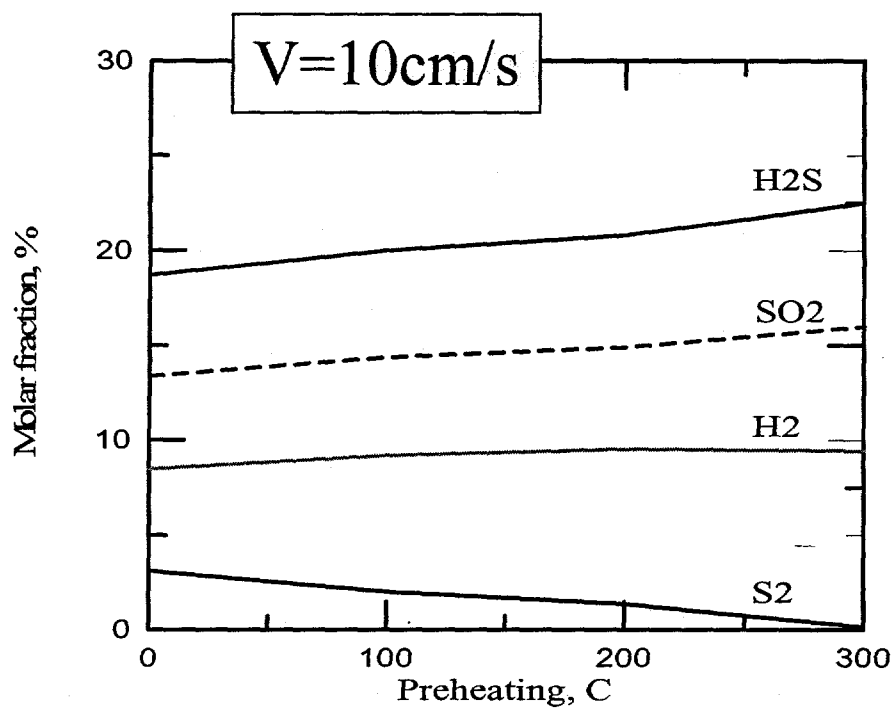


Figure 11. Effect of Preheating of Initial Mixture: $[N_2]=43.7\%$, $[H_2S]=37.5\%$, $[O_2]=18.7\%$
(Equivalence ratio = 3, 30% of $[O_2]$)

APPENDIX B

DESIGN OF A BENCH-SCALE TESTING SYSTEM FOR PRODUCTION OF HYDROGEN FROM THERMAL DECOMPOSITION OF HYDROGEN SULFIDE

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July 2000

1. SUMMARY

The Institute of Gas Technology (IGT) is developing a novel process for hydrogen (H_2) production through the thermal decomposition of hydrogen sulfide (H_2S). The key feature of this process is the superadiabatic combustion (SAC) of a portion of H_2S -oxidant feed gas mixture in a porous medium with high thermal capacity to provide the thermal energy required for the decomposition reaction. The intense heat exchange between the gas and the porous medium ultimately results in flame temperatures that are much higher than the adiabatic combustion temperatures of the feed gas mixture. The high SAC flame temperatures promote the decomposition of H_2S to H_2 and elemental sulfur (S).

A bench-scale testing system is designed for H_2 production from thermal decomposition of 1,400 standard cubic feet per hour (SCFH) of H_2S -oxidant gas mixture. In the proposed testing system, predetermined amounts of feed gas components are mixed and delivered to a packed-bed reactor where H_2S is converted to H_2 and S at high temperatures. Hot off-gas leaving the reactor is cooled with a cooling medium in a condenser where sulfur vapor ($S(g)$) is condensed and collected. Cooled gas is then scrubbed with a caustic solution where H_2S and sulfur dioxide (SO_2) are removed and the cleaned gas is discharged to the atmosphere.

A design package is prepared for the proposed bench-scale testing system. The information required for design, engineering, procurement and installation of this system including the system description, equipment design, and equipment specifications is presented in this report. The estimated total installed cost (TIC) for the bench-scale testing system based on vendor quotations and engineering estimates is \$292,000.

2. DESCRIPTION OF BENCH-SCALE TESTING SYSTEM

The proposed bench-scale testing system is designed to produce H_2 from thermal decomposition of 1,400 standard cubic feet per hour (SCFH) of H_2S and oxidant gas mixture. A process schematic diagram is shown in Figure 2.1. A piping and instrument diagram (P&ID) is shown in Figure 2.2. A brief description of the system is given below.

H_2S , oxygen (O_2) and nitrogen (N_2) feed gases supplied from individual compressed gas cylinders are de-pressurized and delivered at pre-determined flow rates to a mixing chamber (T-101) where the feed gases are thoroughly mixed. The pre-mixed gas mixture is then fed to a reactor (R-101). Three-way valves and by-pass pipings are used to allow the feed gas mixture to be fed to the reactor in an upflow or a downflow mode.

The reactor (R-101) is a vertical, cylindrical tube packed with ¼-inch diameter alumina pellets where H_2 is produced by superadiabatic decomposition of H_2S at high temperatures. The decomposition of H_2S is endothermic and requires high temperatures for the reaction to proceed. In the reactor, a portion of H_2S is combusted with O_2 to provide the thermal energy required for the decomposition reaction. The intense heat exchange between the hot gas mixture and the porous medium allows the accumulation of energy in the solid matrix and consequently results in reactor flame temperatures that are much higher than the adiabatic flame temperatures of the feed

gas mixture. The high reactor temperatures promote the progression of the decomposition reaction.

Off-gas leaving the reactor is maintained at temperatures above the dew point of $S_{(g)}$ to prevent any condensation of $S_{(g)}$ in the reactor. Hot off-gas is fed to a sulfur condenser (E-101) where the gas is cooled and sulfur vapor is condensed and collected. The sulfur condenser is a vertical, tube-and-shell heat exchanger where the off-gas flows downward in the tube side and the cooling medium flows counter-currently in the shell side. Cooled gas is then scrubbed with caustic solution in a countercurrent, multiple-spray type of gas scrubber (T-102) where SO_2 and unreacted H_2S are removed. The cleaned gas is then discharged to the atmosphere.

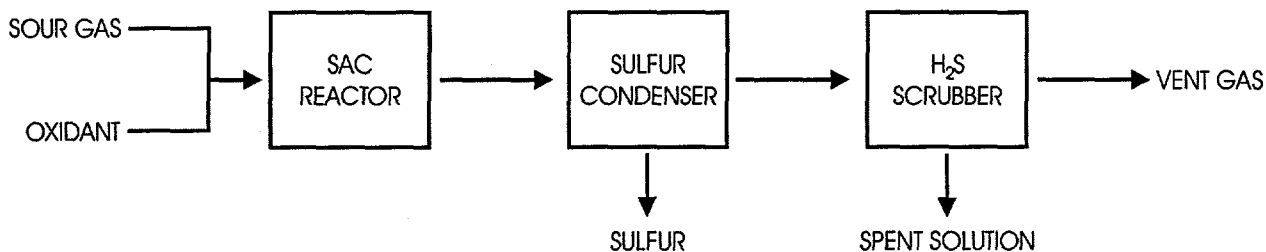


Figure 2.1 Process Schematic Diagram for a Bench-Scale Testing System

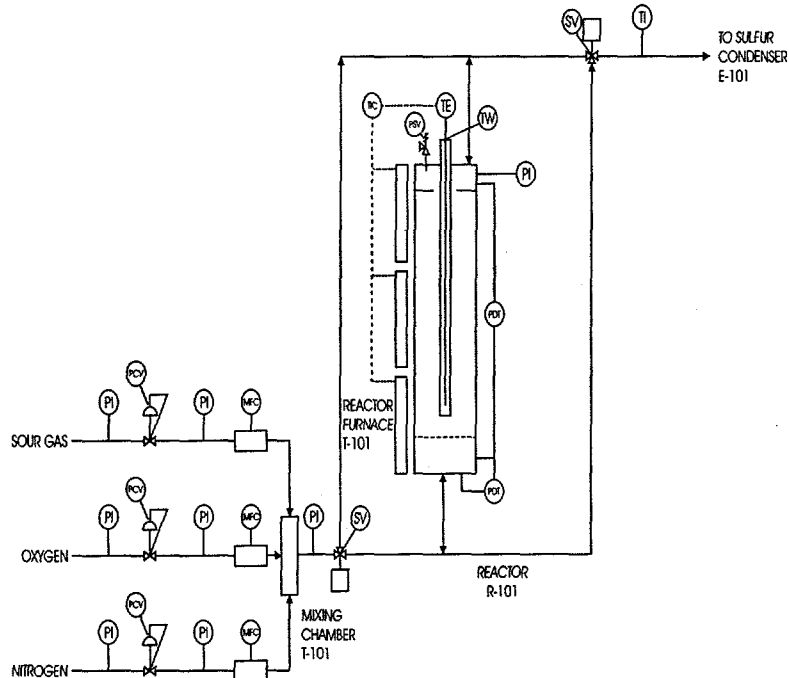


Figure 2.2 PID for a Bench-Scale Testing System

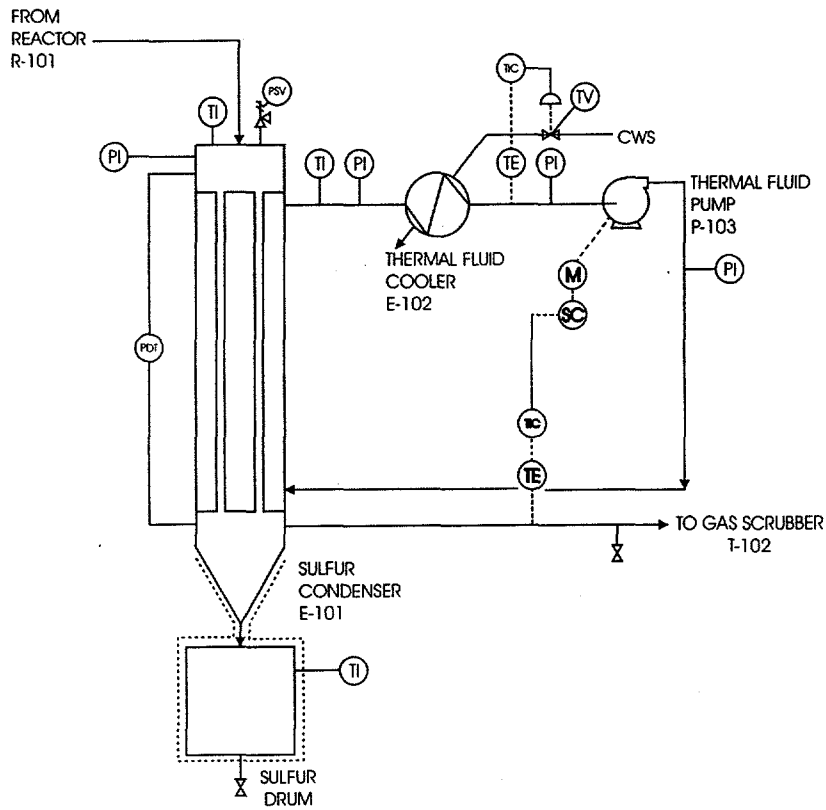


Figure 2.2 PID for a Bench-Scale Testing System

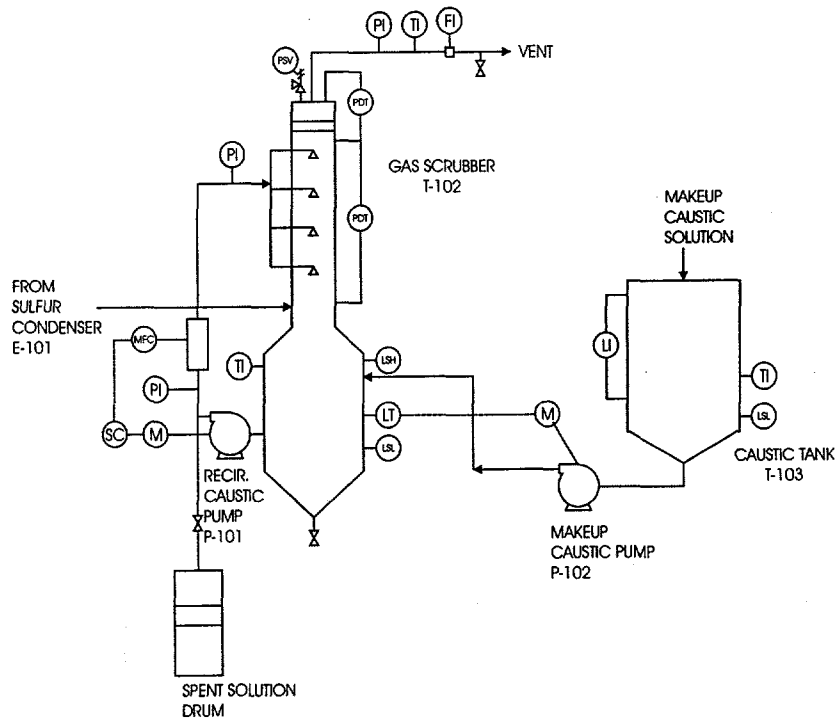


Figure 2.2 PID for a Bench-Scale Testing System

3. DESIGN OF BENCH-SCALE TESTING SYSTEM

The design of major equipment for the proposed lab-scale testing system, including key operating conditions and performance requirements, are presented in this section.

3.1. Reactor (R-101)

The reactor is designed based on the following parameters:

Type	Vertical packed column
Packing Material	¼-inch alumina pellets
Maximum Temperature	2,800°F (1538°C)
Maximum Superficial Gas Velocity	2 ft/s (60 cm/s)
Maximum Interstitial Gas Velocity	5 ft/s (150 cm/s)
Minimum Gas Residence Time	2 sec
Inner Diameter	6 inches (15 cm)

A vertical fixed-bed reactor packed with ¼-inch diameter alumina pellets is used to facilitate the thermal decomposition of H₂S via superadiabatic combustion. The maximum superficial and interstitial gas velocities of 2 ft/s (60 cm/s) and 5 ft/s (150 cm/s), respectively, are used based on modeling and experimental studies conducted at the University of Illinois at Chicago (UIC). The superficial gas velocity is defined based on the feed gas flow rate in an empty reactor column at ambient conditions; the interstitial gas velocity is also defined based on the feed gas flow rate in the interstitial space of the alumina packing at ambient conditions.

A reactor diameter of 6 inches (15 cm) is used so that the data generated from the bench-scale reactor can be used for future scale-up design. A minimum gas residence time of 2 seconds in the packed-bed of the reactor based on the maximum superficial gas velocity is used to ensure complete conversion of decomposition reaction. This results in a packing height of 48 inches. Based on these conditions, the proposed reactor is capable of processing about 1,400 SCFH of total feed gas mixture containing H₂S and oxidant. The estimated pressure drop across the packed-bed at maximum gas throughput ranges from 0.7 to 1.6 psi at average gas temperatures ranging from 1000 to 2500°F (538 to 1371°C).

The reactor consists of a vertical, cylindrical carbon steel shell (21-inch ID x 21.5-inch OD x 72-inch H) lined with 6-inch thick rigid fibrous ceramic insulation. An impervious ceramic tube (6-inch ID x 7-inch OD x 72-inch H) containing 99+% alumina is used as the inner reactor tube to contain the alumina packing and reactor gases. A 30 kW 3-zone, silicon carbide or molybdenum disilicide electric heater is located in the space between the ceramic tube and the insulation to provide auxiliary heat for cold startup and temperature control. Support and hold-down plates are used to support and contain the alumina packing and ceramic insulation. High-temperature gaskets are used in the ceramic-metal joints and the flanged connections to prevent any leakage of reactor gases. Additional information regarding the mechanical design of the proposed reactor is given in Section 4.3 of this report.

All insulation materials with low thermal conductivity are porous. The porosity of castable refractory may vary from 20 to 50% depending on the compositions, densities, and installation and curing methods. The porosity of rigid ceramic fiber insulation, which has much lower thermal conductivity than castable refractory, can be as high as 85%. The porosity of the fixed bed packed with alumina pellets is about 40%. Therefore, an impervious ceramic tube is needed as the inner reactor tube such that all feed and reactor gases flow through the packed bed and no gas will by-pass or channel through the porous insulation layers. Furthermore, the reactor gases containing H₂ may attack the high temperature silicon carbide or molybdenum disilicide heating elements, which reduces the efficiency of heating elements. The ceramic tube prevents any direct contact of heating elements with reactor gases.

A carbon steel shell is placed outside of the inner reactor tube to prevent the reactor gases from leaking to the atmosphere, should there be a rupture or a crack in the inner reactor tube. The outer metal shell is lined with layers of rigid fibrous ceramic insulation such as Zircar AL-30AAH and ALC. These low-density (less than 30 lb/ft³) insulation materials have lower thermal conductivity and provide better thermal insulation than castable refractory at high temperatures.

The alumina pellets are randomly packed and supported by a perforated grid plate. A hold-down plate is used at the top of the reactor to prevent the packing pellets from being blown out of the reactor. A thin layer of high-temperature insulation blanket is used to cover the inner wall of the reactor tube to minimize the effect of differential thermal expansion between the ceramic tube wall and alumina pellets. The instrumentation for the reactor includes thermocouples placed inside a thermowell located along the axis of the reactor, a pressure indicator, a differential pressure transmitter for pressure drop across the packing, and a pressure relief valve. A set of three-way valves located at the inlet and outlet of the reactor and by-pass pipings is used to allow the feed gas mixture to be fed to the reactor in an upflow or a downflow mode.

3.2. Sulfur Condenser (E-101)

The design of the sulfur condenser is summarized as follows:

Type	Vertical, tube-and-shell
Flow Pattern	Countercurrent
Heat Duty	32,000 Btu/h
Feed Gas Flow Rate	110 lb/h, in tube side
Sulfur Vapor Condensed	40 lb/h
Inlet Gas Temperature	800°F (427°C)
Outlet Gas Temperature	300°F (149°C)
Cooling Water Flow Rate	3190 lb/h, in shell side
Tube Dimensions	(7) 1-inch D x 72-inch L
Shell Dimensions	6-inch D x 72-inch L
Material of Construction	Stainless Steel

The sulfur condenser is a vertical, downflow tube-and-shell heat exchanger where hot off-gas from the reactor (R-101) is cooled and S_(g) is condensed in the tube side. Liquid sulfur (S_(l)) is

drained by gravity and collected in an electrically traced sulfur drum. Temperatures of the liquid sulfur are controlled at about 300°F (149°C) to maintain a low viscosity for the liquid sulfur.

One concern of using cooling water as the cooling medium for the sulfur condenser is that the water inlet temperature is much lower than the temperatures of the condenser off-gas and liquid sulfur. This large temperature difference may cause some temperature control problems such as over cooling the gas and $S_{(l)}$, which can result in potential plugging due to increased viscosity of $S_{(l)}$ at lower temperatures. This problem can be overcome by using a waste heat boiler type of sulfur condenser, which is the conventional design for most commercial-scale units, or a thermal fluid system such as Dowtherm with the inlet and outlet temperatures of the thermal fluid maintained close to the temperature of $S_{(l)}$. Both systems are complicated and expensive due to the need of additional equipment, instrumentation, and control. The use of a thermal fluid system also requires a much larger sulfur condenser due to the decreased driving force for heat transfer, i.e., the log mean temperature difference.

3.3. Gas Scrubber (T-102)

The design of the gas scrubber is summarized as follows:

Type	Vertical, countercurrent spray column
Feed Gas Flow Rate	1,990 ft ³ /h
H ₂ S Concentration	44 mol %
Feed Gas Temperature	300°F (149°C)
Scrubbing Liquid	20 wt % caustic solution
Liquid Flow Rate	320 lb/h
Liquid/Acid Gas Loading	50 gal/1000 SCF
Dimensions of Spray Column	6-inch D x 102-inch H
Number of Spray Nozzles	4
Material of Construction	Carbon steel

Off-gas leaving the sulfur condenser (E-101) is scrubbed with caustic solution in the gas scrubber where unreacted H₂S and SO₂ are removed. The condenser off-gas contains trace amount (less than 0.1 vol %) of $S_{(g)}$ which may be condensed in the scrubber when the gas is cooled. This precludes the use of a packed or a tray column due to the potential plugging from sulfur condensation. A spray column is used because of its low capital cost, easy maintenance, operational flexibility, and low pressure drop. Multiple spray nozzles are used to improve the removal efficiency. Caustic solution is selected as the scrubbing liquid because of its high removal efficiency and low liquid-to-gas loading requirement which is about 6 times lower than that for potassium carbonate solution. This would simplify the handling and disposal of spent scrubbing liquid. The diameter of the gas scrubber is determined from the flooding velocity calculations for a spray column. The height of the scrubber is determined by calculations of transfer height and numbers of transfer unit based on liquid droplet size and an empirical correlation for mass transfer coefficient for a spray column.

4. EQUIPMENT INFORMATION FOR BENCH-SCALE TESTING SYSTEM

The equipment list, equipment summary, and equipment specifications for the proposed bench-scale testing system are presented in this section.

4.1. Equipment List

The major equipment for the proposed lab-scale testing system is shown in Table 4.1.

Table 4.1. Equipment List for a Bench-Scale Testing System

Equipment No	Equipment Description
E-101	Sulfur Condenser
E-102	Thermal Fluid Cooler
P-101	Recirculating Caustic Pump
P-102	Makeup Caustic Pump
P-103	Thermal Fluid Pump
R-101	Reactor
T-101	Mixing Chamber
T-102	Gas Scrubber
T-103	Caustic Tank

4.2. Equipment Summary

A summary of major equipment for the bench-scale testing system is given in Table 4.2.

Table 4.2. Equipment Summary for a Bench-Scale Testing System

Equip No.	Equipment Name	Qty	Description
E-101	Sulfur Condenser	1	Vertical tube-and-shell heat exchanger, 32,000 Btu/h heat duty, 11 ft ² heat transfer surface area, all stainless steel. 110 lb /h process gas is cooled in tube side from 800°F to 300°F and 40 lb/h sulfur vapor is condensed with city water in shell side.
E-102	Thermal Fluid Cooler	1	Tube-and-shell heat exchanger, 32,000 Btu/h heat duty, 8 ft ² heat transfer surface area, 1,210 lb /h Dowtherm A is cooled from 300°F to 250°F by city water.
P-101	Recirculating Caustic Pump	1	Centrifugal pump rated for 2 gpm 20 wt % caustic solution at 1.2 specific gravity, 130°F and 60 psi differential pressure, flooded suction, all carbon steel, equipped with variable speed motor and drive.

Table 4.2. Equipment Summary for a Lab-Scale Testing System—cont'd

Equip No.	Equipment Name	Qty	Description
P-102	Makeup Caustic Pump	1	Centrifugal pump rated for 1 gpm 20 wt %caustic solution at 1.2 specific gravity, 80°F and 30 psi differential pressure. all carbon steel, equipped with motor and drive.
P-103	Thermal Fluid Pump	1	Centrifugal pump rated for 3 gpm Dowtherm A at 1.0 specific gravity, 250°F and 10 psi differential pressure, flooded suction, all carbon steel, equipped with variable speed motor and drive.
R-101	Reactor	1	<u>Outer Shell</u> : vertical carbon steel, 21" ID x 21.5" OD x 72" H, lined with 6" thick fibrous ceramic insulation. <u>Inner Tube</u> : vertical impervious ceramic tube, 6" ID x 7" OD x 72" H, packed with ¼" alumina pellets, 2,800°F maximum temperature, 3 psig internal pressure. <u>Heating Element</u> : 3-zone, 2,800°F, located outside of inner tube, complete with instrumentation and control.
T-101	Mixing Chamber	1	Mixing chamber for 2 mol/h hydrogen sulfide and 2 mol/h air.
T-102	Gas Scrubber	1	Countercurrent multiple-spray column, 6" D x 102" H spray section and 12" D x 72" H liquid reservoir section. 1990 ft ³ /h process gas containing 44 vol% H ₂ S at 300°F is scrubbed with 320 lb/h 20 wt% caustic solution.
T-103	Caustic Tank	1	800-gal carbon steel storage tank for 20 wt % caustic solution.

4.3. Equipment Specifications

The specifications of major equipment for the bench-scale testing system are given in the following tables.

EQUIPMENT SPECIFICATION FOR SULFUR CONDENSER (E-101)

1. Introduction

- 1.1. The Institute of Gas Technology (IGT) is constructing a lab-scale unit for the production of H₂ from the thermal decomposition of H₂S. This specification covers the requirements for furnishing a sulfur condenser to be used for this project. The vendor shall supply one sulfur condenser in accordance with the following specifications and attached drawings.

2. General Description

- 2.1. The sulfur condenser is a vertical, countercurrent tube-and-shell heat exchanger where the feed gas flows downward in the tube side and the cooling medium, such as Dowtherm thermal fluid, flows in the shell side. The feed gas is cooled and S_(g) is condensed, drained, and collected.

3. Design Data

- 3.1. General
- | | |
|--------------------------|---|
| Type | Vertical, countercurrent tube-and-shell |
| Heat Duty | 32,000 Btu/h |
| Material of Construction | * |
| Type of Service | Continuous |

3.2. Service conditions and Performance Requirements

	Tube Side	Shell Side
Fluid	Process gas	Dowtherm A
Flow Rate, lb/h	110	1,200
Sulfur Vapor Condensed, lb/h	40	
Inlet Temperature, °F	800	250
Outlet Temperature, °F	300	300
Inlet Pressure, psig	1	40
Outlet Pressure, psig	*	*
Density, lb/ft³	0.03	62
Specific Heat, Btu/lb-°F	0.26	0.53
Thermal Conductivity, Btu/ft-°F-h	0.026	0.08
Viscosity, cp	0.03	0.3

* Vender to recommend.

4. Site Data

- 4.1. Location
Institute of Gas Technology
1700 South Mount Prospect Road
Des Plaines, Illinois 60018
The unit will be located indoors.
- 4.2. Power Available
110/230/460 volts, 60 Hz, 1-phase and 3-phase.
- 4.3. Area Specification
To be provided by IGT

5. Details of Construction

- 5.1 A preliminary design of the condenser is shown in the attached Figure 4.3.1-A and Table 4.3.1-A, which are considered to be part of this specification. The vendor is free to recommend other types of heat exchange equipment.
- 5.2. The condenser shall be designed to allow for easy disassembling for inspection, cleaning and maintenance.
- 5.3. The condenser shall be designed and constructed to accommodate for differential thermal expansions of the tubes and shell.
- 5.4. Corrosion allowance should be provided for the wall thickness calculations.
- 5.5. The vendor shall perform his own structural calculations to finalize the design, and to recommend the appropriate, cost effective material for construction. The final design shall be in compliance with all applicable codes.
- 5.6. The vendor shall submit final drawings showing all structural details as part of the quotation.

6. Performance Guarantee

- 6.1. The vendor shall guarantee the equipment to meet the specification requirements for a period of 12 months from the date of initial operation or 18 months from the date of shipping.
- 6.2. Changes mandated by substandard performance shall be made promptly at the vendor's expense.

7. Quotation

- 7.1. The vendor shall provide a quotation including firm fixed price and delivery schedule good for 60 days.
- 7.2. The vendor shall identify and explain any exceptions or deviations made with respect to the specification requirements.
- 7.3. The vendor shall provide data as requested with the quotation.

Table 4.3.1-A. Nozzle Schedule for Sulfur Condenser (E-101)

Nozzle No.	Size, inch	Service
1	2	Gas Inlet
2	0.5	Temperature Indicator
3	0.5	Differential Pressure Transmitter
4	2	Pressure Relief
5	1	Dowtherm Outlet
6	0.5	Pressure Indicator
7	1	Dowtherm In
8	1	Drain
9	2	Gas Outlet
10	0.5	Temperature Indicator
11	0.5	Differential Pressure Transmitter
12	2	Liquid Sulfur Outlet

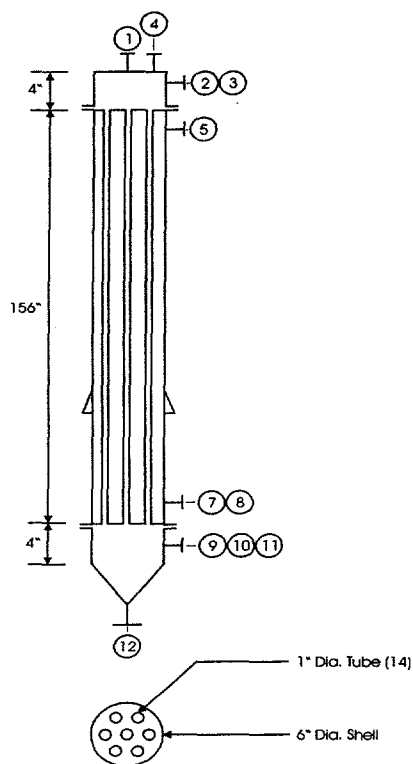


Figure 4.3.1-A Sulfur Condenser (E-101)

EQUIPMENT SPECIFICATION FOR THERMAL FLUID COOLER (E-102)

1. Introduction

- 1.1. The Institute of Gas Technology (IGT) is constructing a bench-scale unit for the production of H_2 from thermal decomposition of H_2S . This specification covers the requirements for furnishing a thermal fluid cooler to be used for this project. The thermal fluid cooler is a tube-and-shell heat exchanger where hot Dowtherm fluid is cooled by city water. The vendor shall supply one thermal fluid cooler in accordance with the following specifications.

2. Design Data

2.1. General

Type	Tube-and-shell
Heat Duty	32,000 Btu/h
Material of Construction	*
Type of Service	Continuous

2.2. Service Conditions and Performance Requirements

Fluid	Dowtherm A	City water
Flow Rate, lb/h	1,210	1,100
Inlet Temperature, °F	300	70
Outlet Temperature, °F	250	100
Inlet Pressure, psig	40	40
Outlet Pressure, psig	*	*
Density, lb/ft³	62	62
Specific Heat, Btu/lb-°F	0.53	1.0
Thermal Conductivity, Btu/ft-°F-h	0.08	0.36
Viscosity, cp	0.3	0.8

3. Site Data

- 3.1. Location Institute of Gas Technology
1700 South Mount Prospect Road
Des Plaines, Illinois 60018
The unit will be installed indoors.
- 3.2. Power Available 110/230/460 volts, 60 Hz, 1-phase and 3-phase.
- 3.3. Area Specification To be provided by IGT

4. Details of Construction

- 4.1. The condenser shall be designed to allow for easy disassembling for inspection, cleaning, and maintenance.
- 4.2. The condenser shall be designed and constructed to accommodate differential thermal expansions of the tubes and shell.
- 4.3. Corrosion allowance shall be provided for the wall thickness calculations.
- 4.4. The vendor shall perform his own structural calculations to finalize the design, and to recommend the appropriate and cost effective material for construction. The final design shall be in compliance with all applicable codes.
- 4.5. The vendor shall submit final drawings showing all structural details as part of the quotation.

5. Performance Guarantee

- 5.1. The vendor shall guarantee the equipment to meet the specification requirements for a period of 12 months from the date of initial operation or 18 months from the date of shipping.
- 5.2. Changes mandated by substandard performance shall be made promptly at the vendor's expense.

6. Quotation

- 6.1. The vendor shall provide a quotation including firm fixed price and delivery schedule good for 60 days.
- 6.2. The vendor shall identify and explain any exceptions or deviations made with respect to the specification requirements.
- 6.3. The vendor shall provide data as requested with the quotation.

* Vendor to recommend.

SPECIFICATION FOR RECIRCULATING CAUSTIC PUMP (P-101)

1. Introduction

- 1.1. The Institute of Gas Technology (IGT) is constructing a bench-scale unit for the production of H₂ from thermal decomposition of H₂S. This specification covers the requirements for furnishing a recirculating caustic pump to be used for this project. The vendor shall supply one recirculating caustic pump in accordance with the following specifications.

2. General Description

- 2.1. Process gas stream is scrubbed with caustic solution in a countercurrent spray column where H₂S and SO₂ are removed from the gas stream. The recirculating caustic pump provides caustic solution to the spray nozzles.

3. Design Data

- 3.1. Service Conditions and Performance Requirements

Type	Centrifugal pump
Fluid Handled	20 wt% caustic solution
Capacity	2 gpm
Differential Pressure	60 psi
Suction Pressure	2 psig, flooded
Temperature	130°F
Specific Gravity	1.2
Viscosity	1 cp
Motor	Variable speed
Type of Service	Continuous

4. Site Data

- 4.1. Location

Institute of Gas Technology
1700 South Mount Prospect Road
Des Plaines, Illinois 60018
The unit will be installed indoors.
- 4.2. Power Available

110/230/460 volts, 60 Hz, 1-phase and 3-phase.
--

4.3. Area Specification To be provided by IGT

5. Performance Guarantee

- 5.1. The vendor shall guarantee the equipment to meet the specification requirements for a period of 12 months from the date of initial operation or 18 months from the date of shipping.
- 5.2. Changes mandated by substandard performance shall be made promptly at the vendor's expense.

6. Quotation

- 6.1. The vendor shall provide a quotation including firm fixed price and delivery schedule good for 60 days.
- 6.2. The vendor shall identify and explain any exceptions or deviations made with respect to the specification requirements.
- 6.3. The vendor shall provide data as requested with the quotation.

EQUIPMENT SPECIFICATION FOR MAKEUP CAUSTIC PUMP (P-102)

1. Introduction

- 1.1. The Institute of Gas Technology (IGT) is constructing a bench-scale unit for the production of H₂ from thermal decomposition of H₂S. This specification covers the requirements for furnishing a makeup caustic pump to be used for a gas scrubber. The vendor shall supply one makeup caustic pump in accordance with the following specifications.

2. General Description

- 2.1. Fresh caustic solution is pumped from a storage tank to a gas scrubber for maintaining a constant liquid level in the scrubber.

3. Design Data

- 3.1. Service Conditions and Performance Requirements
 - Type Centrifugal pump
 - Fluid Handled 20 wt% caustic solution
 - Capacity 1 gpm
 - Differential Pressure 30 psi
 - Suction Pressure 2 psig, flooded
 - Temperature ambient
 - Specific Gravity 1.2
 - Viscosity 1 cp

Motor
Type of Service

Constant speed
Intermittent

4. Site Data

- 4.1. Location Institute of Gas Technology
1700 South Mount Prospect Road
Des Plaines, Illinois 60018
The unit will be installed indoors.
- 4.2. Power Available 110/230/460 volts, 60 Hz, 1-phase and 3-phase.
- 4.3. Area Specification To be provided by IGT

5. Performance Guarantee

- 5.1. The vendor shall guarantee the equipment to meet the specification requirements for a period of 12 months from the date of initial operation or 18 months from the date of shipping.
- 5.2. Changes mandated by substandard performance shall be made promptly at the vendor's expense.

6. Quotation

- 6.1. The vendor shall provide a quotation including firm fixed price and delivery schedule good for 60 days.
- 6.2. The vendor shall identify and explain any exceptions or deviations made with respect to the specification requirements.
- 6.3. The vendor shall provide data as requested with the quotation.

SPECIFICATION FOR THERMAL FLUID PUMP (P-103)

1. Introduction

- 1.1. The Institute of Gas Technology (IGT) is constructing a bench-scale unit for the production of H_2 from thermal decomposition of H_2S . This specification covers the requirements for furnishing a thermal fluid pump to be used for this project. The vendor shall supply one thermal fluid pump in accordance with the following specification.

2. General Description

- 2.1. Thermal fluid is used as the cooling medium in a condenser. Returned hot thermal fluid leaving the condenser is cooled by city water in a cooler. Cooled

thermal fluid leaving the cooler is then pumped by the thermal fluid pump and returned to the condenser.

3. Design Data

3.1. Service Conditions and Performance Requirements

Type	Centrifugal pump
Fluid Handled	Dowtherm A
Capacity	3 gpm
Differential Pressure	10 psi
Suction Pressure	2 psig, flooded
Temperature	250°F
Specific Gravity	1
Viscosity	0.3 cp
Motor	Variable speed
Type of Service	Continuous

4. Site Data

- 4.1. Location Institute of Gas Technology
1700 South Mount Prospect Road
Des Plaines, Illinois 60018
The unit will be installed indoors.
- 4.2. Power Available 110/230/460 volts, 60 Hz, 1-phase and 3-phase.
- 4.3. Area Specification To be provided by IGT

5. Performance Guarantee

- 5.1. The vendor shall guarantee the equipment to meet the specification requirements for a period of 12 months from the date of initial operation or 18 months from the date of shipping.
- 5.2. Changes mandated by substandard performance shall be made promptly at the vendor's expense.

6. Quotation

- 6.1. The vendor shall provide a quotation including firm fixed price and delivery schedule good for 60 days.
- 6.2. The vendor shall identify and explain any exceptions or deviations made with respect to the specification requirements.
- 6.3. The vendor shall provide data as requested with the quotation.

EQUIPMENT SPECIFICATION FOR REACTOR (R-101)

1. Introduction

- 1.1. The Institute of Gas Technology (IGT) is constructing a bench-scale testing system for the production of H_2 from thermal decomposition of H_2S . This specification covers the requirements for a reactor to be used for converting H_2S into H_2 and elemental sulfur using superadiabatic combustion in a packed-bed reactor. The vendor shall supply one reactor in accordance with the following specifications and attached drawings.

2. General Description

- 2.1. A preliminary design of the reactor is shown in the attached Figure 4.3.6-A and Table 4.3.6-A.
- 2.2. The reactor is a vertical, cylindrical steel vessel (21" ID x 21.5" OD x 72" H) lined with 6"-thick low thermal conductivity ceramic insulation. An impervious ceramic tube (6" ID x 7" OD x 72" H) is used as the inner tube to contain the alumina packing and reactor gases. An electric heater is located in the space between the ceramic tube and the insulation.
- 2.3. Support and hold-down plates are used to support and contain the alumina packing and ceramic insulation.
- 2.4. High-temperature gaskets are used to prevent leakage of reactor gases.
- 2.5. Feed gas mixture containing H_2S and oxidant is fed to the packed-bed reactor where H_2S is decomposed into H_2 and sulfur at high temperatures. Raw gas leaving the reactor contains H_2 , elemental sulfur, H_2S , SO_2 , N_2 , and water vapor ($H_2O_{(g)}$).

3. Design Data

- | | |
|--------------------------|-----------------------------|
| 3.1. Inner Reactor Tube | |
| Type | Vertical cylindrical tube |
| Material of Construction | Impervious ceramics |
| Overall Dimensions | 6" ID x 7" OD x 72" H |
| Reactor Temperature | 2,800°F max. |
| Off-Gas Temperature | 800°F min. |
| Reactor Pressure | 3 psig max. |
| 3.2. Packing | (To be provided by others) |
| Packing Material | ¼" diameter alumina pellets |
| Packing Height | 60 inches |
| Packing Weight | 130 lb |
| 3.3. Heater | |
| Type | Electrical |
| Total Heat Duty | 30 KW |
| Temperature | 2,800°F max. |

Heating Zones

(3) 16" long heating zones

3.4. Insulation

Hot Face Temperature

2,800°F max.

Cold Face Temperature

200°F

Hot Face Insulation

2" thick Zircar AL-30AAH or equivalent

Intermediate Insulation

2" thick Zircar ALC or equivalent

Cold Face Insulation

2" thick Zircar Alumina-Silica or equivalent

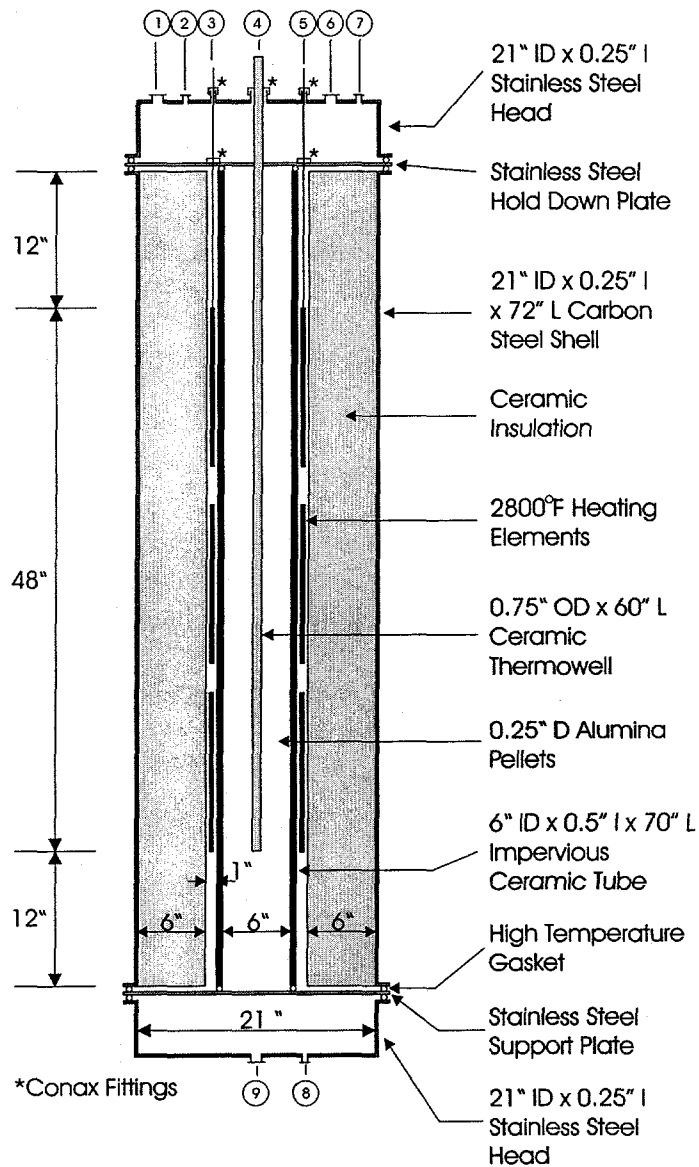


Figure 4.3.6-A Reactor (R-101)

4. Site Data

4.1. Location Institute of Gas Technology
1700 South Mount Prospect Road
Des Plaines, Illinois 60018
The unit will be installed indoors.

4.2. Power Available 110/230/460 volts, 60 Hz, 1-phase and 3-phase.

4.3. Area Specification To be provided by IGT

5. Details of Construction

5.1 The vendor is free to recommend other designs or materials of construction.

5.2 The vendor shall provide all instrumentation, control and mounting/supporting assembly required for the electric heater.

5.3 The reactor shall be designed to allow easy disassembling for inspection, cleaning and maintenance.

5.4 The vendor shall perform his own structural calculations to finalize the design, and to recommend the appropriate and cost effective material for construction. The final design shall be in compliance with all applicable codes.

5.5 The vendor shall submit final drawings showing all structural details as a part of the quotation.

6. Performance Guarantee

6.1 The vendor shall guarantee the equipment to meet the specification requirements for a period of 12 months from the date of initial operation or 18 months from the date of shipping.

6.2 Changes mandated by substandard performance shall be made promptly at the vendor's expense.

7. Quotation

7.1 The vendor shall provide a quotation including firm fixed price and delivery schedule good for 60 days.

7.2 The vendor shall identify and explain any exceptions or deviations made with respect to the specification requirements.

7.3 The vendor shall provide data as requested with the quotation.

Table 4.3.6-A. Details of Nozzle Connection for Reactor (R-101)

Nozzle No.	Size, in	Service
1	2	Pressure Relief
2	0.5	Differential Pressure Transmitter
3	0.5	Heater Wiring
4	0.75	Thermowell
5	0.5	Heater Wiring
6	2	Gas Outlet
7	0.5	Pressure Indicator
8	0.5	Differential Pressure Transmitter
8	2	Gas Inlet

SPECIFICATION FOR MIXING CHAMBER (T-101)

1. Introduction

1.1. The Institute of Gas Technology (IGT) is constructing a bench-scale unit for the production of H₂ from thermal decomposition of H₂S. This specification covers the requirements for furnishing a mixing chamber to be used for mixing feed gas streams. The vendor shall supply one mixing chamber in accordance with the following specification.

2. General Description

2.1. Pre-determined amounts of H₂S, O₂, and N₂ gases supplied from gas cylinders are thoroughly mixed in a gas chamber and then fed to packed-bed reactor.

3. Design Data

3.1. Service Conditions and Performance Requirements

Type	Gas mixing chamber
Feed Gas	2 mol/h H ₂ S, 0.4 mol/h O ₂ , 1.6 mol/h N ₂
Temperature	Ambient
Type of Service	Continuous

4. Site Data

4.1. Location	Institute of Gas Technology 1700 South Mount Prospect Road Des Plaines, Illinois 60018 The unit will be installed indoors.
4.2. Power Available	110/230/460 volts, 60 Hz, 1-phase and 3-phase.
4.3. Area Specification	To be provided by IGT

5. Performance Guarantee

- 5.1. The vendor shall guarantee the equipment to meet the specification requirements for a period of 12 months from the date of initial operation or 18 months from the date of shipping.
- 5.2. Changes mandated by substandard performance shall be made promptly at the vendor's expense.

6. Quotation

- 6.1. The vendor shall provide a quotation including firm fixed price and delivery schedule good for 60 days.
- 6.2. The vendor shall identify and explain any exceptions or deviations made with respect to the specification requirements.
- 6.3. The vendor shall provide data as requested with the quotation.

EQUIPMENT SPECIFICATION FOR GAS SCRUBBER (T-102)

1. Introduction

- 1.1. The Institute of Gas Technology (IGT) is constructing a bench-scale unit for the production of H_2 from thermal decomposition of H_2S . This specification covers the requirements for furnishing a gas scrubber to be used for the removal of H_2S and SO_2 from a gas stream using aqueous alkaline solution. The vendor shall supply one gas scrubber in accordance with the following specification and the attached drawings.

2. General Description

- 2.1 Feed gas enters the bottom of the scrubber where H_2S and SO_2 are removed by contact countercurrently with scrubbing solution. Clean gas leaving the top of the scrubber and is discharged to the atmosphere.
- 2.2 The absorber is a vertical, countercurrent spray column equipped with multiple spray nozzles.

3. Design Data

- 3.1. General
 - Gas-Liquid Contact Vertical, countercurrent multiple-spray column.
 - Material of Construction Carbon steel
 - Type of Service Continuous
- 3.2. Feed Gas

Composition	Process gas containing H ₂ S, SO ₂ , elemental sulfur, H ₂ , N ₂ , and H ₂ O _(g) .
Flow Rate	1,990 ft ³ /h
H ₂ S Concentration	44 mol %
Temperature	300°F
Pressure	1 psig
Density	0.06 lb/ft ³
Viscosity	0.02 cp

3.3. Scrubbing Liquid	
Composition	20 wt % caustic solution
Flow Rate	320 lb/h
Temperature	70°F
Density	76 lb/ft ³
Viscosity	1 cp

4. Site Data

4.1. Location	Institute of Gas Technology (IGT) 1700 South Mount Prospect Road Des Plaines, Illinois 60018 The unit will be installed indoors.
4.2. Power Available	110/230/460 volts, 60 Hz, 1-phase and 3-phase
4.3. Area Specification	To be provided by IGT

5. Details of Construction

- 5.1 A preliminary design of the scrubber is shown in the attached Figure 4.3.8-A and Table 4.3.8-A, which are considered to be part of this specification. The vendor is free to recommend other types of scrubbing equipment.
- 5.2 The equipment shall be designed to allow easy disassembling for inspection, cleaning and maintenance.
- 5.3 The vendor shall perform his own structural calculations to finalize the design, and to recommend the appropriate and cost effective material for construction. The final design shall be in compliance with all applicable codes.
- 5.4 The vendor shall submit final drawings showing all structural details as a part of the quotation.

6. Performance Guarantee

- 6.1 The vendor shall guarantee the equipment to meet the specification requirements for a period of 12 months from the date of initial operation or 18 months from the date of shipping.

6.2. Changes mandated by substandard performance shall be made promptly at the vendor's expense.

7. **Quotation**

- 7.1. The vendor shall provide a quotation including firm fixed price and delivery schedule good for 60 days.
- 7.2. The vendor shall identify and explain any exceptions or deviations made with respect to the specification requirements.
- 7.3. The vendor shall provide data as requested with the quotation.

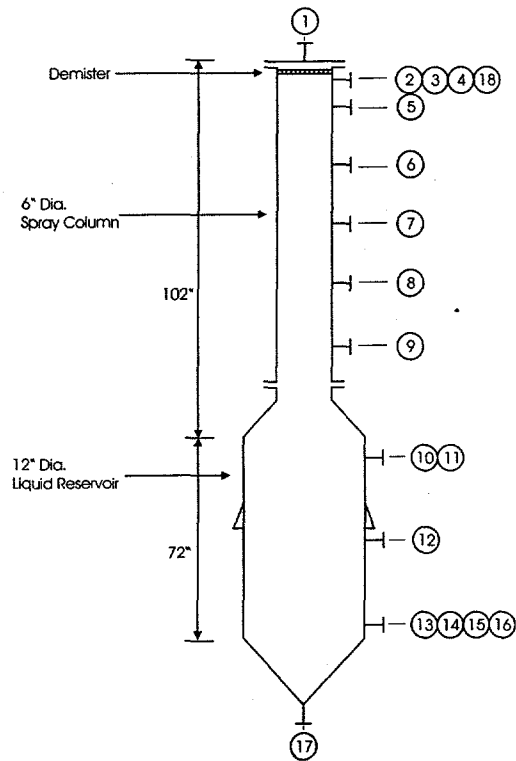


Figure 4.3.8-A Gas Scrubber (T-102)

Table 4.3.8-A. Nozzle Schedule for Gas Scrubber (T-102)

Nozzle No.	Size, in	Service
1	2	Gas Out
2	0.5	Pressure Differential Transmitter
3	0.5	Temperature Indicator
4	2	Pressure Relief
5	2	Liquid In
6	2	Liquid In
7	2	Liquid In
8	2	Liquid In
9	2	Gas In
10	0.5	Pressure Differential Transmitter
11	0.5	Liquid Level Switch
12	0.5	Temperature Indicator
13	2	Liquid Out
14	0.5	Liquid Level Switch
15	0.5	Liquid Level Switch
16	6	Hand Hole
17	2	Drain
18	0.5	Pressure Indicator

EQUIPMENT SPECIFICATION FOR CAUSTIC TANK (T-103)

1. Introduction

1.1. The Institute of Gas Technology (IGT) is constructing a bench-scale unit for the production of H₂ from thermal decomposition of H₂S. This specification covers the requirements for furnishing a caustic tank to be used for the storage of caustic solution. The vendor shall supply one caustic tank in accordance with the following specification and the attached drawings.

2. Design Data

- 2.1. Material Handled
- | | |
|-------------|---------------------------------|
| Liquid | 20 wt% aqueous caustic solution |
| Pressure | Atmospheric |
| Temperature | 130°F |
| Viscosity | 1 cp |
| Density | 76 lb/ft ³ |
- 2.2. Tank
- | | |
|--------------------------|----------------------|
| Type | Vertical cylindrical |
| Capacity | 800 gal |
| Material of Construction | Carbon steel |

Service

Continuous

3. Site Data

- 3.1. Location Institute of Gas Technology (IGT)
1700 South Mount Prospect Road
Des Plaines, Illinois 60018
The unit will be installed indoors.
- 3.2. Power Available 110/230/460 volts, 60 Hz, 1-phase and 3-phase.
- 3.3. Area Specification **

4. Details of Construction

- 4.1 A preliminary design of the scrubber is shown in the attached Figure 4.3.9-A and Table 4.3.9-A, which are considered to be part of this specification.
- 4.2. The equipment shall be designed to allow for easy disassembling for inspection, cleaning, and maintenance.
- 4.3. The vendor shall perform his own structural calculations to finalize the design and to recommend the appropriate and cost effective material for construction. The final design shall be in compliance with all applicable codes.
- 4.4. The vendor shall submit final drawings showing all structural details as part of the quotation.

5. Performance Guarantee

- 5.1. The vendor shall guarantee the equipment to meet the specification requirements for a period of 12 months from the date of initial operation or 18 months from the date of shipping.
- 5.2. Changes mandated by substandard performance shall be made promptly at the vendor's expense.

6. Quotation

- 6.1. The vendor shall provide a quotation including firm fixed price and delivery schedule good for 60 days.
- 6.2. The vendor shall identify and explain any exceptions or deviations made with respect to the specification requirements.
- 6.3. The vendor shall provide data as requested with the quotation.

** IGT to provide.

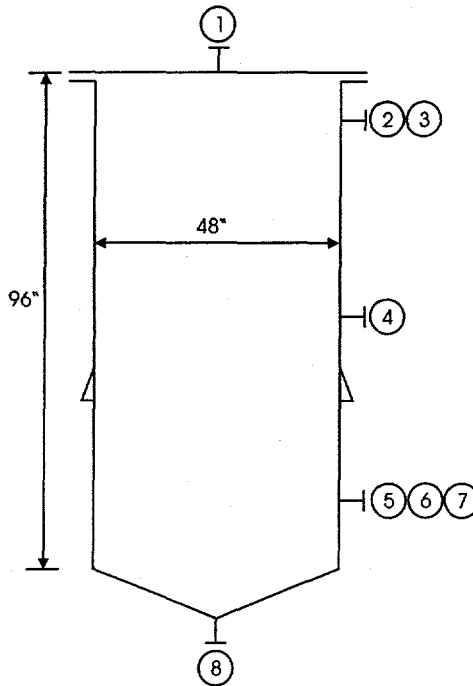


Figure 4.3.9-A Caustic Tank (T-103)

Table 4.3.9-A. Nozzle Schedule for Caustic Tank (T-103)

Nozzle No.	Size, inch	Service
1	2	Liquid In
2	0.5	Liquid Level Switch
3	0.5	Liquid Level Indicator
4	0.5	Temperature Indicator
5	0.5	Liquid Level Switch
6	0.5	Liquid Level Indicator
7	2	Liquid Out
8	2	Drain

4.4. Cost Estimate

The cost estimates for the proposed bench-scale testing system are presented in this section. The total purchased equipment cost (Table 4.4.1) is \$94,300. The estimated total installed cost (Table 4.4.2) is \$292,000. The total installed cost is estimated using a conventional factored cost estimate method. Vender quotations are attached at the end of this appendix.

Table 4.4.1. Purchased Equipment Cost for a Bench-Scale Testing System

Equipment No.	Equipment Description	Purchased Cost, \$	Source
E-101	Sulfur Condenser	10,000	1, 2
E-102	Thermal Fluid Cooler	4,000	2
P-101	Recirc. Caustic Pump	4,000	1
P-102	Makeup Caustic Pump	1,500	1
P-103	Thermal Fluid Pump	4,000	2
R-101	Reactor	60,000	1, 2
T-101	Mixing Chamber	500	2
T-102	Gas Scrubber	5,300	1
T-103	Caustic Tank	5,000	1
Total		94,300	

1. Vendor quotation
2. Engineering estimate

Table 4.4.2. Total Installed Cost for a Bench-Scale Testing System

	2000 Dollars
Direct Costs	
Purchased Equipment	94,300
Equipment Installation	18,900
Installed Instrumentation & Control	40,000
Installed Electrical	10,000
Installed Piping	10,000
Installed Structural Steel	10,000
Total Direct Costs	183,200
Indirect Costs	
Design, Engineering & Supervision	40,000
Construction Costs	20,000
Total Indirect Costs	60,000
Direct & Indirect Costs	243,200
Contingency	48,800
TOTAL INSTALLED COSTS	292,000

VENDOR QUOTATIONS



ZIRCAR PRODUCTS, INC.

SALES OFFICE

P.O. BOX 458

FLORIDA, NEW YORK 10921-0458

TEL: (914)-651-6600 FAX: (914)-651-0441

Email: dch@zircar.com

From: David C. Hoskins – Sales Engineer Ext.226

TO: Bob Sheng	DATE: 7/28/00
FAX NO.: 630-969-6929	COUNTRY: USA
COMPANY: IGT	
NO. OF PAGES INCLUDING THIS ONE: 1	

Dear Bob:

I still do not have all my numbers together, but I will share what I do have so far:

Material costs: Heating elements, straps, clamps \$4500
9" ID x 21" OD x 72" insulating system with AL 30AA hot face \$22,000

A AL-30AAH hot face will be more. I will have to take an AL-300AA system oversize it so we can high fire and sinter it down then machine out the ID and OD. Could add another 3 or 4 thousand for the H designation.

Still need steel and process tube costs and assembly costs. Who will do the engineered drawings? That is a cost that will need to be incurred.

At this point I might guess \$50,000 excluding the beads and six foot process tube.

Best regards,

David Hoskins
Sales Engineer



VESUVIUS MCDANEL

510 Ninth Avenue
Beaver Falls, PA 15010-4700
Telephone: 724-843-8300 Fax: 724-843-5644

Proposal

Contact: T. Robert Sheng	From: Marti Monaco
Company: Institute of Gas Technology	Phone: EXT 238
Address: 436A West 75th Street Downers Grove, IL 60516 USA	E-mail: marti_monaco@vesuvius.com
Phone: 630-969-7878	
FAX: 630-969-6929	Date: 07/07/2000

Proposal #: O2000-1543

Please refer to proposal # when placing order.

Line #	Item Description	Item Number	Item Qty	Unit Price	Extended Price	Availability
1.	99.8% Alumina-6.5" OD X 6" ID X 60" LG	98A315030060000	1	\$2,567.27	\$2,567.27	Negotiable
2.	99.8% Alumina-5" OD X 4.625" ID X 4" LG	98A313931004000	1	\$283.20	\$283.20	Negotiable
3.	99.8% Alumina-5.375" DIAM X .5" THICK	To be determined	1	\$525.00	\$525.00	Negotiable
4.	99.8% Alumina-1" OD X .75" ID X 60" LG	98A310931060000	1	\$331.58	\$331.58	Negotiable

Terms: Net 30
FOB: Beaver Falls

HUDSON BOILER & TANK COMPANY

STEEL FABRICATORS AND ERECTORS

1725 WEST HUBBARD STREET • CHICAGO, ILLINOIS 60622

PHONE: 312 - 666 - 4780 • FAX: 312 - 666 - 5145

WEBSITE: [http:// www.hudsonboiler.com](http://www.hudsonboiler.com)

To:	Bob Sheng	From:	Lou Wodka
Company:	Institute of Gas Technology	Company:	Hudson Boiler & Tank C
Fax:	(708)768-0501	Fax:	(312) 666-5145
Date:	July 12, 2000	Pages:	1
Memo:		Quote Number:	3606

We propose to fabricate (1) gas scrubber (T-101) per Figure 1 and Table 1 consisting of 12" diameter shell reducing to 6" diameter shell with cones, fittings, flanges, demister and supporting lugs. All fittings below 2" diameter are to be couplings, 2" and over are flanged nozzles except where noted. Price is \$5,300.00 FOB Hudson.

Fabrication of (1) Caustic Tank (T-102) per Figure 1 and Table 1 consisting of 48" O.D. shell X 8'-0 long on straight shell with 3/4" top blind flange bolted to 3/4" flange, cone bottom, fittings, flanges, and support lugs. All fittings below 2" diameter are to be couplings, 2" and over to be flanged nozzles except where noted. Price is \$4,980.00 FOB Hudson.

Thank you for the opportunity of bidding on your requirements.

Very truly yours,



Lou Wodka

HUDSON BOILER & TANK COMPANY

STEEL FABRICATORS AND ERECTORS

1725 WEST HUBBARD STREET • CHICAGO, ILLINOIS 60622

PHONE: 312 - 666 - 4780 • FAX: 312 - 666 - 5145

WEBSITE: [http:// www.hudsonboiler.com](http://www.hudsonboiler.com)

To: Bob Sheng

From: Lou Wodka

Company: Institute of Gas Technology

Company: Hudson Boiler & Tank Co.

Fax: (708)768-0501

Fax: (312) 666-5145

Date: June 26, 2000

Pages: 1

Memo:

Quote Number: 3578

We propose to fabricate (1) Sulfur Condenser per your Figure 1 and Table 1 consisting of 6" diameter shell and (7) 1" diameter tubes. Shell to be 6'-0 high with flanged cap on top, support lugs, tube sheets in interior, and flanged cone bottom. Price is \$3,936.00 FOB Hudson.

Fabrication of Scrubber per your Figure 1 and Table 1 consisting of 30" diameter flanged shell with blind flange on top with fittings, support lugs, and flanged cone bottom with fittings. Price is \$7,957.00 FOB Hudson.

Thank you for the opportunity of bidding on your requirements.

Very truly yours,



Lou Wodka

Item 1

Brooks Instrument Model 5853i,

Model Code: 5853iABD1D1D4BA VALID
 Maximum Pressure: 1,500 psig @ 150 F
 Body Material: 316L
 Full Scale Flow: >200 TO 450 <= 90 (N2 Eq.)
 Valve Type/Seat: N.C. 30 TO 290 PSID/KALREZ <=200 PSIG
 O-Ring Material: PTFE
 PC Bd/IO/Soft Start: -20mA IN 4-20mA & 5v OUT/DISAB
 Cable Length: TBD
 Process Connection: 1/2 COMPR. TUBE 1 1/16-12
 Full Scale Flow: 13 scfm(368.16 slpm)
 Process Gas: Hydrogen Sulfide
 Inlet Pressure: 55 psig(69.7 psia)
 Outlet Pressure: 5 psig(19.7 psia)
 Cal. Ref. Temp. 21.1 Deg. C.
 Soft Start: Enable Disable
 5 Volt Ref.: Enabled
 Attitude: 1 HORIZONTAL (H)
 Customer P/N: _____

(Kalrez recommended)

Part Number	Description	Qty	Unit Price	Ext. Price
5853iABD1D1D4BA	<u>MFC</u>	<u>1</u>	<u>\$2988.36</u>	

2000-0711-BA01
Quote#:

Delivery: 6 weeks ARD

Total Price: _____

Engineering Information:

Orifice Size: 0.048 in.
Restrictor Size: M

Soft Errors: (None)

Special Instructions:

Optional Cable

Description: D-Connector for use with Brooks Secondary Electronics

Part Number: S124Z__AAA

- 576 = 5' Cable, Unit Price \$74.52
- 577 = 10' Cable, Unit Price \$81.00
- 578 = 25' Cable, Unit Price \$88.56
- 579 = 50' Cable, Unit Price \$99.36

* preliminary operating conditions used for quotation purposes on items 1-3

page D-23
Brooks catalog

Quote To:

Date: 07-11-2000 Time: 12:52:48 Rev: 8.6

*Item 2

Brooks Instrument Model 5851i, Industrial Mass Flow Controller

Model Code: 5851iA1BR2G2DEA VALID
 Maximum Pressure: 1,500 psig @ 150 F
 Body Material: VAR 316L
 Valve Type/Seat: N.C./VITON
 O-Ring Material: Viton
 Elect. Conn./In Out: D-Conn/4-20mA 4-20mA
 Cable Length: TBD
 Process Connection: 1/2" Compression
 Full Scale Flow: 3 scfm(84960 sccm)
 Process Gas: Oxygen
 Inlet Pressure: 55 psig(69.7 psia)
 Outlet Pressure: 5 psig(19.7 psia)
 Cal. Ref. Temp. 21.1 Deg. C.
 Soft Start: Disable
 5 Volt Ref.: Enabled
 Attitude: 1 HORIZONTAL (H)
 Customer P/N: _____

Part Number	Description	Qty	Unit Price	Ext. Price
5851iA1BR2G2DEA	MFC	1	\$1983.96	

Quote#: 2000-0711-BA01 Delivery: 4 weeks ARO Total Price: _____

Engineering Information:

Orifice Size: 0.076 in. Flow Type: SUPER-CRITICAL
 Restrictor Type: SINTERED ELEMENT
 Restrictor Size: G 1-40u & 2-60u(G per sizing)
 Calibration: >50-100 SLPM, UP TO 90 PSIG
 Assembly: STANDARD ASSEMBLY
 O.E.M. Account: BROOKS HATFIELD

Soft Errors: (None)

Special Instructions:

Optional Cable

Description: D-Connector for use with Brooks Secondary Electronics

Part Number: S124Z__ _AAA

- 576 = 5' Cable, Unit Price \$74.52
- 577 = 10' Cable, Unit Price \$81.00
- 578 = 25' Cable, Unit Price \$88.56
- 579 = 50' Cable, Unit Price \$99.36

Quote To:

Date: 07-11-2000 Time: 12:53:44 Rev: 8.6

* Item 3

Brooks Instrument Model 5853i,

Model Code: 5853iABA1D1D4BA VALID
 Maximum Pressure: 1,500 psig @ 150 F
 Body Material: 316L
 Full Scale Flow: >200 TO 450 <= 90 (N2 Eq.)
 Valve Type/Seat: N.C. 30 TO 290 PSID/VITON
 O-Ring Material: VITON
 PC Bd/IO/Soft Start: -20mA IN 4-20mA & 5v OUT/DISAB
 Cable Length: TBD
 Process Connection: 1/2 COMPR. TUBE 1 1/16-12
 Full Scale Flow: 10 scfm(283.2 slpm)
 Process Gas: Nitrogen
 Inlet Pressure: 55 psig(69.7 psia)
 Outlet Pressure: 5 psig(19.7 psia)
 Cal. Ref. Temp. 21.1 Deg. C.
 Soft Start: Enable Disable
 5 Volt Ref.: Enabled
 Attitude: 1 HORIZONTAL (H)
 Customer P/N: _____

Part Number	Description	Qty	Unit Price	Ext. Price
5853iABA1D1D4BA	<u>MFC</u>	<u>1</u>	<u>\$ 2739.96</u>	

Unit

Quote#: 2000-0711-BA01 Delivery: 6 weeks ARO Total Price: _____

Engineering Information:

Orifice Size: 0.048 in.
 Restrictor Size: M

Soft Errors: (None)

Special Instructions:

Optional Cable

Description: D-Connector for use with Brooks Secondary Electronics

Part Number: S124Z__AAA

- 576 = 5' Cable, Unit Price \$74.52
- 577 = 10' Cable, Unit Price \$81.00
- 578 = 25' Cable, Unit Price \$88.56
- 579 = 50' Cable, Unit Price \$99.36

page D-23

Quote #: 2000-0711-BA01
Company: IGT

Brooks Instrument Secondary Electronics

<u>Item 4</u>		<u>Unit Price</u>
Model Number:	0154BEE2BC1A	\$2354.40
Description:	<ul style="list-style-type: none">• 4 Channel Power Supply/Controller• Panel Mount Model• 110V - 50/60 Hz Power Supply• 24 VDC Output Power to MFC• 4-20 mA Input/Output Signal to MFC	

Shipment: 3-4 weeks ARO
FOB: Hatfield, PA
Terms: Net 30 or Credit Card
Brooks Instrument C/O Control Plus Inc.
257 N. West Avenue, Elmhurst, IL 60126

Great Lakes Analytical, Inc.


4805 Sheffield Ave., Suite A
Hammond, IN. 46327

Phone: (219) 933-1076
Fax: (219) 933-1096

TO: Institute of Gas Technology 436 A 75th Street Downers Grove, IL 60516 Attn: Bob Sheng	QUOTATION #: <u>071800B</u>
	DATE: <u>July 18, 2000</u> TERMS: <u>Net 30</u>
	PROPOSED SHIPPING DATE: <u>3 to 4 weeks</u>
	INQUIRY NO: <u>(630)969-7878</u>

ITEM	QTY.	DESCRIPTION	UNIT PRICE	TOTAL
Draeger Instruments				
1	1	P/N 4543000 Polytron 2 XP Ex, Combustible Gas 0-100% LEL (sold with sensor PR and relays, Poison Resistant, NEMA 7 Enclosure, Explosion Proof Design, UL approved, Class 1, Div 1, Group B, C, D).....	\$950.00	\$950.00
2	2	P/N 4543200 Polytron 2 XP Tox w/ relays, (order sensor separately, NEMA 7 Enclosure, Explosion Proof Design, UL approved, Class 1, Div 1, Group B, C, D CENELEC approved, EEx d [ia] T6).....	\$1,120.00	\$2,240.00
3	1	P/N 6809610 Draeger Sensor Hydrogen Sulfide (H2S).....	\$385.00	\$385.00
4	1	P/N 6809660 Draeger Sensor Sulfur Dioxide (SO2).....	\$385.00	\$385.00
5	1	P/N 4509314 Calibration Adapter.....	\$38.00	\$38.00
TOTAL.....				\$3,998.00
<p>Please Address Order To: Draeger Safety, Inc. C/o Great Lakes Analytical, Inc. 101 Technology Dr. Pittsburgh, PA. 15275</p>				

The prices and terms on this quotation are not subject to verbal changes or other agreement unless approved in writing by the Home Office of the Seller. All quotations and agreements are contingent upon strikers, accidents, fires, availability of materials and all other causes beyond our control. Prices are based on costs and conditions existing on date of quotation and are subject to change by the Seller before final acceptance. Typographical and stenographic errors subject to correction. Purchaser agrees to accept either overage or shortage not in excess of ten percent to be charged for pro-rata. Purchaser assumes liability for patent and copyright infringement when goods are made to Purchaser's specifications. When quotation specifies materials to be furnished by the purchaser, ample allowance must be made for reasonable spoilage and material must be of suitable quality to facilitate efficient production. Conditions not specifically stated herein shall be governed by established trade customs. Terms inconsistent with stated herein which may appear on Purchaser's formal order will not be binding on the Seller.

Great Lakes Analytical, Inc. 4805 Sheffield Ave., Suite A Hammond, IN. 46327 Phone: (219) 933-1076 Fax (219) 933-1096	 _____ Technical Sales Representative	July 18, 2000 _____ Date
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QUOTATION

a world of liquid handling solutions

QUOTATION

Phone: 312/666-2210

1312 West Lake Street, Chicago, IL 60607

Fax: 312/666-3384

To: Institute of Gas Technology

436A W. 75th St.
Downers Grove, IL 60516

Attention: Bob Sheng
Phone: 630/969-7878
Fax: 630/969-6929

Quote # N-8926

Reference: Budget Quote on Spray
Column

Date: 7/11/00

Page: 1 of 1

ITEM	QTY	DESCRIPTION	PRICE	EXTENDED
1	1	Eco Gear Pump Model GA4-ACT-KKU 316 Stainless Steel W/Carbon Bearings, Wearplates & Teflon Single Mechanical Seal. Driven By A 5 HP/1750/3/60/230-460v/Inverter Duty Motor. Pump & Motor Mounted On A Steel Base W/Coupling, Guard & Risers Complete.	\$ 2,699.00	\$ 2,699.00
2	1	Baldor Series 15H General Purpose Inverter, 5 HP/230v (For Above Pump Speed Control)	\$ 1,315.00	\$ 1,315.00
3	1	Eco Gear Pump 316 GA2-ACT-KKU Stainless Steel W/Carbon Bearings, Wearplates & Teflon Single Mechanical Seal. Driven By A 1/2 HP/1750/3/60/230-460v/TEFC Constant Speed Motor. Pump & Motor Mounted On A Steel Base W/Coupling, Guard & Risers Complete.	\$ 1,487.00	\$ 1,487.00
4	1	Schlumberger/Neptune Coriolis Mass Flow Meter 316 Stainless Steel W/ 1/2" ANSI Flanges & NexGen SFT100 Mass Flow Transmitter W/LCD Display & Function Keys and 4-20mA Output.	\$ 6,575.00	\$ 6,475.00
TOTAL				\$ 12,076.00

Terms and Conditions:

- This quote is valid for 30 days.
- D. J. INC. Standard Terms and conditions, a copy of which is available on request, apply to all goods quoted herein.
- F.O.B.: Don Johns, Inc. - Chicago
- Terms: Net 30 Days
- Delivery: 4 Weeks ARO

Best Regards,
Brian Byrne
Brian Byrne

Prices and specifications subject to change without notice.

www.donjohns.com

APPENDIX C

UIC PROPOSAL FOR PHASE 2

A Proposal Submitted to IGT

Institute of Gas Technology
1700 South Mount Prospect Road
Des Plaines, IL 60018

MODELING OF HYDROGEN AND SULFUR PRODUCTION BY SUPERADIABATIC COMBUSTION OF HYDROGEN SULFIDE

Phase 2 of the IGT Program

Prepared by: Prof. Alexander A. Fridman
Dr. Alexander F. Gutsol
Prof. Lawrence A. Kennedy
Dr. Alexei V. Saveliev

Date Submitted:	October 17, 2000
Amount Requested:	\$ 109,500
Period of Research:	May 1, 2001 - June 30, 2002

MODELING OF HYDROGEN AND SULFUR PRODUCTION BY SUPERADIABATIC COMBUSTION OF HYDROGEN SULFIDE

1. Background and Principal UIC Modeling Results of Phase 1

Research interest in filtration combustion (FC) has been driven by numerous applications such as utilization of low calorific fuels [1], low emission burners [2] and pollution control devices. Recent novel applications include fuel reforming and processing in the ultra-rich superadiabatic combustion waves [3].

In Phase 1 of this program filtration combustion waves in H₂S/air mixtures were modeled within the one-dimensional approach taking into account multi-step chemistry and separate energy equations for the gas and solid phases [4]. The superadiabatic wave propagation is a complex phenomenon, and many factors that influence wave properties, in particular the heat loss rate, interfacial heat exchange or effective heat conductivity of the porous medium, must be accurately specified. We developed a numerical model to describe combustion wave characteristics in a coordinate system moving together with the wave front. Two chemical kinetic mechanisms were used. The first one (developed by Frenklach's group) is more appropriate under combustion conditions (moderately high equivalence ratios), the second kinetic mechanism has been developed at UIC to describe more accurately the partial oxidation of H₂S (ultra-high equivalence ratio). The products of partial H₂S oxidation, H₂ and S₂ are dominants for ultra-rich superadiabatic combustion, which is a fuel reforming actually. The chemistry in the combustion wave was modeled, and species and temperatures profiles were predicted. A database of hydrogen and sulfide conversion in a wide range of equivalence ratios and other process parameters was produced.

Filtration combustion in porous media differs substantially from combustion in a homogeneous media. The difference is the heat transfer between filtrated gas and the porous medium under conditions of active interfacial heat transfer. FC also differs from flames stabilized within a porous body in that FC is an inherently transient process. These differences lead to positive or negative enthalpy fluxes between the reacting gas and the solid carcass, resulting in combustion temperatures in excess or below the adiabatic one for the supply mixture. Combustion waves in the porous body, including excess enthalpy (superadiabatic) flames, have been the focus of many recent experimental and theoretical studies [5-10]. However, almost all of these studies were limited to the case of very lean mixtures. To fully exploit FC potential applications, numerical models need to be extended to the practically important limit of rich and ultra-rich filtration combustion of gases, addressing the issues of multi-step kinetics [11], heterogeneous reactions [12], pore level mechanisms of combustion [13], and adequate heat and mass transport phenomena in porous media.

Ultra-lean filtration combustion results in complete burnout of the hydrocarbon fuel with the formation of carbon dioxide and water. Thus, both the composition of the final products and the heat release are well defined. In contrast with the ultra-lean case, the combustion products of rich waves are not clearly defined. In this case, fuel is only partially oxidized in the filtration wave and the total heat release could be kinetically controlled by the degree of the partial combustion. As a result, the chemical kinetics, heat release and heat transfer are strongly coupled in the ultra rich wave making it more complicated and challenging phenomenon than the ultra-lean wave. Previous analyses [5-10] of the FC waves were based upon a model in which the gas phase chemical reactions were approximated by a single-step kinetic mechanism for combustion.

In Phase 1 of this program the numerical model was developed for description of superadiabatic combustion (SAC) of ultra-rich H₂S/air mixtures [4]. Modeling studies of H₂S decomposition through SAC were conducted based upon computational models of filtration combustion waves in a porous medium developed earlier for ultra-rich filtration combustion of methane/air mixtures. These include numerical programs for unsteady simulation of ultra-rich combustion waves with multi-step chemical mechanisms. Superadiabatic combustion of ultra-rich H₂S/air mixtures is represented within a one-dimensional, non-steady model, including separate energy equations for the gas and porous medium. The boundary conditions for the gas are imposed at the inlet and the exit of the reactor. Standard reaction flux/pathway and gradient sensitivity analysis techniques are applied at each step to identify important reaction pathways. The model allows the prediction of process performance (i.e., overall H₂S conversion, H₂/H₂O selectivity, S₂/SO₂ selectivity, etc) over a range of operating conditions, including equivalence ratios, flow rates, and other packed-bed reactor parameters.

Certain products, oxygen, sulfur dioxide, and sulfur, correlate fairly well with thermodynamic predictions. Others, notably hydrogen, diverges over the whole range of rich mixtures. Hydrogen in the products is present after stoichiometry and maximizes at $\phi=2$ to achieve a maximum conversion rate of 20% based on the hydrogen sulfide input. Its production fell rather gently thereafter to where nothing is gained by equivalence ratio of 5.5. The concentration of unreacted hydrogen sulfide rises linearly with equivalence ratio at post-stoichiometry. Some sulfur based products peaked at the extremities: sulfur dioxide at stoichiometry (100% conversion), and elemental sulfur (50% conversion) at $\phi=4$. Finally, the formation of sulfuric acid in ultra-lean combustion was qualitatively verified. Detailed modeling results were presented in a final report submitted to IGT (see Appendix A).

2. Objectives of Numerical Modeling in Phase 2

The main objective of UIC activities in Phase 2 is to provide guidelines for the operation of the bench-scale reactor unit according to a test plan and also to analyze the experimental results and provide recommendations for the next phase of the program. In Phase 2 the previously developed numerical model of rich and ultra-rich filtration combustion (FC) of H₂S-containing fuel/oxidant gas mixtures will be modified as necessary. Work will include the following:

- *Further Development of the Simulation Model and Programming Complex for Detailed Kinetic and Heat Transfer Modeling.*
- *Detailed Reactor Modeling Application for the Bench-Scale Unit Operation.*
- *Application of the Improved Detailed Process Modeling for Interpretation and Analysis of the Experimental Results.*
- *Application of the Improved Detailed Process Modeling in Comparison with the Experimental Results Obtained during Bench-Scale Testing for Technical Feasibility Verification.*

3. Computational Approach

Theoretical studies will be conducted based upon computational models of filtration combustion of waves in a porous medium developed for ultra-rich filtration combustion of hydrogen sulfide developed in Phase 1 of the project [4]. These include numerical programs for unsteady simulation of ultra-rich combustion waves with multi-step chemical mechanisms [14].

3.1 Computational Model

Superadiabatic combustion of ultra-rich H₂S/air mixture will be represented within a one-dimensional, non-steady model. The combustion wave propagation in an inert, packed bed is described by the system of conservation equations for gas energy, solid medium energy, mass fractions of gas species, and mass flow rates. Further details are provided in references 6 and 15.

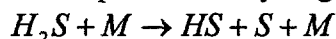
The major factors controlling the combustion wave behavior under filtration in an inert porous medium are: (i) the heat deposition in the gas phase due to fuel oxidation, (ii) the forced convection of fuel/air mixture, (iii) the longitudinal effective heat conductivity of the porous medium, (iv) the intense interfacial heat exchange between gas and solid phase, and (v) the heat exchange between the porous medium and surroundings. The factors (i)-(iv) are accurately represented within the one-dimensional approach due to the high degree of radial uniformity of the combustion wave front found in the measurements for the reactors under consideration. The factor (v) can be taken into account only parametrically, via the heat exchange in solid state energy equation, within a one-dimensional approach due to its explicit multi-dimensional nature.

The one-dimensional laminar flame code PREMIX is used following modification for the above-described problem. The adaptive placement of the grid points is done to resolve accurately the gradient and the curvature of the gas temperature and species profiles. We have found that 70-100 grid points provide sufficiently accurate solutions. The numerical algorithm implemented in the PREMIX code has been used to find the combustion wave velocity u .

The Chemkin subroutines are used to implement the chemical kinetics description [16] and the Transport subroutine [17] to calculate gas properties.

3.2 Kinetic Mechanisms of Ultra-Rich Hydrogen Sulfide Combustion

Two chemical kinetic mechanisms have been used in Phase 1 [4]. The first one (developed by the Frenklach's group), which includes 17 species and 58 reactions, is more appropriate under combustion conditions (moderately high equivalence ratios). The second kinetic mechanism has been developed at UIC to describe more accurately the partial oxidation of H₂S (ultra-high equivalence ratio). In the second kinetic mechanism the thermal decomposition of hydrogen sulfide



is described with a rate constant.

In Phase 2 we propose to modify kinetic mechanisms by taking into account the heterogeneous chemical reactions on the surface of pellets.

4. Work plan

4.1. Further Development of the Simulation Model and Programming Complex for Detailed Kinetic and Heat Transfer Modeling.

Previously developed numerical model of rich and ultra-rich filtration combustion (FC) of H₂S-containing fuel/oxidant gas mixtures will be modified. The most important improvement of the code is related to taking into account the heterogeneous chemical reactions on the surface of pellets. This will provide an additional control on the process temperature to increase conversion of hydrogen sulfide.

To simulate different inlet fuel gas compositions (H₂S-rich, H₂S-lean, simulated gas composition from a typical refinery, etc.), new reactions will be included to describe the kinetic mechanism.

Period of Performance: 5 months (May 2001 – September 2001).

4.2. Detailed Reactor Modeling Application for the Bench-Scale Unit Operation

The simulation model and programming complex developed in Phase 1 of the project (as well as improved versions of the code during the initial stages of Phase 2), will be applied for the selection of most suitable parameters, within the ranges specified in IGT's Test Plan, for the operation of the bench-scale unit and for the definition of the structure and properties of filtration combustion waves including reaction and chemical product information in this bench-scale unit. The model should predict process performance (i.e., overall H₂S conversion, H₂/H₂O selectivity, S₂/SO₂ selectivity, etc) over a range of operating conditions, including equivalence ratios, flow rates, and other packed-bed reactor parameters.

Period of Performance: 5 months (May 2001 – September 2001).

4.3. Application of the Improved Detailed Process Modeling for Interpretation and Analysis of the Experimental Results Obtained during Bench-Scale Testing.

The simulation model and programming complex developed in Phase 2 will be applied for interpretation of experimental results obtained during the bench-scale unit operation as well as for optimization of hydrogen sulfide conversion and other process characteristics.

Period: 9 months (October 2001 – June 2002).

4.4. Application of the Improved Detailed Process Modeling in Comparison with the Experimental Results Obtained during Bench-Scale Testing for Technical Feasibility Verification.

Experimental results will be compared with model simulations, further enhancing the reliability of the numerical model to provide further insight into technical feasibility of the process and guidelines for scale-up options in the next phase of the program.

Period of Performance: 7 months (December 2001 – June 2002).

Research Team

- Professor Alexander Fridman, Principal Investigator
- Professor Lawrence Kennedy
- Dr. Alexander Gutsol
- Dr. Alexei Saveliev
- Graduate student Mr. Alexander Shirokov.

The research group from the University of Illinois at Chicago has extensive experience in physical and numerical modeling of non-reacting and reacting flows, combustion and pollutant

chemistry, superadiabatic combustion, soot formation and plasma decomposition of H₂S. This group carried out the modeling work in Phase 1 of the project. The project implementation will involve joint efforts of two UIC laboratories: *Energy Systems Laboratory*, directed by Prof. Lawrence A. Kennedy and *High Temperature Laboratory*, directed by Prof. Alexander A. Fridman. Professor Kennedy's technical interests include the broad areas of combustion, non-equilibrium processes, fluid and thermal sciences. Combustion phenomena of Dr. Kennedy's recent research interests are superadiabatic filtration flames at porous inert media with emphasis on ultra-rich self-sustained flames for fuel processing and reforming. Developed experimental and numerical capabilities in filtration combustion are focused on wave chemical properties and heat-transfer characteristics. With more than 10 years of experience in superadiabatic combustion of gases the research group of Prof. Kennedy brings solid background for the research project. Prof. Fridman theoretical research has involved both fundamental and applied aspects of high-temperature and high-energy chemistry, plasma and laser chemistry, plus their applications to energy systems, nuclear safety, hydrogen production, and environmental-control technologies. Working at Kurchatov Institute of Atomic Energy (1979-1995), Alexander directed the development of the theoretical basis for microwave plasmolysis of hydrogen sulfide. Prof. Fridman and his co-workers have developed a kinetic mechanism of H₂S decomposition, which will be applied in the proposed project.

Facilities

The following equipment of the UIC will be available for the proposed research:

- Modern computational facilities; Two Silicon Graphics workstations and a Hewlett Packard workstation, Pentium PC's are in the laboratories. Centralized mainframe and access to the Illinois supercomputing facilities at UIUC center are available as required.

ESTIMATED BUDGET

Faculty – 1 summer month –	\$12,500
Research scientists – together 6 mo. –	\$30,000
Graduate student – 1 year	\$16,000
Materials and supplies	\$1,000
Total direct cost	\$59,500
Approximate indirect cost	\$50,000
Total	\$109,500

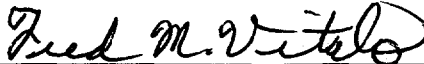
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APPENDIX D

COST PROPOSAL FOR PHASE 2

APPLICATION FOR FEDERAL ASSISTANCE

1. TYPE OF SUBMISSION <i>Application</i> <input type="checkbox"/> Construction <input checked="" type="checkbox"/> Non-Construction		2. DATE SUBMITTED 10/19/2000	Applicant Identifier 18601-06																																																																																
		State Applicant Identifier	Federal Identifier																																																																																
5. APPLICANT INFORMATION																																																																																			
Legal Name: Institute of Gas Technology		Organizational Unit:																																																																																	
Address (give city, county, state, and zip code): 1700 South Mount Prospect Road Des Plaines, IL 60018-1804		Name and telephone number of person to be contacted on matters involving this application (give area code) Technical: Francis Lau (847) 768-0592 Budgetary: Mary Ann Edgell (847) 768-0759 Contractual: Mary Ann Edgell (847) 768-0759																																																																																	
6. EMPLOYER IDENTIFICATION NUMBER (EIN): 3 6 - 2 1 7 0 1 3 7		7. TYPE OF APPLICANT: (enter appropriate letter in box) N																																																																																	
8. TYPE OF APPLICATION: <input type="checkbox"/> New <input checked="" type="checkbox"/> Continuation <input type="checkbox"/> Revision If Revision, enter appropriate letter(s) in box(es): <input type="checkbox"/> <input type="checkbox"/> A. Increase Award B. Decrease Award C. Increase Duration D. Decrease Duration Other (specify):		A. State H. Independent School Dist. B. County I. State Controlled Institution of Higher Learning C. Municipal J. Private University D. Township K. Indian Tribe E. Interstate L. Individual F. Intermunicipal M. Profit Organization G. Special District N. Other (Specify) <u>Not-for-Profit</u>																																																																																	
10. CATALOG OF FEDERAL DOMESTIC ASSISTANCE NUMBER: 8 1 . 0 8 7 TITLE:		9. NAME OF FEDERAL AGENCY: U. S. Department of Energy Golden Field Office																																																																																	
12. AREAS AFFECTED BY PROJECT (cities, counties, states, etc.): Des Plaines, Cook County, Illinois		11. DESCRIPTIVE TITLE OF APPLICANT'S PROJECT: Production of Hydrogen by Superadiabatic Decomposition of Hydrogen Sulfide - Phase 2																																																																																	
13. PROPOSED PROJECT: Start Date 01/01/2001 12/31/2002		14. CONGRESSIONAL DISTRICTS OF: a. Applicant b. Project 6th 6th																																																																																	
15. ESTIMATED FUNDING: <table border="1" style="width:100%; border-collapse: collapse;"> <tr> <td style="width:20%;">a. Federal</td> <td style="width:10%;">\$</td> <td style="width:10%;"></td> <td style="width:10%;"></td> <td style="width:10%;"></td> <td style="width:10%;"></td> <td style="width:10%;"></td> <td style="width:10%;"></td> <td style="width:10%;"></td> <td style="width:10%;"></td> </tr> <tr> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td style="text-align: right;">845,036.00</td> </tr> <tr> <td>b. Applicant</td> <td>\$</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td style="text-align: right;">.00</td> </tr> <tr> <td>c. State</td> <td>\$</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td style="text-align: right;">.00</td> </tr> <tr> <td>d. Local</td> <td>\$</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td style="text-align: right;">.00</td> </tr> <tr> <td>e. Other</td> <td>\$</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td style="text-align: right;">211,259.00</td> </tr> <tr> <td>f. Program Income</td> <td>\$</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td style="text-align: right;">.00</td> </tr> <tr> <td>g. TOTAL</td> <td>\$</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td style="text-align: right;">1,056,295.00</td> </tr> </table>		a. Federal	\$																		845,036.00	b. Applicant	\$.00	c. State	\$.00	d. Local	\$.00	e. Other	\$								211,259.00	f. Program Income	\$.00	g. TOTAL	\$								1,056,295.00	16. IS APPLICATION SUBJECT TO REVIEW BY STATE EXECUTIVE ORDER 12372 PROCESS? a. YES. THIS PREAPPLICATION/APPLICATION WAS MADE AVAILABLE TO THE STATE EXECUTIVE ORDER 12372 PROCESS FOR REVIEW ON: DATE _____ b. NO. <input checked="" type="checkbox"/> PROGRAM IS NOT COVERED BY E.O. 12372 <input type="checkbox"/> OR PROGRAM HAS NOT BEEN SELECTED BY STATE FOR REVIEW	
a. Federal	\$																																																																																		
									845,036.00																																																																										
b. Applicant	\$.00																																																																										
c. State	\$.00																																																																										
d. Local	\$.00																																																																										
e. Other	\$								211,259.00																																																																										
f. Program Income	\$.00																																																																										
g. TOTAL	\$								1,056,295.00																																																																										
17. IS THE APPLICANT DELINQUENT ON ANY FEDERAL DEBT? <input type="checkbox"/> Yes If "Yes," attach an explanation. <input checked="" type="checkbox"/> No		18. TO THE BEST OF MY KNOWLEDGE AND BELIEF, ALL DATA IN THIS APPLICATION/PREAPPLICATION ARE TRUE AND CORRECT. THE DOCUMENT HAS BEEN DULY AUTHORIZED BY THE GOVERNING BODY OF THE APPLICANT AND THE APPLICANT WILL COMPLY WITH THE ATTACHED ASSURANCES IF THE ASSISTANCE IS AWARDED.																																																																																	
a. Typed Name of Authorized Representative Fred M. Vitalo		b. Title Director, Contract Services																																																																																	
d. Signature of Authorized Representative 		c. Telephone number (847) 768-0761																																																																																	
e. Date Signed 10/18/00																																																																																			

Federal Assistance Budget Information

OMB Burden Disclosure Statement

Public reporting burden for this collection of information is estimated to average 1.87 hours per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Office of Information Resources Management Policy, Plans and Oversight, Records Management Division, HR-422 - GTN, Paperwork Reduction Project (1910-0400), U.S. Department of Energy, 1000 Independence Avenue, S.W., Washington, DC 20585; and to the Office of Management and Budget (OMB), Paperwork Reduction Project (1910-0400), Washington, DC 20503.

1. Program/Project Identification No. DE-FC36-99GO10450	2. Program/Project Title Production of Hydrogen by Superadiabatic Decomposition - Phase 2
3. Name and Address Institute of Gas Technology 1700 South Mount Prospect Road Des Plaines, IL 60018-1804	4. Program/Project Start Date 01/01/2000
	5. Completion Date 12/31/2002

SECTION A - BUDGET SUMMARY

Grant Program Function or Activity (a)	Federal Catalog No. (b)	Estimated Unobligated Funds		New or Revised Budget		
		Federal (c)	Non-Federal (d)	Federal (e)	Non-Federal (f)	Total (g)
1. Phase 2	81-087	\$	\$	\$845,036	\$211,259	\$1,056,295
2.						
3.						
4.						
5. TOTALS		\$	\$	\$845,036	\$211,259	\$1,056,295

SECTION B - BUDGET CATEGORIES

6. Object Class Categories	Grant Program, Function or Activity				Total (5)
	(1)Federal	(2)Non-Federal	(3)	(4)	
a. Personnel	\$141,355	\$35,339	\$	\$	\$176,694
b. Fringe Benefits					
c. Travel	\$6,038	\$1,510			\$7,548
d. Equipment	\$248,000	\$62,000			\$310,000
e. Supplies	\$12,000	\$3,000			\$15,000
f. Contractual	\$87,600	\$21,900			\$109,500
g. Construction					
h. Other					
i. Total Direct Charges	\$494,993	\$123,749			\$618,742
j. Indirect Charges	\$350,042	\$87,511			\$437,553
k. TOTALS	\$845,035	\$211,260	\$	\$	\$1,056,295
7. Program Income	\$	\$	\$	\$	\$

U.S. DEPARTMENT OF ENERGY
GOLDEN FIELD OFFICE



BUDGET EXPLANATION PAGE FOR FORM DOE F 4600.4

Grantee: Institute of Gas Technology Budget Period: 01/01/2001 - 12/31/2002
Grant/Proposal Number: DE-FC36-99GO10450 Amendment Number: _____

Negotiation and administration of Financial Assistance awards will be in accordance with DOE Financial Assistance Rules (10 CFR Part 600). A copy of 10 CFR 600 may be obtained electronically through the Golden Field Office Home Page at <http://www.eren.doe.gov/golden/applicationdocs.html>. Post award forms and other reference documents may also be obtained electronically through the above Internet address.

1. **BUDGET INFORMATION**

THE FOLLOWING INFORMATION MUST BE SUPPLIED AND MUST INCLUDE ALL PROJECT COSTS INCLUDING DOE REQUESTED FUNDING AND ANY RECIPIENT COST SHARE. Please provide detailed data to support each cost category as follows. The information can either be provided in the Applicants format or included on this form.

a. **PERSONNEL**

1. Identify, by title and name, each position to be supported under the proposed award.
 Rachid Slimane, Principal Chemical Engineer, Professional Level II
 Brett Williams, Assistant Materials Engineer, Professional Level I
 Osman Akpolat, Research Associate, Technical Level I
 Francis Lau, Director, Process Engineering, Professional Level V

2. Briefly specify the duties of professionals to be compensated under this project and provide resumes for each individual.

R. Slimane - project supervision
 B. Williams - set up analysis system and shakedown testing
 F. Lau - program management

3. State the amounts of time, such as hours, to be expended by each position, their base pay rate and total direct compensation under this project. Provide the amounts of time by tasks as proposed in the Statement of Work.

Position/Person	Time	X	Rate	=
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Please see attached Direct Labor Details.

Direct Labor Total Program

10/17/2000

GTI Proposal No. 18601-06
DE-FC36-99GO10450 Phase 2

Category	Phase 2 Year 1												Total
	Jan-01	Feb-01	Mar-01	Apr-01	May-01	Jun-01	Jul-01	Aug-01	Sep-01	Oct-01	Nov-01	Dec-01	
Tech Lev I	0	0	0	0	0	0	160	160	160	96	96	96	768
	\$0	\$0	\$0	\$0	\$0	\$0	\$2,191	\$2,191	\$2,300	\$1,380	\$1,380	\$1,380	\$10,822
	13.69	13.69	13.69	13.69	13.69	13.69	13.69	13.69	14.38	14.38	14.38	14.38	
Prof Lev I	0	0	0	0	0	0	160	160	160	96	96	96	768
	\$0	\$0	\$0	\$0	\$0	\$0	\$4,356	\$4,356	\$4,574	\$2,744	\$2,744	\$2,744	\$21,518
	27.23	27.23	27.23	27.23	27.23	27.23	27.23	27.23	28.59	28.59	28.59	28.59	
Prof Lev II	12	12	12	12	20	20	20	20	46	40	40	88	342
	\$515	\$515	\$515	\$515	\$858	\$858	\$858	\$858	\$2,071	\$1,801	\$1,801	\$3,962	\$15,127
	42.88	42.88	42.88	42.88	42.88	42.88	42.88	42.88	45.03	45.03	45.03	45.03	
Prof Lev V	4	4	4	4	4	4	4	4	30	8	8	56	134
	\$326	\$326	\$326	\$326	\$326	\$326	\$326	\$326	\$2,564	\$684	\$684	\$4,787	\$11,327
	81.41	81.41	81.41	81.41	81.41	81.41	81.41	81.41	85.48	85.48	85.48	85.48	
Task Totals:	16	16	16	16	24	24	344	344	396	240	240	336	2012
	\$841	\$841	\$841	\$841	\$1,184	\$1,184	\$7,731	\$7,731	\$11,509	\$6,609	\$6,609	\$12,873	\$ 58,794

Direct Labor Total Program

10/17/2000

GTI Proposal No. 18601-06
DE-FC36-99GO10450 Phase 2

Category	Phase 2 Year 2												Total
	Jan-02	Feb-02	Mar-02	Apr-02	May-02	Jun-02	Jul-02	Aug-02	Sep-02	Oct-02	Nov-02	Dec-02	
Tech Lev I	96	96	96	96	96	96	0	0	0	0	0	0	576
	\$1,380	\$1,380	\$1,380	\$1,380	\$1,380	\$1,380	\$0	\$0	\$0	\$0	\$0	\$0	\$8,280
	14.38	14.38	14.38	14.38	14.38	14.38	14.38	14.38	15.1	15.1	15.1	15.1	
Prof Lev I	96	96	96	96	96	96	0	0	0	0	0	0	576
	\$2,744	\$2,744	\$2,744	\$2,744	\$2,744	\$2,744	\$0	\$0	\$0	\$0	\$0	\$0	\$16,464
	28.59	28.59	28.59	28.59	28.59	28.59	28.59	28.59	30.02	30.02	30.02	30.02	
Prof Lev II	72	72	72	76	72	110	52	52	16	16	16	40	666
	\$3,242	\$3,242	\$3,242	\$3,422	\$3,242	\$4,953	\$2,341	\$2,341	\$756	\$756	\$756	\$1,891	\$30,184
	45.03	45.03	45.03	45.03	45.03	45.03	45.03	45.03	47.28	47.28	47.28	47.28	
Prof Lev V	40	40	40	44	40	120	94	94	58	58	58	40	726
	\$3,419	\$3,419	\$3,419	\$3,761	\$3,419	\$10,257	\$8,035	\$8,035	\$5,206	\$5,206	\$5,206	\$3,590	\$62,972
	85.48	85.48	85.48	85.48	85.48	85.48	85.48	85.48	89.75	89.75	89.75	89.75	
Task Totals:	304	304	304	312	304	422	146	146	74	74	74	80	2544
	\$10,785	\$10,785	\$10,785	\$11,307	\$10,785	\$19,334	\$10,376	\$10,376	\$5,962	\$5,962	\$5,962	\$5,481	\$ 117,900

Direct Labor Details

10/17/2000

GTI Proposal No. 18601-06
DE-FC36-99GO10450 Phase 2

Task # 1

Category	Jan-01	Feb-01	Mar-01	Apr-01	May-01	Jun-01	Jul-01	Aug-01	Sep-01	Total
Tech Lev I	0	0	0	0	0	0	160	160	160	480
	\$0	\$0	\$0	\$0	\$0	\$0	\$2,191	\$2,191	\$2,300	\$6,682
	13.69	13.69	13.69	13.69	13.69	13.69	13.69	13.69	14.38	
Prof Lev I	0	0	0	0	0	0	160	160	160	480
	\$0	\$0	\$0	\$0	\$0	\$0	\$4,356	\$4,356	\$4,574	\$13,286
	27.23	27.23	27.23	27.23	27.23	27.23	27.23	27.23	28.59	
Prof Lev II	8	8	8	8	8	8	8	8	8	72
	\$343	\$343	\$343	\$343	\$343	\$343	\$343	\$343	\$360	\$3,104
	42.88	42.88	42.88	42.88	42.88	42.88	42.88	42.88	45.03	
Task Totals:	8	8	8	8	8	8	328	328	328	1032
	\$343	\$343	\$343	\$343	\$343	\$343	\$6,890	\$6,890	\$7,234	\$ 23,072

Direct Labor Details

10/17/2000

GTI Proposal No. 18601-06
DE-FC36-99GO10450 Phase 2

Task # 2

Category	Phase 2 Year 1								Total
	May-01	Jun-01	Jul-01	Aug-01	Sep-01	Oct-01	Nov-01	Dec-01	
Prof Lev II	8	8	8	8	8	8	8	8	64
	\$343	\$343	\$343	\$343	\$360	\$360	\$360	\$360	\$2,812
	42.88	42.88	42.88	42.88	45.03	45.03	45.03	45.03	
Task Totals:	8	8	8	8	8	8	8	8	64
	\$343	\$343	\$343	\$343	\$360	\$360	\$360	\$360	\$ 2,812

Direct Labor Details

10/17/2000

GTI Proposal No. 18601-06
DE-FC36-99GO10450 Phase 2

Task # 3

Category	Oct-01	Nov-01	Dec-01	Jan-02	Feb-02	Mar-02	Apr-02	May-02	Jun-02	Total
Tech Lev I	96	96	96	96	96	96	96	96	96	864
	\$1,380	\$1,380	\$1,380	\$1,380	\$1,380	\$1,380	\$1,380	\$1,380	\$1,380	\$12,420
	14.38	14.38	14.38	14.38	14.38	14.38	14.38	14.38	14.38	
Prof Lev I	96	96	96	96	96	96	96	96	96	864
	\$2,744	\$2,744	\$2,744	\$2,744	\$2,744	\$2,744	\$2,744	\$2,744	\$2,744	\$24,696
	28.59	28.59	28.59	28.59	28.59	28.59	28.59	28.59	28.59	
Prof Lev II	24	24	24	24	24	24	24	24	24	216
	\$1,081	\$1,081	\$1,081	\$1,081	\$1,081	\$1,081	\$1,081	\$1,081	\$1,081	\$9,729
	45.03	45.03	45.03	45.03	45.03	45.03	45.03	45.03	45.03	
Task Totals:	216	216	216	216	216	216	216	216	216	1944
	\$5,205	\$5,205	\$5,205	\$5,205	\$5,205	\$5,205	\$5,205	\$5,205	\$5,205	\$ 46,845

Direct Labor Details

10/17/2000

GTI Proposal No. 18601-06
DE-FC36-99GO10450 Phase 2

Task # 5

Category	Jun-02	Jul-02	Aug-02	Sep-02	Oct-02	Nov-02	Total
Prof Lev II	12	12	12	12	12	12	72
	\$540	\$540	\$540	\$567	\$567	\$567	\$3,321
	45.03	45.03	45.03	47.28	47.28	47.28	
Prof Lev V	54	54	54	54	54	54	324
	\$4,616	\$4,616	\$4,616	\$4,847	\$4,847	\$4,847	\$28,389
	85.48	85.48	85.48	89.75	89.75	89.75	
Task Totals:	66	66	66	66	66	66	396
	\$5,156	\$5,156	\$5,156	\$5,414	\$5,414	\$5,414	\$ 31,710

Direct Labor Details

10/17/2000

GTI Proposal No. 18601-06
DE-FC36-99GO10450 Phase 2

Task # 6

Category	Task 6 Year 1												Total	
	Jan-01	Feb-01	Mar-01	Apr-01	May-01	Jun-01	Jul-01	Aug-01	Sep-01	Oct-01	Nov-01	Dec-01		
Prof Lev II	4	4	4	4	4	4	4	4	4	30	8	8	8	86
	\$172	\$172	\$172	\$172	\$172	\$172	\$172	\$172	\$172	\$1,351	\$360	\$360	\$360	\$3,807
	42.88	42.88	42.88	42.88	42.88	42.88	42.88	42.88	42.88	45.03	45.03	45.03	45.03	
Prof Lev V	4	4	4	4	4	4	4	4	4	30	8	8	8	86
	\$326	\$326	\$326	\$326	\$326	\$326	\$326	\$326	\$326	\$2,564	\$684	\$684	\$684	\$7,224
	81.41	81.41	81.41	81.41	81.41	81.41	81.41	81.41	81.41	85.48	85.48	85.48	85.48	
Task Totals:	8	8	8	8	8	8	8	8	8	60	16	16	16	172
	\$498	\$498	\$498	\$498	\$498	\$498	\$498	\$498	\$498	\$3,915	\$1,044	\$1,044	\$1,044	\$ 11,031

Direct Labor Details

10/17/2000

GTI Proposal No. 18601-06
DE-FC36-99GO10450 Phase 2

Task # 6

Task 6 Year 2

Category	Jan-02	Feb-02	Mar-02	Apr-02	May-02	Jun-02	Jul-02	Aug-02	Sep-02	Oct-02	Nov-02	Dec-02	Total
Prof Lev II	4	4	4	8	4	30	4	4	4	4	4	40	114
	\$180	\$180	\$180	\$360	\$180	\$1,351	\$180	\$180	\$189	\$189	\$189	\$1,891	\$5,249
	45.03	45.03	45.03	45.03	45.03	45.03	45.03	45.03	47.28	47.28	47.28	47.28	
Prof Lev V	4	4	4	8	4	30	4	4	4	4	4	40	114
	\$342	\$342	\$342	\$684	\$342	\$2,564	\$342	\$342	\$359	\$359	\$359	\$3,590	\$9,967
	85.48	85.48	85.48	85.48	85.48	85.48	85.48	85.48	89.75	89.75	89.75	89.75	
Task Totals:	8	8	8	16	8	60	8	8	8	8	8	80	228
	\$522	\$522	\$522	\$1,044	\$522	\$3,915	\$522	\$522	\$548	\$548	\$548	\$5,481	\$ 15,216

4. Supply rate verification documentation (e.g., labor distribution report).

Please see to Reference A-2

b. FRINGE BENEFITS

1. Indicate the basis for computation of rates, including the types of benefits to be provided, the rate(s) used, and the cost base for each rate.

See Reference A-2

2. Are the fringe cost rates approved by a Federal Agency? If so, identify the agency, period of applicability, and date of latest rate agreement or audit and provide the approval letter.

No

c. TRAVEL

Identify total Foreign and Domestic Travel as separate items.

1. Indicate the estimated number of trips, number of travelers, names/positions of travelers, number of days per trip, point of origin, destination, and purpose of travel.

Please see the attached Travel Schedule.

2. For each trip, itemize the estimate of transportation and/or subsistence costs, including airfare, mileage, rental car expenses, lodging costs, and per diem.

Please refer to Travel Schedule

3. Specify the basis for computation of each type of travel expense (e.g., current airline ticket quotes, past trips of a similar nature, federal government or organization travel policy, etc.) and supply supporting information (e.g., quotes, previous invoices, historical data, etc.).

REFERENCE A-2 - Basis for Labor Cost Estimates

A breakdown of labor cost estimate by personnel classification is given in the attached table. The rates given for labor classifications are current GTI average hourly rates including fringe benefits for the labor classification shown.

For manpower deployment purposes, it is assumed that an average employee's productive year is 1920 hours, and a productive man-month is 160 hours.

The labor rates for GTI's FY 2000 (September 1999 through August 2000) are labor category rates. All labor rates for each year thereafter are escalated by 5.0%.

The following fringe benefits are included in the average hourly rates given in the labor cost estimate tables:

1. Employer contribution to social security (FICA)
2. GTI contribution to employee's Retirement Program
3. Base Medical Insurance provided by GTI
4. Major Medical Insurance paid for by GTI
5. Disability Insurance paid for by GTI
6. Hartford Life Insurance Co., life insurance paid for by GTI for non-union employees
7. Life insurance paid for by GTI for union employees
8. Unemployment tax paid for by GTI
9. Dental Insurance paid for by GTI
10. Holidays, vacation, illness and administrative leave

Reference: A-Trv
 Basis for Direct Cost Estimate
 10/17/2000

GTI Proposal No. 18601-06
 DE-FC36-99GO10450 Phase 2

TRAVEL SCHEDULE

Task No	No. of People	No. of Days	Destination **	Airfare	Ground Trans	Per Diem	Total Cost	Purpose
1	2	3	Denver, CO	\$ 2,736.00	\$ 210.00	\$ 828.00	\$ 3,774.00	Annual Hydrogen Program Review Meeting
4	2	3	Denver, CO	\$ 2,736.00	\$ 210.00	\$ 828.00	\$ 3,774.00	Annual Hydrogen Program Review Meeting

Grand Total: \$ 7,548.00

**** All trips are round trip from Chicago, unless otherwise noted.**

Basis: Travel cost estimates are based on current air fares listed in the Official Airline Guide (OAG) and car rental and living expenses are based on IGT standards.

Please see Reference A-1

- d. **EQUIPMENT** - As defined at 10 CFR 600.101 and 10 CFR 600.202, "Equipment".
1. Itemize the equipment and briefly justify the need for the items of equipment to be purchased as they apply to the Statement of Work.

Please see attached Equipment Detail

2. Indicate the estimated unit cost and number of units for each item to be purchased.

Please see Equipment Detail

3. Provide the basis for the equipment cost estimates (e.g., vendor quotes, published price lists, prior purchases of similar or like items, etc.) and supply supporting information (e.g., vendor quotes, previous invoices, historical data, published price list, etc.).

Please see Equipment Detail and Reference A-1

- e. **SUPPLIES** - As defined at 10 CFR 600.101 and 10 CFR 600.202, "Supplies".
1. Identify the materials and supplies and briefly justify the need for each item as they apply to the Statement of Work.

Please see the attached Materials Detail

2. Indicate the estimated unit cost and number of units for each item to be purchased.

Please see Materials Detail

REFERENCE A-1 - Basis for Direct Cost Estimate

The estimated cost given for materials, supplies, and equipment items are approximate, based on the best information we have in hand from manufacturers' or supplier's published price catalogs, from past experience in purchase of similar items, from verbal or written quotes, or from engineering estimates.

Selection of vendors for commercially available items is made on the basis of competitive bidding, whenever possible, product quality and the vendor's ability to deliver the item when required.

Selection of subcontractors and consultants are made on the basis of competitive bidding, whenever possible. Selection is also based on technical experience and the ability to deliver the work required within the time required.

Travel cost estimates are based on living expenses as allowed by the Federal Travel Regulations (41 CFR Chapter 301), car rental (based on GTI standards) and current air fares listed in the Official Airline Guide.

Reference: A-Equ
Basis for Direct Cost Estimate
10/17/2000

GTI Proposal No. 18601-06
DE-FC36-99GO10450 Phase 2

EQUIPMENT

Cost Task	Name/Description	Vendor	Quote Code*	Total
1	Total installed cost of a SAC reactor system	To be selected	WQ	300,000
1	Gas chromatograph	HP	VQ	10,000
Total Equipment:				<u>\$ 310,000.00</u>

* Quote Codes: VQ=Verbal Quote, WQ=Written Quote, CA=Catalog Price, EE=Engineering Estimate, CI=Current Invoice

DIRECT MATERIALS

Cost Task	Name/Description	Vendor	Quote Code*	Total
1	gases, valves, parts, etc.	Various	EE	5,000
3	gases, valves, parts, etc.	Various	EE	10,000
Total Direct Materials:				<u>\$ 15,000.00</u>

* Quote Codes: VQ=Verbal Quote, WQ=Written Quote, CA=Catalog Price,
EE=Engineering Estimate, CI=Current Invoice

3. Provide the basis for the material cost estimates (e.g., vendor quotes, prior purchases of similar or like items, published price list, etc.) and supply supporting information (e.g. quotes, previous invoices, historical data, published price list, etc.).

Please see Reference A-1

f. **CONTRACTUAL**

1. Provide a Statement of Work and cost proposal for each selected contractors/subgrantee and supply the following:

<u>Contractor/Subgrantee</u>	<u>Competitively selected:</u> <u>Cost</u>	<u>Work Description</u>
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Please see Subcontractor Detail and attached proposal

<u>Contractor/Subgrantee</u>	<u>Non-competitively selected*:</u> <u>Cost</u>	<u>Work Description</u>	<u>Sole Source Justification</u>
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* For each non-competitively selected contractor or subgrantee, have the contractor and subgrantee complete a GO-PF20, Budget Information Page For Form DOE F 4600.4 and attach them to this form.

Reference: A-Sub
Basis for Direct Cost Estimate
10/17/2000

GTI Proposal No. 18601-06
DE-FC36-99GO10450 Phase 2

SUBCONTRACTORS

Cost Task	Name/Description	Vendor	Quote Code*	Total
2	University of Illinois at Chicago (UIC)	UIC	WQ	109,500

Total Subcontractors: \$ 109,500.00

* Quote Codes: VQ=Verbal Quote, WQ=Written Quote, CA=Catalog Price, EE=Engineering Estimate, CI=Current Invoice

A Proposal Submitted to IGT

Institute of Gas Technology

1700 South Mount Prospect Road

Des Plaines, IL 60018

MODELING OF HYDROGEN AND SULFUR PRODUCTION BY SUPERADIABATIC COMBUSTION OF HYDROGEN SULFIDE

Phase 2 of the IGT Program

Prepared by: Prof. Alexander A. Fridman
Dr. Alexander F. Gutsol
Prof. Lawrence A. Kennedy
Dr. Alexei V. Saveliev

Date Submitted:	October 17, 2000
Amount Requested:	\$ 109,500
Period of Research:	May 1, 2001 - June 30, 2002

MODELING OF HYDROGEN AND SULFUR PRODUCTION BY SUPERADIABATIC COMBUSTION OF HYDROGEN SULFIDE

1. Background and Principal UIC Modeling Results of Phase 1

Research interest in filtration combustion (FC) has been driven by numerous applications such as utilization of low calorific fuels [1], low emission burners [2] and pollution control devices. Recent novel applications include fuel reforming and processing in the ultra-rich superadiabatic combustion waves [3].

In Phase 1 of this program filtration combustion waves in H_2S /air mixtures were modeled within the one-dimensional approach taking into account multi-step chemistry and separate energy equations for the gas and solid phases [4]. The superadiabatic wave propagation is a complex phenomenon, and many factors that influence wave properties, in particular the heat loss rate, interfacial heat exchange or effective heat conductivity of the porous medium, must be accurately specified. We developed a numerical model to describe combustion wave characteristics in a coordinate system moving together with the wave front. Two chemical kinetic mechanisms were used. The first one (developed by Frenklach's group) is more appropriate under combustion conditions (moderately high equivalence ratios), the second kinetic mechanism has been developed at UIC to describe more accurately the partial oxidation of H_2S (ultra-high equivalence ratio). The products of partial H_2S oxidation, H_2 and S_2 are dominants for ultra-rich superadiabatic combustion, which is a fuel reforming actually. The chemistry in the combustion wave was modeled, and species and temperatures profiles were predicted. A database of hydrogen and sulfide conversion in a wide range of equivalence ratios and other process parameters was produced.

Filtration combustion in porous media differs substantially from combustion in a homogeneous media. The difference is the heat transfer between filtrated gas and the porous medium under conditions of active interfacial heat transfer. FC also differs from flames stabilized within a porous body in that FC is an inherently transient process. These differences lead to positive or negative enthalpy fluxes between the reacting gas and the solid carcass, resulting in combustion temperatures in excess or below the adiabatic one for the supply mixture. Combustion waves in the porous body, including excess enthalpy (superadiabatic) flames, have been the focus of many recent experimental and theoretical studies [5-10]. However, almost all of these studies were limited to the case of very lean mixtures. To fully exploit FC potential applications, numerical models need to be extended to the practically important limit of rich and ultra-rich filtration combustion of gases, addressing the issues of multi-step kinetics [11], heterogeneous reactions [12], pore level mechanisms of combustion [13], and adequate heat and mass transport phenomena in porous media.

Ultra-lean filtration combustion results in complete burnout of the hydrocarbon fuel with the formation of carbon dioxide and water. Thus, both the composition of the final products and the heat release are well defined. In contrast with the ultra-lean case, the combustion products of rich waves are not clearly defined. In this case, fuel is only partially oxidized in the filtration wave and the total heat release could be kinetically controlled by the degree of the partial combustion. As a result, the chemical kinetics, heat release and heat transfer are strongly coupled in the ultra rich wave making it more complicated and challenging phenomenon than the ultra-lean wave. Previous analyses [5-10] of the FC waves were based upon a model in which the gas phase chemical reactions were approximated by a single-step kinetic mechanism for combustion.

In Phase 1 of this program the numerical model was developed for description of superadiabatic combustion (SAC) of ultra-rich H₂S/air mixtures [4]. Modeling studies of H₂S decomposition through SAC were conducted based upon computational models of filtration combustion waves in a porous medium developed earlier for ultra-rich filtration combustion of methane/air mixtures. These include numerical programs for unsteady simulation of ultra-rich combustion waves with multi-step chemical mechanisms. Superadiabatic combustion of ultra-rich H₂S/air mixtures is represented within a one-dimensional, non-steady model, including separate energy equations for the gas and porous medium. The boundary conditions for the gas are imposed at the inlet and the exit of the reactor. Standard reaction flux/pathway and gradient sensitivity analysis techniques are applied at each step to identify important reaction pathways. The model allows the prediction of process performance (i.e., overall H₂S conversion, H₂/H₂O selectivity, S₂/SO₂ selectivity, etc) over a range of operating conditions, including equivalence ratios, flow rates, and other packed-bed reactor parameters.

Certain products, oxygen, sulfur dioxide, and sulfur, correlate fairly well with thermodynamic predictions. Others, notably hydrogen, diverges over the whole range of rich mixtures. Hydrogen in the products is present after stoichiometry and maximizes at $\phi=2$ to achieve a maximum conversion rate of 20% based on the hydrogen sulfide input. Its production fell rather gently thereafter to where nothing is gained by equivalence ratio of 5.5. The concentration of unreacted hydrogen sulfide rises linearly with equivalence ratio at post-stoichiometry. Some sulfur based products peaked at the extremities: sulfur dioxide at stoichiometry (100% conversion), and elemental sulfur (50% conversion) at $\phi=4$. Finally, the formation of sulfuric acid in ultra-lean combustion was qualitatively verified. Detailed modeling results were presented in a final report submitted to IGT (see Appendix A).

2. Objectives of Numerical Modeling in Phase 2

The main objective of UIC activities in Phase 2 is to provide guidelines for the operation of the bench-scale reactor unit according to a test plan and also to analyze the experimental results and provide recommendations for the next phase of the program. In Phase 2 the previously developed numerical model of rich and ultra-rich filtration combustion (FC) of H₂S-containing fuel/oxidant gas mixtures will be modified as necessary. Work will include the following:

- *Further Development of the Simulation Model and Programming Complex for Detailed Kinetic and Heat Transfer Modeling.*
- *Detailed Reactor Modeling Application for the Bench-Scale Unit Operation.*
- *Application of the Improved Detailed Process Modeling for Interpretation and Analysis of the Experimental Results.*
- *Application of the Improved Detailed Process Modeling in Comparison with the Experimental Results Obtained during Bench-Scale Testing for Technical Feasibility Verification.*

3. Computational Approach

Theoretical studies will be conducted based upon computational models of filtration combustion of waves in a porous medium developed for ultra-rich filtration combustion of hydrogen sulfide developed in Phase 1 of the project [4]. These include numerical programs for unsteady simulation of ultra-rich combustion waves with multi-step chemical mechanisms [14].

3.1 Computational Model

Superadiabatic combustion of ultra-rich H₂S/air mixture will be represented within a one-dimensional, non-steady model. The combustion wave propagation in an inert, packed bed is described by the system of conservation equations for gas energy, solid medium energy, mass fractions of gas species, and mass flow rates. Further details are provided in references 6 and 15.

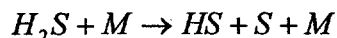
The major factors controlling the combustion wave behavior under filtration in an inert porous medium are: (i) the heat deposition in the gas phase due to fuel oxidation, (ii) the forced convection of fuel/air mixture, (iii) the longitudinal effective heat conductivity of the porous medium, (iv) the intense interfacial heat exchange between gas and solid phase, and (v) the heat exchange between the porous medium and surroundings. The factors (i)-(iv) are accurately represented within the one-dimensional approach due to the high degree of radial uniformity of the combustion wave front found in the measurements for the reactors under consideration. The factor (v) can be taken into account only parametrically, via the heat exchange in solid state energy equation, within a one-dimensional approach due to its explicit multi-dimensional nature.

The one-dimensional laminar flame code PREMIX is used following modification for the above-described problem. The adaptive placement of the grid points is done to resolve accurately the gradient and the curvature of the gas temperature and species profiles. We have found that 70-100 grid points provide sufficiently accurate solutions. The numerical algorithm implemented in the PREMIX code has been used to find the combustion wave velocity u .

The Chemkin subroutines are used to implement the chemical kinetics description [16] and the Transport subroutine [17] to calculate gas properties.

3.2 Kinetic Mechanisms of Ultra-Rich Hydrogen Sulfide Combustion

Two chemical kinetic mechanisms have been used in Phase 1 [4]. The first one (developed by the Frenklach's group), which includes 17 species and 58 reactions, is more appropriate under combustion conditions (moderately high equivalence ratios). The second kinetic mechanism has been developed at UIC to describe more accurately the partial oxidation of H₂S (ultra-high equivalence ratio). In the second kinetic mechanism the thermal decomposition of hydrogen sulfide



is described with a rate constant.

In Phase 2 we propose to modify kinetic mechanisms by taking into account the heterogeneous chemical reactions on the surface of pellets.

4. Work plan

4.1. Further Development of the Simulation Model and Programming Complex for Detailed Kinetic and Heat Transfer Modeling.

Previously developed numerical model of rich and ultra-rich filtration combustion (FC) of H₂S-containing fuel/oxidant gas mixtures will be modified. The most important improvement of the code is related to taking into account the heterogeneous chemical reactions on the surface of pellets. This will provide an additional control on the process temperature to increase conversion of hydrogen sulfide.

To simulate different inlet fuel gas compositions (H₂S-rich, H₂S-lean, simulated gas composition from a typical refinery, etc.), new reactions will be included to describe the kinetic mechanism.

Period of Performance: 5 months (May 2001 – September 2001).

4.2. Detailed Reactor Modeling Application for the Bench-Scale Unit Operation

The simulation model and programming complex developed in Phase 1 of the project (as well as improved versions of the code during the initial stages of Phase 2), will be applied for the selection of most suitable parameters, within the ranges specified in IGT's Test Plan, for the operation of the bench-scale unit and for the definition of the structure and properties of filtration combustion waves including reaction and chemical product information in this bench-scale unit. The model should predict process performance (i.e., overall H₂S conversion, H₂/H₂O selectivity, S₂/SO₂ selectivity, etc) over a range of operating conditions, including equivalence ratios, flow rates, and other packed-bed reactor parameters.

Period of Performance: 5 months (May 2001 – September 2001).

4.3. Application of the Improved Detailed Process Modeling for Interpretation and Analysis of the Experimental Results Obtained during Bench-Scale Testing.

The simulation model and programming complex developed in Phase 2 will be applied for interpretation of experimental results obtained during the bench-scale unit operation as well as for optimization of hydrogen sulfide conversion and other process characteristics.

Period: 9 months (October 2001 – June 2002).

4.4. Application of the Improved Detailed Process Modeling in Comparison with the Experimental Results Obtained during Bench-Scale Testing for Technical Feasibility Verification.

Experimental results will be compared with model simulations, further enhancing the reliability of the numerical model to provide further insight into technical feasibility of the process and guidelines for scale-up options in the next phase of the program.

Period of Performance: 7 months (December 2001 – June 2002).

Research Team

- Professor Alexander Fridman, Principal Investigator
- Professor Lawrence Kennedy
- Dr. Alexander Gutsol
- Dr. Alexei Saveliev
- Graduate student Mr. Alexander Shirokov.

The research group from the University of Illinois at Chicago has extensive experience in physical and numerical modeling of non-reacting and reacting flows, combustion and pollutant chemistry, superadiabatic combustion, soot formation and plasma decomposition of H₂S. This group carried out the modeling work in Phase 1 of the project. The project implementation will involve joint efforts of two UIC laboratories: *Energy Systems Laboratory*, directed by Prof. Lawrence A. Kennedy and *High Temperature Laboratory*, directed by Prof. Alexander A. Fridman. Professor Kennedy's technical interests include the broad areas of combustion, non-equilibrium processes, fluid and thermal sciences. Combustion phenomena of Dr. Kennedy's recent research interests are superadiabatic filtration flames at porous inert media with emphasis on ultra-rich self-sustained flames for fuel processing and reforming. Developed experimental and numerical capabilities in filtration combustion are focused on wave chemical properties and heat-transfer characteristics. With more than 10 years of experience in superadiabatic combustion of gases the research group of Prof. Kennedy brings solid background for the research project. Prof. Fridman theoretical research has involved both fundamental and applied aspects of high-temperature and high-energy chemistry, plasma and laser chemistry, plus their applications to energy systems, nuclear safety, hydrogen production, and environmental-control technologies. Working at Kurchatov Institute of Atomic Energy (1979-1995), Alexander directed the development of the theoretical basis for microwave plasmolysis of hydrogen sulfide. Prof. Fridman and his co-workers have developed a kinetic mechanism of H₂S decomposition, which will be applied in the proposed project.

Facilities

The following equipment of the UIC will be available for the proposed research:

- Modern computational facilities; Two Silicon Graphics workstations and a Hewlett Packard workstation, Pentium PC's are in the laboratories. Centralized mainframe and access to the Illinois supercomputing facilities at UIUC center are available as required.

ESTIMATED BUDGET

Faculty – 1 summer month –	\$12,500
Research scientists – together 6 mo. –	\$30,000
Graduate student – 1 year	\$16,000
Materials and supplies	\$1,000
Total direct cost	\$59,500
Approximate indirect cost	\$50,000
Total	\$109,500

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20. Chernysheva, A.V., Basevich, V. Ya., Vedenev V.I., and Arutyunov, V.S., *Izv. Acad. Nauk SSSR, Ser. Khim.* No. 9: 1956-1966 (1990).

2. For each proposed procurement contract and subgrant for which a contractor/subgrantee selection has not been made complete the following:

<u>Cost Estimate</u>	<u>Basis for the Cost Estimate*</u>	<u>Work Description</u>
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* Identify the basis of the cost estimate (e.g., quotes, prior subcontracts, etc.) and supply supporting information (e.g., quotes, previous invoices, historical data, etc.).

g. CONSTRUCTION

1. Identify the proposed construction costs and identify the subcontractor/subgrantee to perform the construction.

No construction is proposed

2. Provide a Statement of Work and either a cost proposal or a completed GO-PF20 Budget Information Page For Form DOE F 4600.4 for each selected contractors/subgrantee. For proposed procurement contract and subgrant for which a contractor/subgrantee selection has not been made provide work scope and basis of cost estimate. If non-competitively selected provide a sole source justification.

h. OTHER

1. Identify other costs and briefly justify the need for each cost item proposed relative to the work scope.

No other costs are proposed

2. Indicate the estimated unit cost and number of units for each item proposed.

3. Provide the basis for the cost estimates (e.g., vendor quotes, prior purchases of similar or like items, published price list, etc.) and supply the supporting information (e.g., quotes, previous invoices, historical data, published price list, etc.).

i. INDIRECT CHARGES

1. State the amounts and percentages used for calculation of indirect costs.

Overhead = 120% x \$176,694 = \$212,694

G&A = 25% x \$830,775 = \$207,694

FCCOM (Labor) = 7.55% x \$176,694 = \$13,340

FCCOM (G&A) - 0.54% x \$830,775 = \$4,486

2. Are the indirect cost rates approved by a Federal Agency? If so, identify the agency and date of latest rate agreement or audit and supply the approved rate agreement.

Please see attached rate approval letter

3. If indirect cost rates are not approved by a Federal Agency, state the basis for the proposed indirect cost rates and provide a rate proposal.

2. ADDITIONAL INFORMATION

a. COST SHARE

1. Identify the percentage and amount of cost sharing proposed by each project participant. Cost sharing from other Federal sources can not be counted as non-Federal Recipient contributions. Non-Federal sources include private, state or local Government, or any sources that were not originally derived from Federal funds.

It is anticipated that 20% (\$211,259) cost share will be provided by GRI. A letter of commitment will be forwarded upon receipt.

REFERENCE A-3 - Basis for Overhead and G&A Estimate

GTI presently operates under negotiated provisional indirect rates subject to post audit adjustment for all of its cost reimbursement type Government contracts. The cognizant agency performing audits for all Government contracts is the Defense Contract Audit Agency, 635 Butterfield Road, Suite 210A, Oakbrook Terrace, Illinois 60181-4041, (630) 268-8590.

The Indirect expense rate of 120% is applied to direct labor, and a separate G&A expense rate of 25% is applied to the total direct and indirect cost excluding direct utility costs. The G&A rate consists of three major components, namely - G&A Expense - B&P Expense - and IR&D Expense.

The indirect expense pools included the following elements:

1. Administrative expenses.
2. Salaries and related fringe benefits for vacation, sickness and administrative leave for Administrative staff
3. Office supplies, telephone, postage, insurance, legal and accounting fees, safety & health, employment expenses and photocopying.
4. Occupancy costs.
5. Library services.
6. Depreciation of facilities and equipment.

All costs allocated to the operation of the GTI Education Division are excluded from the overhead for Government contracts.



SEP 27 2000

Mr. Fred M. Vitalo
Director, Contracts Services
Gas Technology Institute (GTI)
1700 South Mount Prospect Road
Des Plaines, IL 60018

Dear Mr. Vitalo:

The U.S. Department of Energy hereby approves the following provisional rates for billing purposes as requested by your letter dated September 13, 2000. The rates are approved for your Fiscal Year 2001 beginning September 1, 2000, and ending August 31, 2001, and supersede any prior approvals.

INDIRECT COST RATES:

Table with 3 columns: Indirect Cost Pool, Billing Rate, Allocation Base. Rows include Overhead (120.00%), G&A (25.00%), and Subcontract G&A (13.00%).

BASIS FOR ALLOCATION:

- (a) Direct Labor Dollars Including Fringe Benefits
(b) Total Cost Input Less Direct Utility Costs
(c) Applicable to Subcontract Costs when Total Subcontract Costs Exceed 50% of Total Estimated Cost

Pending establishment of final indirect cost rates, you may bill for indirect expenses using the above rates for the period specified for existing Government contracts, grants, or cooperative agreements. However, this approval shall not change any monetary ceiling, contract obligation, or specific cost allowance or disallowance provided for in such awards. Additionally, if any award contains indirect rate ceilings, and these ceilings are less than the above rates, the lesser rates shall prevail.

Acceptance of these provisional rates for billing purposes does not imply final acceptance nor commit the Government to any specific rate in final rate negotiations.

Nothing herein shall be construed to prejudice, waive, or in any other way affect any rights of the Government under the provisions of any contracts, grants, or other cooperative agreements respecting limitation of the Government's obligation thereunder.

This agreement is effective as of the date of this letter. Questions regarding this agreement should be directed to Ms. Pat Sienko at (412) 386-4986.

Sincerely,

A handwritten signature in cursive script that reads "Andrew J. Ferlic". The signature is written in dark ink and is positioned above the printed name.

Andrew J. Ferlic
Cognizant Contracting Officer
Indirect Cost Rate Management

**FACILITIES CAPITAL
COST OF MONEY FACTORS COMPUTATION**

Effective
through 07/01/2000 through 12/31/2000

CONTRACTOR: Institute of Gas Technology			ADDRESS: 1700 South Mount Prospect Road Des Plaines, IL 60018-1804				
BUSINESS UNIT:							
COST ACCOUNTING PERIOD:	1. APPLICABLE COST OF MONEY RATE %	2. ACCUMULATION & DIRECT DISTRIBUTION OF N.B.V.	3. ALLOCATION OF UNDISTRIBUTED	4. TOTAL NET BOOK VALUE	5. COST OF MONEY FOR THE COST ACCOUNTING PERIOD	6. ALLOCATION BASE FOR THE PERIOD	7. FACILITIES CAPITAL COST OF MONEY FACTORS
August 31, 2000	7.25%						
BUSINESS UNIT FACILITIES CAPITAL	RECORDED	4,812,646	BASIS OF ALLOCATION	COLUMNS 2+3	COLUMNS 1 X 4	IN UNIT(S) OF MEASURE	COLUMNS 5+6
	LEASED PROPERTY						
	CORPORATE OR GROUP	1,318,096					
	TOTAL	6,130,742					
	UNDISTRIBUTED						
	DISTRIBUTED	6,130,742					
		↓					
OVERHEAD POOLS	Research	4,812,646		4,812,646	348,917	4,621,000	0.0755
G&A EXPENSE POOLS	G & A Expense	1,318,096		1,318,096	95,562	17,510,000	0.0054
TOTAL		6,130,742		6,130,742	444,479	////////	////////

2. Identify the source of the Applicant's cost share (e.g., corporate equity, loan, etc.).

3. Identify the type (e.g., in-kind, cash, etc.) of cost share contributions and supply funding commitment letters from each contributor. Note that "cost sharing" is not limited to cash investment. In-kind contributions (e.g., contribution of services or property; donated equipment, buildings, or land; donated supplies; or unrecovered indirect costs) incurred as part of the project may be considered as all or part of the cost share.

It is anticipated that GRI's cost share will be in the form of cash:

b. FINANCIAL CAPABILITY

1. Document applicant's compliance with Financial Management System specifications per 10 CFR 600.121.

2. Provide current financial statements for the applicant. If the statements are audited, provide the complete audit report with footnotes.

September 27, 2000

Francis S. Lau
Director, Process Development & Engineering
Gas Technology Institute
1700 S. Mt. Prospect Rd
Des Plaines, IL 60018

Subject: Hydrogen Production by Superadiabatic Combustion of Hydrogen Sulfide

Dear Francis:

I am writing to express our continued interest in your efforts to develop a novel process for the production of hydrogen based on the superadiabatic combustion (SAC) of hydrogen sulfide-containing waste streams. We do see a commercial opportunity and a market need for hydrogen in the Refining and IGCC technologies that could be partially met by the hydrogen provided by your process. In addition, we do believe there is merit in exploring the opportunity afforded by such technology for Natural Gas producers to co-produce hydrogen from H₂S, though we believe this opportunity to be more limited than that offered in Refining.

Based on the progress you have made in Phase 1, we share your enthusiasm to continue your efforts towards moving this process one step closer to commercialization in a Phase 2 program. We understand that in Phase 2 you will develop the necessary experimental data to demonstrate the technical and economical viability of the SAC H₂S decomposition process. We believe that such undertaking is critical for successful demonstration and future commercialization of the process.

This letter is to confirm that UOP is interested to participate in GTI's proposal accompanying your final report for Phase 2 "Production of Hydrogen by Superadiabatic Decomposition of Hydrogen Sulfide," Contract No. DE-FC36-99GO10450. We will continue to serve in an industry advisory role, and we will provide assistance as you conduct technical and economic viability of the SAC process.

We wish you the best of luck in the selection of your proposal.

Best Regards,



Mark Schott
Senior Technology Manager
UOP LLC