

**SULPHUR PLANT TAIL GAS  
INCINERATORS IN ALBERTA**

**COMPUTER SIMULATION FOR  
INCINERATOR OPTIMIZATION**

Prepared for:  
Petroleum Technology Alliance Canada  
Calgary, Alberta

Prepared by:  
Bruce Klint, P.Eng.  
Ming Yu,

**Sulphur Experts Inc.**  
Western Research  
Calgary, Alberta  
Canada

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**Sulphur**

**eXperts**  
Western Research

Petroleum Technology Alliance Canada  
500 5<sup>th</sup> Avenue SW  
Suite 700, Chevron Plaza  
Calgary, Alberta  
T2P 3L5

Project No. C504  
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**Attention : Dennis Gaudet**  
**Reference : Sulphur Plant Tail Gas Incinerator In Alberta**  
**Computer Simulation for Incinerator Optimization**

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Sulphur Experts Inc. conducted a detailed study of the operation and simulation of the thermal tail gas incinerators commonly employed in Claus sulphur recovery units. The purpose of this study was to review and update the existing INCWRD incinerator simulation program to allow for more accurate simulation of these systems. This study also investigated new technology and process approaches for optimization of thermal incinerators.

The complete results of this work are included in the following report. If you have any questions about the information contained in this report, please contact us by phone at 403-215-8400, by fax at 403-215-8419 or by email at [help@sulphurexperts.com](mailto:help@sulphurexperts.com).

Yours truly,  
**Sulphur Experts Inc.**  
Western Research

Bruce Klint, P.Eng.  
Manager - Engineering

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**Sulphur Experts Inc.**

**USA Office**  
2819 University Blvd.  
Tyler Texas 75713-0307, USA  
Tel: +1 903-894-6029  
Fax: +1 903-894-6029

**Head Office**  
Suite 102, 12 Manning Close N.E.  
Calgary, Alberta, T2E 7N5, Canada  
Tel: +1 403-215-8400  
Fax: +1 403-215-8419

**European Office**  
Amperestraat 3  
NL 1704 SM Heerhugowaard, The Netherlands  
Tel: +31-72-571-7264  
Fax: +31-72-571-7347

## Summary

All sulphur recovery units (SRUs) in the Province of Alberta employ thermal incinerators to treat the tail gas effluent from the SRUs prior to emitting the waste gas to the atmosphere. The purpose of the thermal incinerator is to facilitate the oxidation of all of the common reduced sulphur compounds ( $H_2S$ , COS,  $CS_2$  and sulphur vapour) to  $SO_2$  prior to release to the atmosphere.

Since 1980, many thermal incinerators in the province have conducted “incinerator optimization” studies in order to identify opportunities to reduce fuel gas consumption by reducing the operating temperature of these systems while continuing to meet the environmental emission requirements of the plant. The “traditional” approach to these optimization studies was based primarily on a combined thermodynamic and kinetic incinerator model (INCWRD) which has been in use since ca. 1980.

The original incinerator model was based on a limited set of test data which had been gathered in the late 1970's. This work expanded the test set to include plant test data gathered from 1980 to 2004 which allowed for more accurate and representative kinetic correlations for modelling the oxidation efficiency of TRS compounds in these thermal incinerators.

The results from this study have allowed for the compilation of updated correlations for the oxidation of  $H_2S$ , COS,  $CS_2$  and  $H_2$ . Also, this work allowed for the derivation of an kinetic correlation for the oxidation of CO for the first time. The use of these correlations in the update incinerator simulation model will allow for more accurate and effective calculations to support new incinerator optimization programs.

Additionally, this study investigated the use of new incinerator technology to realize new opportunities for incinerator optimization. In past works, these incinerators were optimized only for incinerator temperature, essentially a one dimensional optimization approach. These new concepts allow for a “multi-dimensional” optimization approach which includes the use of better system mixing (turbulence) and more system residence time as well as investigating methods for reducing the amount of the undesired pollutants in the SRU waste gas. The case studies completed in this work suggest that these approaches will identify more and larger opportunities for optimization of thermal incinerator in order to reduce fuel gas consumption and  $CO_2$  emissions.

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## 1.0 Introduction

All sulphur recovery units (SRUs) in the Province of Alberta employ thermal incinerators to treat the tail gas effluent from the SRUs prior to emitting the waste gas to the atmosphere. The purpose of the thermal incinerator is to facilitate the oxidation of all of the common reduced sulphur compounds ( $H_2S$ ,  $COS$ ,  $CS_2$  and sulphur vapour) to  $SO_2$  prior to release to the atmosphere. Currently in the Province there is an informal guideline which requires that the maximum Total Reduced Sulphur (TRS) content of the stack effluent be maintained at 300 ppmv or less.

The thermal incinerator also provides significant thermal energy to the SRU tail gas in order to raise the waste gas temperature sufficiently to ensure that the stack plume rises in the atmosphere. This facilitates the effective dispersion of the plume and ensures that the ground level concentration of the  $SO_2$  from the plume does not exceed the Alberta Environment guidelines for this pollutant ( $450 \mu g/m^3$ ).

Due to the very large volumes of SRU tail gas that are treated in these thermal incinerators and the process temperatures required for successful operation, there is a significant amount of plant “fuel gas” consumed in these incinerators.

In previous work it was determined that there is a significant opportunity to reduce the consumption of fuel gas in these systems by optimizing the operation of the incinerators. This “Incinerator Optimization” program has been implemented at many plants in the Province and significant fuel gas savings have been realized as a result.

A key activity in assessing the opportunity to optimize the thermal incinerator is the rigorous modelling of the system with respect to the oxidation of the TRS compounds. A comprehensive research program was completed in the late 1970's on the kinetics of TRS oxidation in these systems. The result of this research program was a rigorous computer model which was used to predict the oxidation efficiency of the TRS compounds at various operating conditions. This computer program, “INCWRD” has been the standard modelling tool used for assessing the TRS oxidation kinetics in these incinerator systems since its' development in the late 1970's.

The purpose of this study was to assess the accuracy of the existing INCWRD program and to assess opportunities to improve the accuracy and applicability of the model by using the large amount of data which has been accumulated on these systems since the original program was completed in 1979.

## 1.2 Project Scope

The specific objectives of the study were to:

- collect and compile operating data on SRU thermal incinerators from existing field studies;
- assess and update the TRS oxidation correlations;
- assess and update the H<sub>2</sub> oxidation correlations;
- assess the new field data to create a new CO oxidation correlation;
- assess the validity of the incinerator mixing factors (K factors) used in the existing model; updating the model as required;
- incorporate all of the updated correlations in a computer modelling program.

## 2.0 Incinerator Reaction Kinetics

The waste gas (tail gas) process streams from Claus sulphur recovery units (SRUs) typically contains several combustible species including  $H_2S$ ,  $COS$  and  $CS_2$  (collectively known as the “total reduced sulphur or TRS species”). These streams also contain elemental sulphur vapour ( $S_v$ ) and  $H_2$  and  $CO$ .

In conventional SRU facilities, a thermal incinerator is employed to oxidize/react these compounds down to acceptably low concentrations prior to venting the waste gas to the atmosphere. The thermal incinerators installed in the many SRU facilities in Alberta typically operate at temperatures in the range of 500 to 600°C in order to ensure that these compounds are adequately converted.

The oxidation rate and efficiency of these compounds is affected strongly by the reaction kinetics in the system including reaction temperature, residence time and extent of mixing. Previous studies by Western Research (1, 2) have provided the basis for detailed empirical correlations for predicting the residual concentrations of these key compounds. These empirical correlations were employed in a computer program (INCWRD) which has been used extensively to model the effects of varying operating parameters on the oxidation of these species (3,4) and allow for the optimization of these incinerator systems.

These original correlations were developed from lab based experiments and were supplemented by field test results to determine the effect of various kinetic factors (primarily mixing) on the reaction kinetics of operating industrial incinerator systems. This original work included plant tests from seven industrial incinerator systems.

Since that time, this kinetic modelling tool has been used to conduct many “Incinerator Optimization” programs with significant success and savings in fuel gas consumption and reduction in  $CO_2$  emissions. A summary report of the historical implementation of this Incinerator Optimization program was presented to PTAC in March, 2005 (5).

A review of the original incinerator kinetic studies suggested that a much larger body of data was available to supplement and (possibly) improve the accuracy of the empirical kinetic correlations which are employed by the INCWRD program. It was one of the primary goals of this study to compile and incorporate this data to allow for a more accurate and versatile modelling of these incinerator systems.



## 2.1 Introduction and Historical Summary

As described earlier, the original kinetic studies in 1975 were based on a combination of lab based and field based experiments (1,2). After compiling and assessing these results, four key correlations were developed for the oxidation of  $\text{H}_2\text{S}$ ,  $\text{COS}$ ,  $\text{CS}_2$  and  $\text{H}_2$ . These original studies also investigated a correlation for the oxidation of  $\text{CO}$ . However, the data did not support a rigorous correlation and none was included in the INCWRD computer program.

These correlations were incorporated into the existing INCWRD computer simulation program and have been used exclusively for all of the incinerator optimization studies conducted to date.

Western Research also compiled data from additional field incinerator studies in the period 1975 to 1979. A review of this data suggested some possible minor changes to the original 1975 correlations. However, the changes were deemed not significant enough to justify changing the model and were therefore never incorporated into the INCWRD computer program. At this date, the current INCWRD computer modelling program contains the correlations determined from the work conducted in 1975 only.

Since the initial implementation of the original Incinerator Optimization program in the Province, Sulphur Experts (and its predecessor companies) have conducted more than 30 field studies on Claus SRU thermal incinerator systems. The data from these field tests represents a significant addition to the total field data base on this topic.

A detailed review of this data was completed in order to assess the existing correlations and use the new data to improve the accuracy and range of those existing correlations. This current research work followed the same philosophy and methods of the prior works and can therefore be considered a natural extension of that work. The development of updated correlations was one of the primary goals of this study.

## 2.2 Field Data Summary

Field data from 13 Claus SRU incinerator systems was collected and compiled for this study. These systems are employed in sulphur recovery units with a very wide range of capacities and feed stocks and the incinerators themselves were of various configurations and arrangements. Table 2.2-1 summarizes the general capacity and plant configurations of these systems.

Table 2.2-1 - Test Plant Descriptions		
Plant No.	SRU Capacity (t/d)	Incinerator Kinetic Design Factor, K
1	600	4
2	100	6
3	525	3
4	165	6
5	50	1
6	10	8
7	700	1
8	3600	4
9	1730	3
10	40	6
11	1270	8
12	480	6
13	350	6

This new data was added to the original 1975 data which provided a data base from a total of 20 plants and more than 200 individual tests.

## 2.3 H<sub>2</sub>S Kinetics

### 1975 Data and Correlation

The original 1975 study provided for a robust H<sub>2</sub>S oxidation correlation based on a relatively large number of field data points. A plot of these results is provided in Figure 2.3-1.

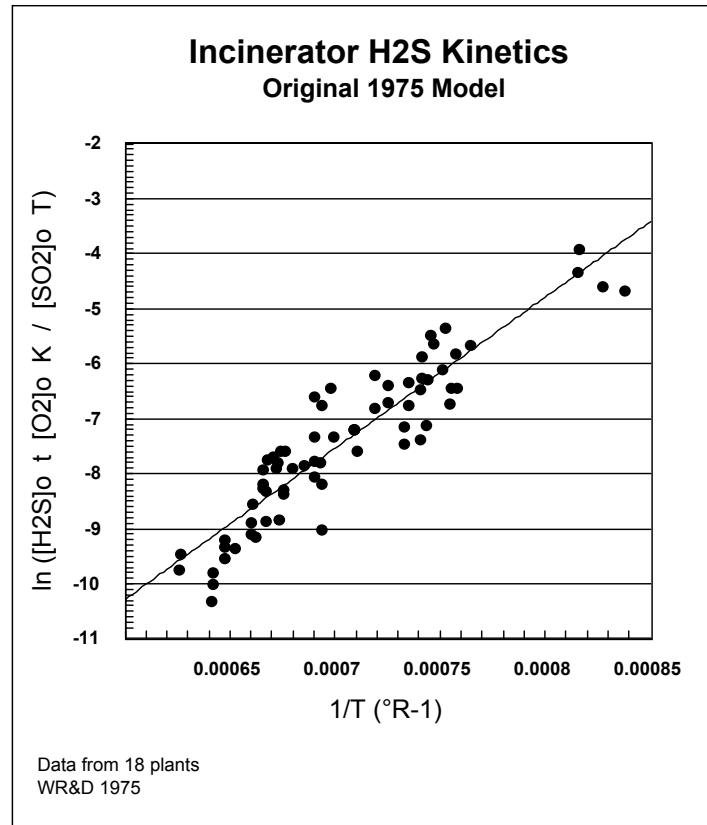


Figure 2.3-1 - H<sub>2</sub>S Kinetics Original 1975 Model

These data yielded the following correlation for the oxidation of H<sub>2</sub>S (4):

$$[\text{H}_2\text{S}]_o = 8.56 \times 10^{-12} [\text{SO}_2]_o T / K \tau [\text{O}_2]_o \exp(25300/T)$$

where ....

[H <sub>2</sub> S] <sub>o</sub>	concentration in the stack gas (ppm)
[SO <sub>2</sub> ] <sub>o</sub>	concentration in the stack gas (ppm)
T	average system temperature (°R)
τ	residence time (s)
K	plant kinetic design factor
[O <sub>2</sub> ]	concentration in the stack gas (vol%)

This correlation was based on the concentration of SO<sub>2</sub> in the stack gas which proved to be more easily attained data and less prone to variation due to upsets in the upstream SRU operation. This was the correlation which was implemented in the original INCWRD model and is still in use today.

### 1979 Data and Correlation

In 1979, additional data was considered, and the correlation was re-worked based on the H<sub>2</sub>S concentration in the SRU waste (tail) gas as opposed to SO<sub>2</sub> in the stack gas. A plot of these results is provided in Figure 2.3-2.

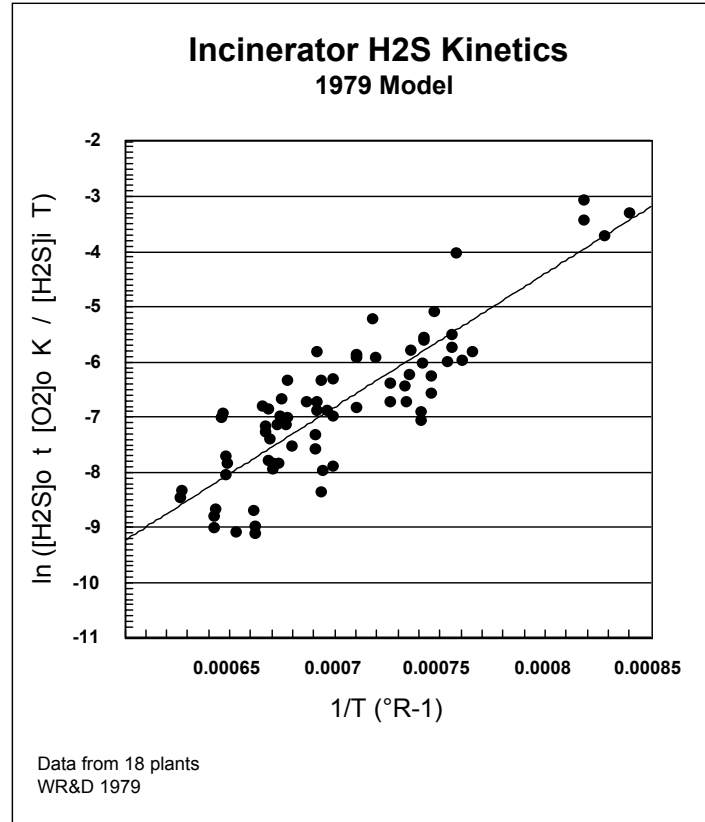


Figure 2.3-2 - H<sub>2</sub>S Kinetics 1979 Model

These data yielded the following correlation for the oxidation of H<sub>2</sub>S (4):

$$[\text{H}_2\text{S}]_o = 5.46 \times 10^{-11} [\text{H}_2\text{S}]_i T / K \tau [\text{O}_2]_o \exp(24955/T)$$

where ....

- [H<sub>2</sub>S]<sub>o</sub> concentration in the stack gas (ppm)
- [H<sub>2</sub>S]<sub>i</sub> concentration in the waste gas (ppm)
- T average system temperature (°R)
- τ residence time (s)
- K plant kinetic design factor
- [O<sub>2</sub>] concentration in the stack gas (vol%)

This correlation was found to provide nearly identical results to the original correlation and therefore was not implemented into the INCWRD program. However, the form of this correlation more closely follows the form of a proper kinetic equation based on first principles which was considered a desirable goal for the current work.

## 2005 Data

The data from 13 additional plant field studies which included more than 150 separate tests was collated and compiled. A plot of the 2005 data is provided in Figure 2.3-3.

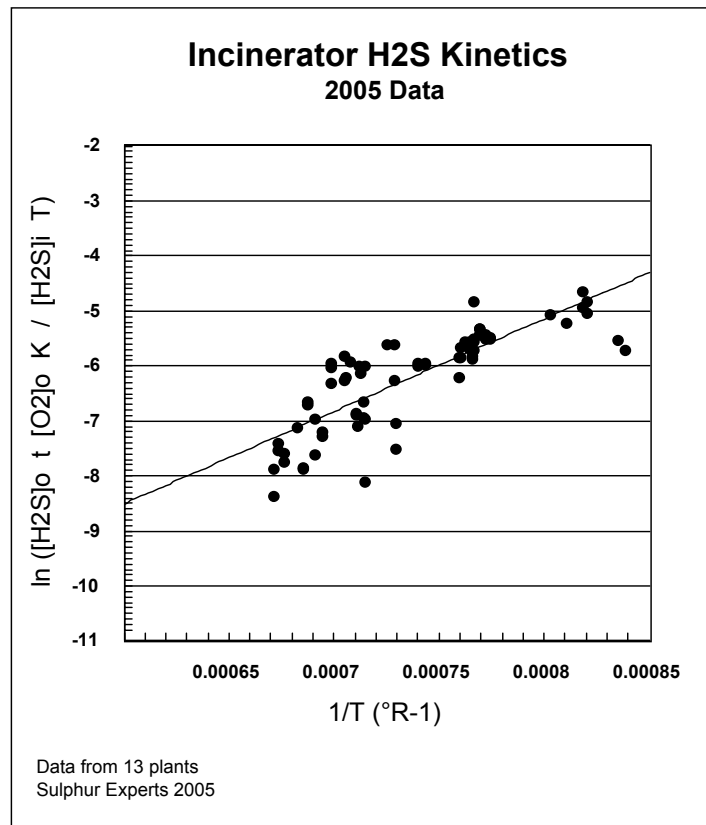


Figure 2.3-3 - H<sub>2</sub>S Kinetics 2005 Data

The 2005 data provided for similar overall results to the earlier work. However, the new 2005 data provided the following additional results and insights:

- the data set included a much large number of data points in the cooler end of the temperature range (down to 380°C or 715°F);
- the data was gathered for a much larger range of H<sub>2</sub>S concentrations in the SRU waste gas;
- the overall results suggested lower residual H<sub>2</sub>S concentrations in the stack gas at the lower end of the temperature scale; in effect the original correlation was over-predicting the residual H<sub>2</sub>S in this temperature range.

Combined 1975 and 2005 Data and Correlation

Ultimately, this style of empirical correlation provides the most utility when the largest possible data set is used. This ensures that the widest range of operating conditions, waste gas compositions and incinerator configurations is properly considered. With this in mind, the original 1975 data was compiled with the 2005 data to provide the following results:

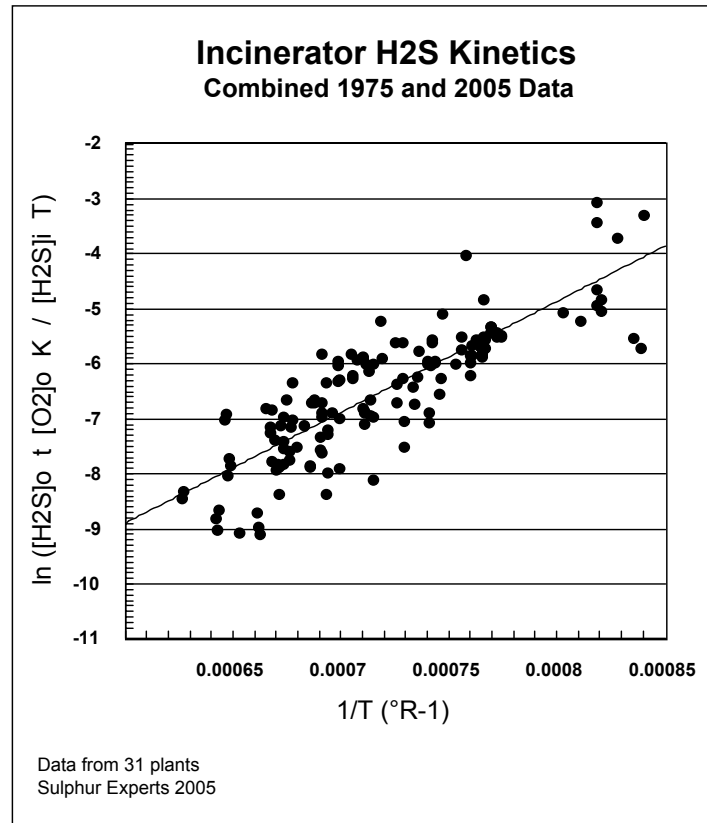


Figure 2.3-4 - H<sub>2</sub>S Kinetics Combined Data

These data yielded the following correlation for the oxidation of H<sub>2</sub>S:

$$[\text{H}_2\text{S}]_o = 7.58 \times 10^{-10} [\text{H}_2\text{S}]_i T / K \tau [\text{O}_2]_o \exp(20200/T)$$

This correlation was based on field data within the following ranges:

[H <sub>2</sub> S] <sub>o</sub>	5 - 310 ppm	(as measured in the stack effluent)
[H <sub>2</sub> S] <sub>i</sub>	470 - 5800 ppm	(as measured in the Claus plant tail gas)
τ	4.3 - 20.0 seconds	(total system - eg. Incinerator plus stack)
[O <sub>2</sub> ]	0.3 - 8.7 mole %	(as measured in the stack effluent)
T	733 - 1030°F or 390 - 555°C	

This 2005 H<sub>2</sub>S correlation is similar in form and function to the original 1975 and 1979 correlations. However, the new 2005 H<sub>2</sub>S correlation does predict moderately different H<sub>2</sub>S residuals in the stack over the range of operating conditions considered in the study.

In order to assess and illustrate the difference between the correlations, a set of simulated results was calculated. These results are presented in Table 2.3-1.

Table 2.3-1 - H <sub>2</sub> S Correlation Comparison K=4							
Case	[H <sub>2</sub> S] Waste Gas (ppm)	Temperature		Excess Oxygen (mole %)	Residence Time (s)	1975 [H <sub>2</sub> S] Stack (ppm)	New [H <sub>2</sub> S] Stack (ppm)
		°C	°F				
1	500	400	752	2	10	362	99
2	500	500	932	2	10	29	13
3	500	600	1112	2	10	4	3
4	6000	400	752	2	10	4344	1193
5	6000	500	932	2	10	348	158
6	6000	600	1112	2	10	50	34

These comparisons clearly indicate that the 2005 correlation predicts lower H<sub>2</sub>S residuals than the 1975/1979 correlations at all operating conditions. The effect is most dramatic at the colder end of the operating range. This appears reasonable as the original 1975/1979 data set included only a very few data points with average incinerator/stack temperatures less than 850°F (455°C). In effect, the 1975 correlation depended on a natural extrapolation to the lower temperatures without significant supporting field measurements.

The more recent field data included a much larger number of data points in the temperature range of 720 to 850°F (ca. 380 to 455°C). Therefore, the 2005 H<sub>2</sub>S correlation is based on actual field measurements in this colder temperature region.

The extension of the H<sub>2</sub>S correlation to lower system temperatures will prove to be very useful in the future because many operators are considering operation of the incinerators at these lower temperatures. The 2005 H<sub>2</sub>S correlation will provide more accurate prediction results for these incinerators.

## 2.4 COS Kinetics

### 1975 Data and Correlation

The original 1975 study for the COS kinetics was based on a relatively small number of tests. A plot of these results is provided in Figure 2.4-1.

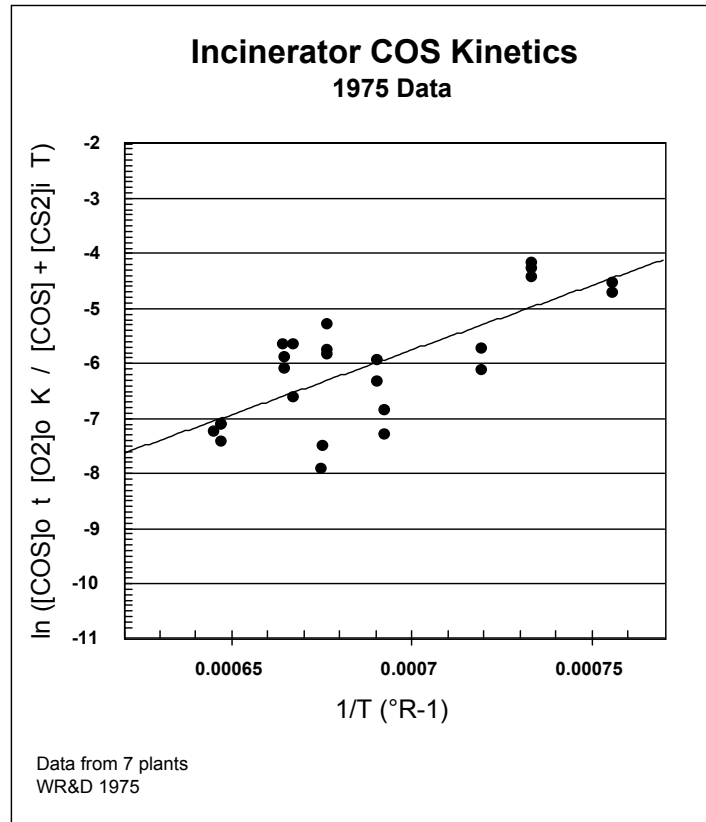


Figure 2.4-1 - COS Kinetics 1975 Model

These data yielded the following correlation for the oxidation of COS (4):

$$[\text{COS}]_o = 9.03 \times 10^{-10} \{[\text{COS}]_i + [\text{CS}_2]_i\} T / K \tau [\text{O}_2]_o \exp (21500/T)$$

where ....

$[\text{COS}]_o$	concentration in the stack gas (ppm)
$[\text{COS}]_i$	concentration in the waste gas (ppm)
$[\text{CS}_2]_i$	concentration in the waste gas (ppm)
T	average system temperature (°R)
$\tau$	residence time (s)
K	plant kinetic design factor
$[\text{O}_2]$	concentration in the stack gas (vol%)

This was the correlation which was implemented in the original INCWRD model and is still in use today.



2005 Data

The data from 13 additional plant field studies which included more than 150 separate tests was collated and compiled. A plot of the 2005 data is provided in Figure 2.4-2.

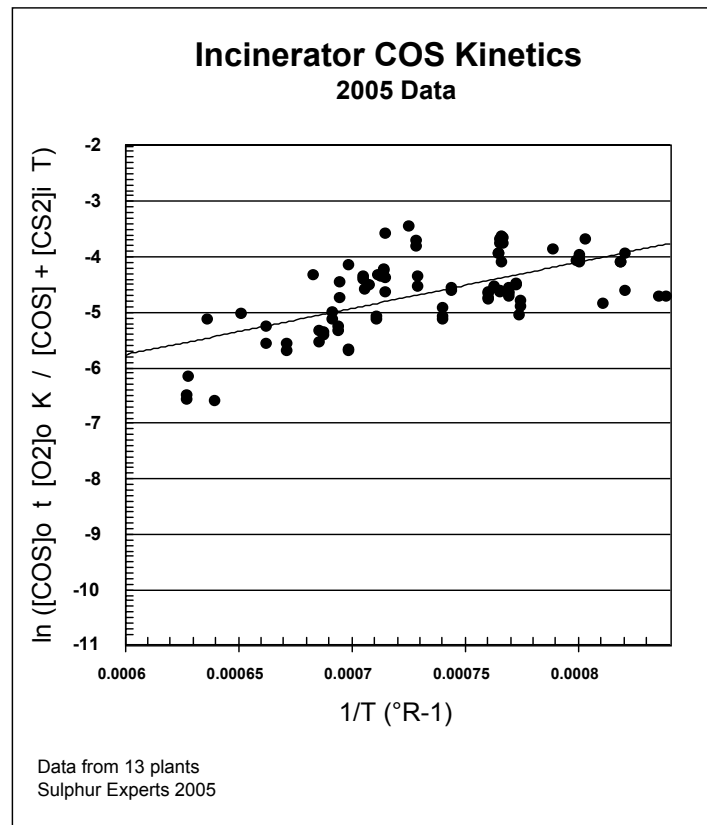


Figure 2.4-2 - COS Kinetics 2005 Data

The data set collected in 2005 yielded a significantly different correlation than the 1975 data and provided the following results:

- the data set included a much large number of data points;
- the data set covered a significantly larger temperature range (390 to 650°C, 730 to 1200°F).

Combined 1975 and 2005 Data and Correlation

The COS oxidation data collected for the 2005 study was combined with the data from the original 1975 study. These results are plotted in Figure 2.4-3.

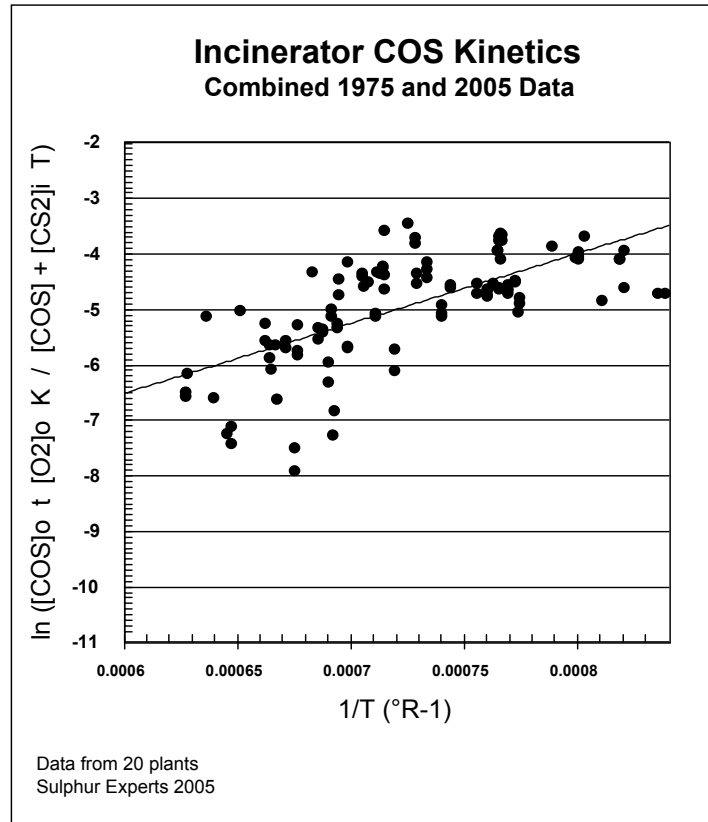


Figure 2.4-3 - COS Kinetics Combined Data

These data yielded the following correlation for the oxidation of H<sub>2</sub>S:

$$[\text{COS}]_o = 7.52 \times 10^{-7} \{[\text{COS}]_i + [\text{CS}_2]_i\} T / K \tau [\text{O}_2]_o \exp (12600/T)$$

This correlation was based on field data within the following ranges:

[COS] <sub>o</sub>	15 - 110 ppm	(as measured in the stack effluent)
[COS] <sub>i</sub>	65 - 235 ppm	(as measured in the Claus plant tail gas)
τ	4.3 - 20.0 seconds	(total system - eg. Incinerator plus stack)
[O <sub>2</sub> ]	1.6 - 8.7 mole %	(as measured in the stack effluent)
T	733 - 1030°F or 390 - 555°C	

The new 2005 COS correlation does predict moderately different COS residuals in the stack over the range of operating conditions considered in the study. In order to assess and illustrate the difference between the correlations, a set of simulated results was calculated. These results are presented in Table 2.4-1.

Case	[COS] Waste Gas (ppm)	Temperature		Excess Oxygen (mole %)	Residence Time (s)	1975 [COS] Stack (ppm)	New [COS] Stack (ppm)
		°C	°F				
1	50	400	752	2	10	35	19
2	50	500	932	2	10	4	6
3	50	600	1112	2	10	1	2
4	500	400	752	2	10	346	187
5	500	500	932	2	10	40	56
6	500	600	1112	2	10	8	22

These comparisons indicate that the 2005 COS correlation predicts lower COS residuals than the 1975/1979 correlations at lower operating temperatures and higher COS residuals at the higher operating temperatures. The difference is most dramatic at the low end of the temperature range.

The effect of this change to the COS correlation will be lower predicted COS residuals in the stack for the plants wishing to optimize to lower average temperatures.

## 2.5 CS<sub>2</sub> Kinetics

### 1975 Data and Correlation

The original 1975 study for the CS<sub>2</sub> kinetics was based on a very small number of tests from a single plant. A plot of these results is provided in Figure 2.5-1.

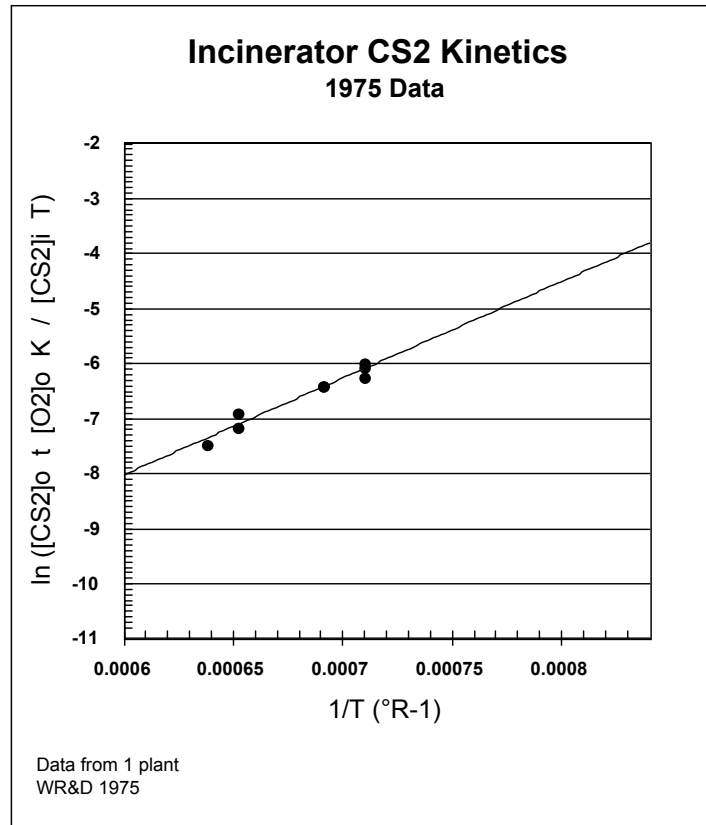


Figure 2.5-1 - CS<sub>2</sub> Kinetics 1975 Data

These data yielded the following correlation for the oxidation of CS<sub>2</sub> (4):

$$[\text{CS}_2]_o = 2.75 \times 10^{-8} [\text{CS}_2]_i T / K \tau [\text{O}_2]_o \exp(18400/T)$$

where ....

- [CS<sub>2</sub>]<sub>o</sub> concentration in the stack gas (ppm)
- [CS<sub>2</sub>]<sub>i</sub> concentration in the waste gas (ppm)
- T average system temperature (°R)
- τ residence time (s)
- K plant kinetic design factor
- [O<sub>2</sub>] concentration in the stack gas (vol%)

This was the correlation which was implemented in the original INCWRD model and is in use today.

2005 Data

The CS<sub>2</sub> data from 13 additional plant field studies which included more than 150 separate tests was collated and compiled. A plot of the 2005 data is provided in Figure 2.5-2.

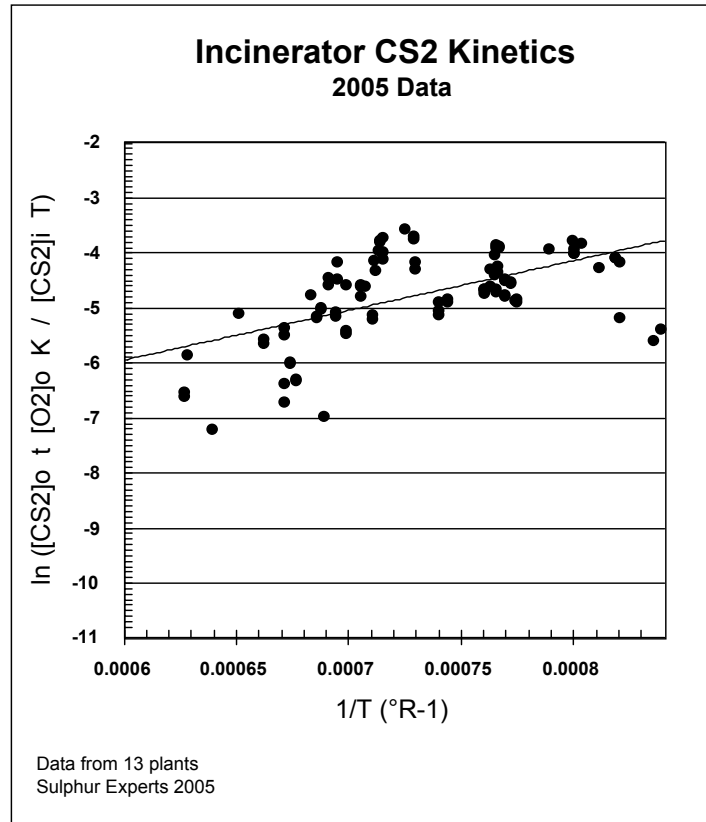


Figure 2.5-2 - CS<sub>2</sub> Kinetics 2005 Data

The CS<sub>2</sub> data set collected in 2005 yielded a significantly different correlation than the 1975 data and had the following important features:

- the data set included a much large number of data points;
- the data set covered a significantly larger temperature range (390 to 650°C, 730 to 1200°F).

Combined 1975 and 2005 Data and Correlation

The CS<sub>2</sub> data collected for the 2005 study was combined with the data from the original 1975 study. These results are plotted in Figure 2.5-3.

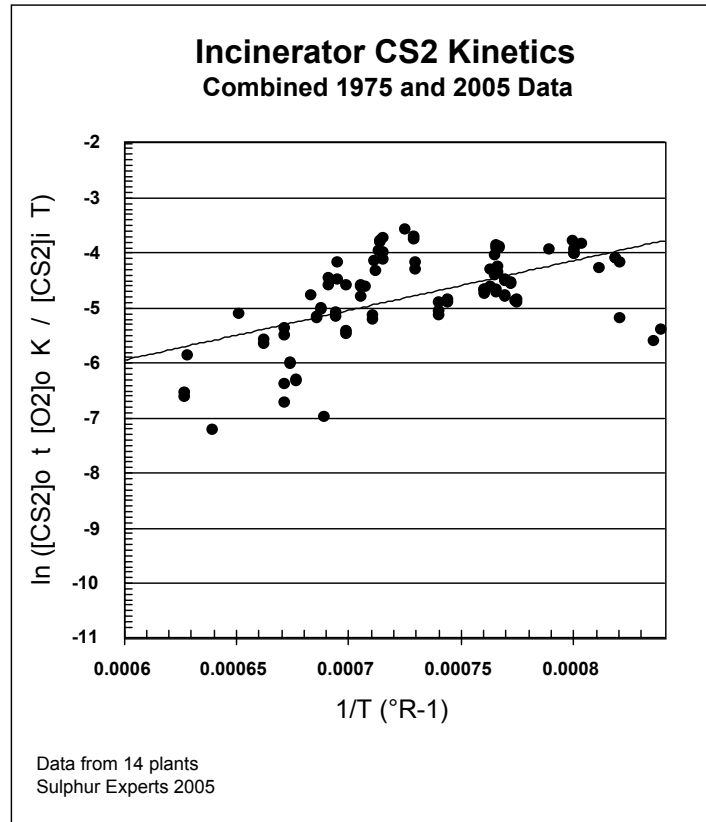


Figure 2.5-3 - CS<sub>2</sub> Kinetics Combined Data

These data yielded the following correlation for the oxidation of CS<sub>2</sub>:

$$[CS_2]_o = 2.76 \times 10^{-6} [CS_2]_i T / K \tau [O_2]_o \exp (10900/T)$$

This correlation was based on field data within the following ranges:

- [COS]<sub>o</sub> 8 - 75 ppm (as measured in the stack effluent)
- [COS]<sub>i</sub> 60 - 900 ppm (as measured in the Claus plant tail gas)
- τ 4.3 - 20.0 seconds (total system - eg. Incinerator plus stack)
- [O<sub>2</sub>] 0.3 - 8.7 mole % (as measured in the stack effluent)
- T 733 - 1030°F or 390 - 555°C

The new 2005 CS<sub>2</sub> correlation does predict significantly different CS<sub>2</sub> residuals in the stack over the range of operating conditions considered in the study. In order to assess and illustrate the difference between the correlations, a set of simulated results was calculated. These results are presented in Table 2.5-1.

Table 2.5-1 - CS <sub>2</sub> Correlation Comparison K=4							
Case	[CS <sub>2</sub> ] Waste Gas (ppm)	Temperature		Excess Oxygen (mole %)	Residence Time (s)	1975 [CS <sub>2</sub> ] Stack (ppm)	New [CS <sub>2</sub> ] Stack (ppm)
		°C	°F				
1	50	400	752	2	10	82	17
2	50	500	932	2	10	13	6
3	50	600	1112	2	10	3	3
4	1000	400	752	2	10	1000	337
5	1000	500	932	2	10	263	121
6	1000	600	1112	2	10	65	56

These comparisons clearly indicate that the 2005 CS<sub>2</sub> correlation predicts lower CS<sub>2</sub> residuals than the 1975/1979 correlations at all operating temperatures.

## 2.6 H<sub>2</sub> Kinetics

### 1975 Data and Correlation

The original 1975 study for the H<sub>2</sub> kinetics was based on a moderate number of tests from a single plant. A plot of these results is provided in Figure 2.6-1.

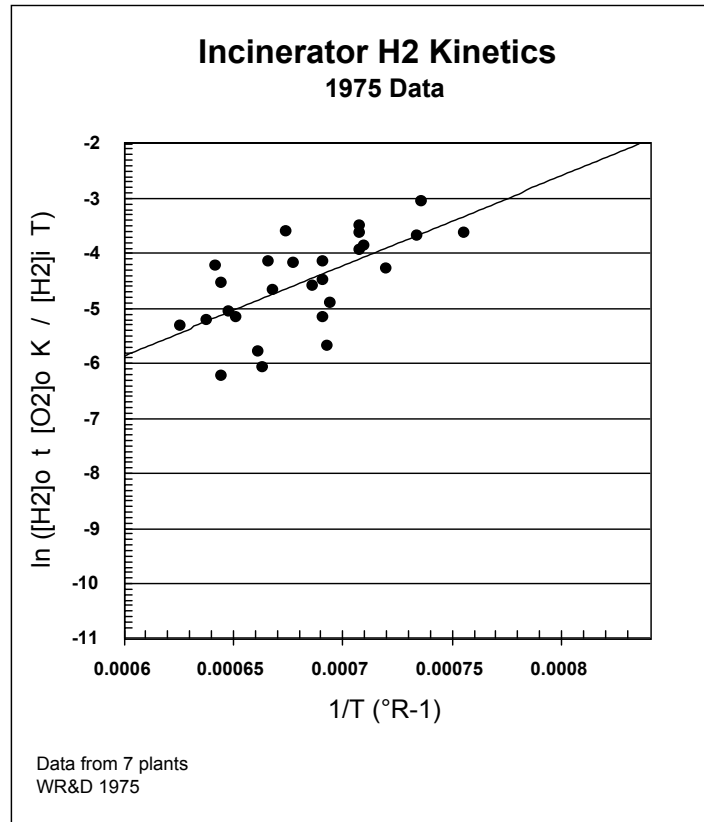


Figure 2.6-1 - H<sub>2</sub> Kinetics 1975 Data

These data yielded the following correlation for the oxidation of H<sub>2</sub>:

$$[H_2]_o = 4.79 \times 10^{-8} [H_2]_i T / K \tau [O_2]_o \exp (18300/T)$$

where ....

- [H<sub>2</sub>]<sub>o</sub> concentration in the stack gas (ppm)
- [H<sub>2</sub>]<sub>i</sub> concentration in the waste gas (ppm)
- T average system temperature (°R)
- τ residence time (s)
- K plant kinetic design factor
- [O<sub>2</sub>] concentration in the stack gas (vol%)

This was the correlation which was implemented in the original INCWRD model and is in use today.



2005 Data

The H<sub>2</sub> data from 13 additional plant field studies which included more than 150 separate tests was collated and compiled. A plot of the 2005 data is provided in Figure 2.6-2.

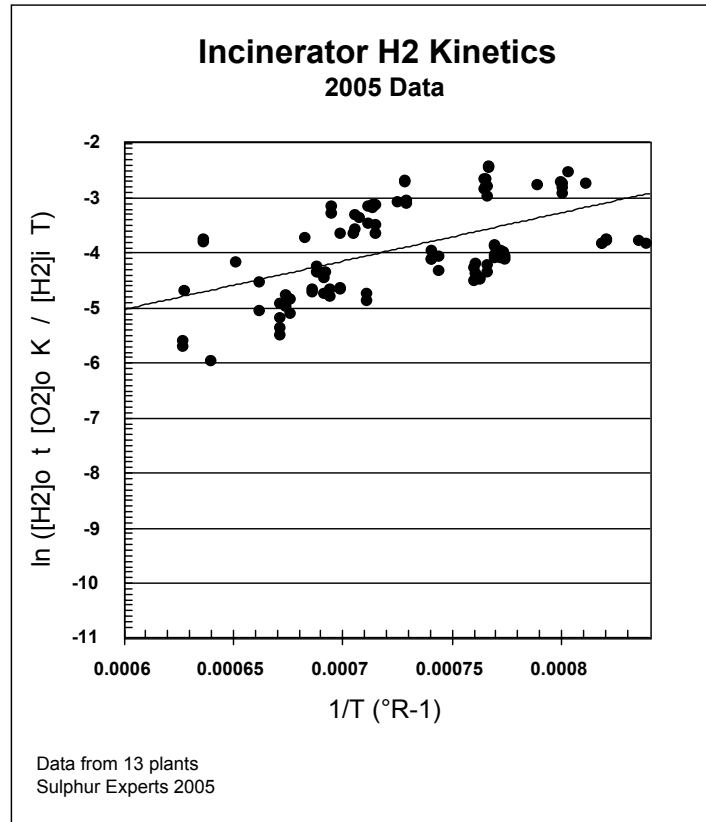


Figure 2.6-2 - H<sub>2</sub> Kinetics 2005 Data

The data set collected in 2005 yielded a moderately different correlation than the 1975 data and had the following important features:

- the data set included a much large number of data points;
- the data set covered a significantly larger temperature range (390 to 650°C, 730 to 1200°F).

Combined 1975 and 2005 Data and Correlation

The data collected for the 2005 study was combined with the data from the original 1975 study. These results are plotted in Figure 2.6-3.

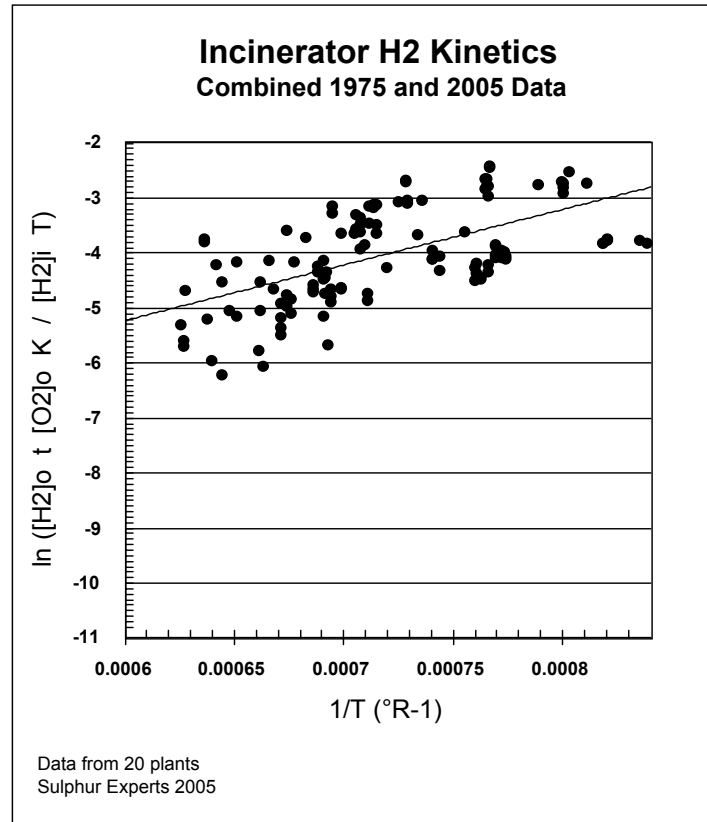


Figure 2.6-3 - H<sub>2</sub> Kinetics Combined Data

These data yielded the following correlation for the oxidation of H<sub>2</sub>:

$$[H_2]_o = 1.23 \times 10^{-5} [H_2]_i T / K \tau [O_2]_o \exp(10100/T)$$

This correlation was based on field data within the following ranges:

[H <sub>2</sub> ] <sub>o</sub>	920 - 9520 ppm	(as measured in the stack effluent)
[H <sub>2</sub> ] <sub>i</sub>	1550 - 20450 ppm	(as measured in the Claus plant tail gas)
τ	4.3 - 20.0 seconds	(total system - eg. Incinerator plus stack)
[O <sub>2</sub> ]	0.3 - 8.7 mole %	(as measured in the stack effluent)
T	733 - 1030°F or 390 - 555°C	

The new 2005 H<sub>2</sub> correlation does predict moderately different H<sub>2</sub> residuals in the stack over the range of operating conditions considered in the study. In order to assess and illustrate the difference between the correlations, a set of simulated results was calculated. These results are presented in Table 2.6-1.

Table 2.6-1 - H <sub>2</sub> Correlation Comparison K=4							
Case	[H <sub>2</sub> Waste Gas (ppm)]	Temperature		Excess Oxygen (mole %)	Residence Time (s)	1975 [H <sub>2</sub> ] Stack (ppm)	New [H <sub>2</sub> ] Stack (ppm)
		°C	°F				
1	5000	400	752	2	10	5000	3898
2	5000	500	932	2	10	2135	1524
3	5000	600	1112	2	10	535	750
4	20000	400	752	2	10	20000	15593
5	20000	500	932	2	10	8539	6096
6	20000	600	1112	2	10	2140	3000

These comparisons clearly indicate that the 2005 H<sub>2</sub> combined correlation predicts lower H<sub>2</sub> residuals than the 1975/1979 correlations at the lower operating temperatures and slightly higher residuals at the higher operating temperatures.

## 2.7 CO Kinetics

The original 1975 study did collect data on the oxidation kinetics for CO. However, a critical review of the data indicated a very poor correlation and relatively small amounts of CO oxidation over the range of conditions tested. Therefore, no correlation for CO kinetics was developed.

### 2005 Data and Correlation

It was a primary goal of this study to re-assess the kinetics of CO oxidation and to determine if a meaningful correlation could be derived. To that end, the CO field data gathered from the 13 plants was compiled. The results from this review are provided in Figure 2.7-1.

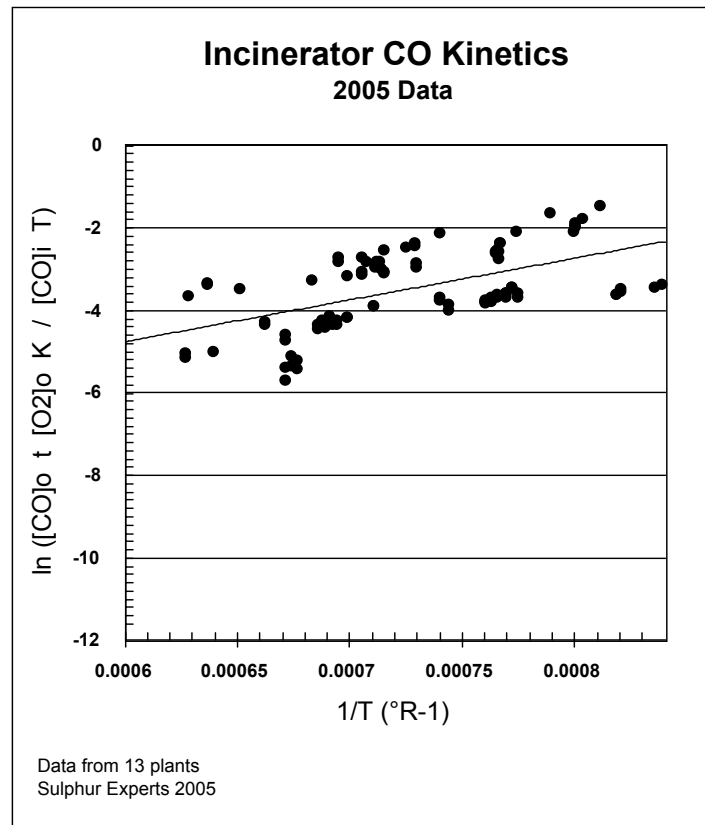


Figure 2.7-1 - CO 2005 Data

These data yielded the following correlation for the oxidation of CO:

$$[\text{CO}]_o = 4.79 \times 10^{-8} [\text{CO}]_i T / K \tau [\text{O}_2]_o \exp (18300/T)$$

where ....

- [CO]<sub>o</sub> concentration in the stack gas (ppm)
- [CO]<sub>i</sub> concentration in the waste gas (ppm)
- T average system temperature (°R)
- τ residence time (s)
- K plant kinetic design factor
- [O<sub>2</sub>] concentration in the stack gas (vol%)

This correlation was based on field data within the following ranges:

[CO] <sub>o</sub>	750 - 9020 ppm	(as measured in the stack effluent)
[COS] <sub>i</sub>	3050- 6810 ppm	(as measured in the Claus plant tail gas)
τ	4.3 - 20.0 seconds	(total system - eg. Incinerator plus stack)
[O <sub>2</sub> ]	1.6 - 8.7 mole %	(as measured in the stack effluent)
T	733 - 1030°F or 390 - 555°C	

Table 2.7-1 summarizes some typical CO results as predicted by the 2005 CO correlation.

Case	[CO] Waste Gas (ppm)	Temperature		Excess Oxygen (mole %)	Residence Time (s)	New [CO] Stack (ppm)
		°C	°F			
1	3000	400	752	2	10	3000
2	3000	500	932	2	10	1508
3	3000	600	1112	2	10	742
4	10000	400	752	2	10	10000
5	10000	500	932	2	10	5027
6	10000	600	1112	2	10	2473

One of the interesting features of CO oxidation in these systems, is that with relatively low incineration temperatures, the CO in the stack effluent is higher than the CO content in the waste gas. This implies that some systems will form CO in the main incinerator burner and that in “cold” systems there is inadequate time or temperature to oxidise the CO to any extent. This is consistent with conventional thought regarding the formation and conversion of CO in thermal incinerators.

### 3.0 Application of New Technology for Incinerator Optimization

In order to investigate more cost effective ways of designing and operating these thermal incinerator systems, several options for utilizing “new technology” were reviewed. The following results and discussions provide details on the utility and economics of implementing these technologies.

#### 3.1 Use of Specialized Claus Catalysts

The emission for TRS compounds from the thermal incinerator is directly related to the concentration of these compounds in the Claus plant waste (tail) gas. The concentration of these compounds in the waste gas is related to a number of factors in the upstream Claus plant including the formation rate of these compounds in the reaction furnace and the extent of conversion of the compounds in the Claus catalyst reactors.

The catalyst typically used in Claus plants is an activated alumina material commercially available from various manufacturers. These catalysts, as a group have a significant capability to convert COS and CS<sub>2</sub> in the process gas. The extent to which they convert COS and CS<sub>2</sub> depends strongly on the operating temperature in the Converter 1 reactor and the condition of the catalyst. Typical COS and CS<sub>2</sub> conversion efficiencies over these catalysts are in the 90 / 75 percent range respectively for start of run conditions.

While these levels of conversion are often adequate for meeting the plant recovery efficiency requirements, there are still measurable levels of COS and CS<sub>2</sub> in the waste gas to the incinerator. For the 13 plants reviewed in this study the COS concentrations in the SRU waste gas ranged from 70 to 816 ppm. The CS<sub>2</sub> concentrations ranged from 60 to 936 ppm. Higher levels of both COS and CS<sub>2</sub> are not uncommon in plants with some measure of catalyst deactivation of the Claus catalyst.

There are also specialized catalysts (titanium dioxide based) which have the ability to better convert the COS and CS<sub>2</sub> at the same operating conditions and are also resistant to some types of normal, ongoing catalyst deactivation. These catalyst are normally employed to improve the overall recovery efficiency in the plant if emissions from COS and CS<sub>2</sub> are a particular problem. This catalyst comes at a significantly higher cost (typically 8 to 10 times the cost of alumina catalyst) and therefore is only used if the recovery efficiency requirements are difficult to meet on an ongoing basis. This type of titania catalyst is also usually employed in the bottom portion of the reaction and is used in conjunction with a top layer of conventional alumina catalyst (typically in a 50:50 ratio). This was the assumed arrangement for these case studies.

Based on preliminary assessments, it was determined that the improved performance of these catalysts could be employed as a method for optimizing the thermal incinerator by simply decreasing the COS and CS<sub>2</sub> “load” to the incinerator. Following is a series of case studies which investigates the impact of the specialized catalyst on the COS and CS<sub>2</sub> content of the SRU tail gas. These results were used to assess the economics comparing the incremental cost of employing these catalyst to the cost savings which would be realized by operating the incinerator at lower temperatures in these cases.

### Specialized Catalyst Case Studies

After reviewing the actual plant configurations used in this study, two “typical” study cases were constructed. These two cases represent a reasonable cross section of the plants compiled for this study. Table 3.1-1 summarizes these cases and the critical data and assumptions for each case.

Case	1A	1B	2A	2B
Description	Lean acid gas		Rich acid gas	
Acid gas [H <sub>2</sub> S] (mole %)	50		80	
Sulphur plant size (t/d)	500	500	500	500
Converter 1 inlet composition				
H <sub>2</sub> S (ppm)	60310	58260	54350	53880
COS (ppm)	2980	3070	5150	5200
CS <sub>2</sub> (ppm)	5080	5040	1910	1880
Converter 1 Catalyst type	Alumina only	Alumina and Titania	Alumina only	Alumina and Titania
Converter 1 Operating Temperature (°C)	340	340	340	340
Converter 1 COS conversion (%)	90	97	92	98
Converter 1 CS <sub>2</sub> conversion (%)	74	95	77	95
Allowable Stack TRS (ppm)	250	250	250	250

Lean Feed plants typically have much higher CS<sub>2</sub> formation rates in the reaction furnace as a result of lower reaction furnace temperatures (6). This was reflected in the process compositions used for these simulated case studies.

Rich feed plants typically have higher COS formation rates and much lower CS<sub>2</sub> formation rates in the reaction furnace as a result of higher furnace temperatures. This was also reflected in the simulated case studies.

The Converter 1 operating conditions chosen were typical of well optimized plants (7). The expected COS and CS<sub>2</sub> conversion rates for the two different catalyst types were determined from data and information available for the open literature (8, 9). These assumptions were in good agreement with data used by Sulphur Experts for the determination of proprietary empirical correlations that are employed in the Sulsim (10) sulphur plant simulation program.

For each case in the study, a detailed plant simulation was completed based on these assumptions. The operation of the incinerator was determined using the H<sub>2</sub>S, COS, CS<sub>2</sub>, H<sub>2</sub> and CO correlations determined in Section 2 of this report. For the sake of realism, the TRS content in the stack gas effluent was maintained at 250 ppm, slightly less than the 300 ppm guideline commonly used for the design and operation of SRU thermal incinerators in Alberta.

These simulations provided the expected incinerator operating conditions for each case and the predicted fuel gas consumption at the optimized incinerator conditions. The value of this fuel gas savings was compared to the increased cost of the specialized catalyst. These results are summarized in Table 3.1-2.

<b>Table 3.1-2 - Specialized Catalyst Case Results</b>				
<b>Case</b>	<b>1A</b>	<b>1B</b>	<b>2A</b>	<b>2B</b>
Description	Lean acid gas		Rich acid gas	
Sulphur plant size (t/d)	500	500	500	500
Converter 1 Catalyst type	Alumina only	Alumina and Titania	Alumina only	Alumina and Titania
Allowable Stack TRS (ppm)	250	250	250	250
Waste gas composition				
H <sub>2</sub> S (ppm)	2330	2320	2820	2820
COS (ppm)	<b>310</b>	<b>110</b>	<b>420</b>	<b>120</b>
CS <sub>2</sub> (ppm)	<b>1380</b>	<b>260</b>	<b>460</b>	<b>100</b>
Incinerator conditions				
Design K Factor	4	4	4	4
Excess oxygen (%)	4	4	4	4
Residence time (s)	10	10	10	10
Temperature (average) (°C)	<b>505</b>	<b>445</b>	<b>475</b>	<b>445</b>
Fuel gas demand (m <sup>3</sup> /d)	25,890	18,120	17130	17020
Stack gas composition				
H <sub>2</sub> S (ppm)	57	173	118	206
COS (ppm)	33	23	62	25
CS <sub>2</sub> (ppm)	160	53	70	20
Cost comparison				
Fuel cost (@ \$370 per 1000 m <sup>3</sup> ) (\$/day)	9,580	6,700	6,340	6295
Fuel savings (\$/day)	---	2,880	---	45
Fuel savings (\$/year)	---	1,008,000	---	15,575
Catalyst costs (material only) <sup>1</sup> (\$)	95,000	400,000	75,000	315,000
Extra catalyst cost (material only) <sup>1</sup> (\$)	---	305,000	---	240,000
CO <sub>2</sub> emissions (t/day)	732	724	196	193
CO <sub>2</sub> emissions (t/year)	256,320	253,406	68,478	67,495
CO <sub>2</sub> savings (t/year)	---	2914	---	983

<sup>1</sup> This incremental cost would be required every 3 to 5 years depending on the plants' typical catalyst change-out schedule.



These case studies revealed some interesting results:

- the fuel gas savings only become significant in cases with COS and CS<sub>2</sub> content is in the high end of the range (more than 1000 ppm in the tail gas with activated alumina catalyst);
- the most dramatic effect occurs when the CS<sub>2</sub> formation is relatively high (those SRUs with lean feeds and/or high hydrocarbon in the acid gas) because the titania catalyst has a more significant effect on the *relative* CS<sub>2</sub> conversion;
- this approach will be very case sensitive and will not be economic for all plants; a detailed knowledge of the waste gas composition is required for an accurate assessment of the opportunity;
- the benefit of the lower realizable temperature is partially off-set by the reduced oxidation efficiency of the H<sub>2</sub> and CO; this effect is more dramatic in rich feed plants which have higher concentrations of H<sub>2</sub> and CO in the waste gas.

Based on the incremental costs associated using the specialized titania catalyst, the expected payout for the Lean acid gas case would be 19 months. This compares favourably to the typical catalyst change-out requirements which typically range from 36 to 60 months. Longer catalyst use would result in a better total savings.

The payout for this particular Rich feed case is not favourable at approximately 42 months. In this case, the use of the specialized catalyst could not be justified on economics alone.

### 3.2 Increasing Incinerator Residence Time

The destruction efficiency of TRS compounds in the incinerator is directly related to the residence time allowed for the reactions. In typical incinerator systems, both the incinerator chamber and the stack contribute volume to the available residence time. In current plant designs, the incinerator system is likely to provide 5 to 20+ seconds of residence time depending on the plant flow conditions.

A simple, but effective method for increasing the TRS destruction is to simply add residence time to the system by providing a larger incinerator volume. It would be possible to add additional volume to an existing incinerator system by simply extending the size of the existing incinerator chamber.

In order to assess the economics of this approach, a simple simulation exercise was completed for several “typical” plant cases. Table 3.2-1 on the following page summarizes the assumptions and results from these cases.

Increasing the effective residence time has a significant effect on both the oxidation efficiency of the TRS compounds and increasing the oxidation of H<sub>2</sub> and CO in the waste gas. This second effect is very important as the energy value of the H<sub>2</sub> and CO provides additional reduction in the fuel gas demand.

These results indicated that the fuel gas savings can be very significant for both the lean and rich acid gas feed cases. Based on the estimated cost of retro-fitting an existing incinerator on a 500 t/d sulphur plant, the payout is very favourable for both cases (less than 2 years). It can be expected that using larger incinerator chamber volumes in a new plant design would also likely have a very favourable payout and should be considered in new plant designs.

<b>Table 3.2-1 - Increasing Incinerator Residence Time Case Results</b>					
<b>Case</b>		<b>1A</b>	<b>1B</b>	<b>2A</b>	<b>2B</b>
<b>Description</b>		<b>Lean acid gas</b>		<b>Rich acid gas</b>	
Sulphur plant size	(t/d)	500	500	500	500
Allowable Stack TRS	(ppm)	250	250	250	250
<b>Waste gas composition</b>					
H <sub>2</sub> S	(ppm)	5720	5720	2820	2820
COS	(ppm)	310	310	420	420
CS <sub>2</sub>	(ppm)	1380	1380	460	460
<b>Incinerator conditions</b>					
Design K Factor		4	4	4	4
Excess oxygen	(%)	4	4	4	4
Residence time	(s)	<b>10</b>	<b>15</b>	<b>10</b>	<b>15</b>
Temperature (average)	(°C)	<b>505</b>	<b>470</b>	<b>475</b>	<b>448</b>
Fuel gas demand	(m <sup>3</sup> /d)	25890	21080	17140	13870
<b>Stack gas composition</b>					
H <sub>2</sub> S	(ppm)	57	71	118	133
COS	(ppm)	33	32	62	56
CS <sub>2</sub>	(ppm)	160	147	70	61
<b>Cost comparison</b>					
Fuel cost (@ \$370 per 1000 m <sup>3</sup> )	(\$/day)	9,580	7,800	6,340	5,130
Fuel savings	(\$/day)	---	1,780	---	1,210
	(\$/year)	---	623,000	---	423,500
Incinerator retro-fit costs (installed)	(\$)	0	950,000	0	750,000
CO <sub>2</sub> emissions	(t/day)	732	724	196	192
	(t/year)	256,320	253,500	68,470	67,030
CO <sub>2</sub> savings	(t/year)	---	2820	---	1440

### 3.3 Improved Burner/Incinerator Mixing

The destruction efficiency of TRS compounds in the incinerator is also directly and proportionally related to the mixing efficiency in the system. The mixing efficiency is affected by many parameters in the system including burner configuration, air pre-mixing techniques, checker wall installation and others. Prior work has indicated that current typical incinerator designs provide a “Design Mixing Factor” (K Factor) up to 8 (2).

More recent research work by combustion engineering companies (6) suggests that design mixing factors up to 20 and higher are possible. In order to assess the value of installing or retro-fitting a newer “high mixing” incinerator system, two cases studies were evaluated. Table 3.3-1 summarizes the assumptions and results from these cases.

<b>Table 3.3-1 - Improved Incinerator Mixing Case Results</b>					
<b>Case</b>		<b>1A</b>	<b>1B</b>	<b>2A</b>	<b>2B</b>
<b>Description</b>		<b>Lean acid gas</b>		<b>Rich acid gas</b>	
Sulphur plant size	(t/d)	500	500	500	500
Allowable Stack TRS	(ppm)	250	250	250	250
<b>Waste gas composition</b>					
H <sub>2</sub> S	(ppm)	5720	5720	2820	2820
COS	(ppm)	310	310	420	420
CS <sub>2</sub>	(ppm)	1380	1380	460	460
<b>Incinerator conditions</b>					
Design K Factor		<b>8</b>	<b>20</b>	<b>8</b>	<b>20</b>
Excess oxygen	(%)	4	4	4	4
Residence time	(s)	10	10	10	10
Temperature (average)	(°C)	448	389	431	382
Fuel gas demand	(m <sup>3</sup> /d)	18,530	11,060	11,890	6625
<b>Stack gas composition</b>					
H <sub>2</sub> S	(ppm)	82	118	142	172
COS	(ppm)	61	27	52	40
CS <sub>2</sub>	(ppm)	137	106	55	38
<b>Cost comparison</b>					
Fuel cost (@ \$370 per 1000 m <sup>3</sup> )	(\$/day)	6,855	3,920	4,400	2,450
Fuel savings	(\$/day)	---	2,935	---	1,950
	(\$/year)	---	1,027,000	---	683,000
Incinerator retro-fit costs (installed)	(\$)	---	1,600,000	---	1,400,000
CO <sub>2</sub> emissions	(t/day)	720	708	189	182
	(t/year)	251,900	247,790	66,160	63,800
CO <sub>2</sub> savings	(t/year)	---	4110	---	2360

Increasing the mixing efficiency of the burner / incinerator system has a significant effect on the oxidation efficiency of the TRS compounds and the oxidation efficiency of H<sub>2</sub> and CO in the waste gas.

These results indicated that the fuel gas savings can be very significant for both the lean and rich acid gas feed cases. Based on the estimated cost of retro-fitting an existing incinerator on a 500 t/d sulphur plant, the estimated payout is 2 years or less depending on the acid gas feed quality. It can be expected that using a modern “high mixing” burner / incinerator in a new plant design would also likely have a very favourable payout and should be considered in new plant designs.

### 3.0 Conclusions

#### Incinerator Kinetic Modelling

- The use of a much extensive plant test data has allowed for a critical review of the original TRS kinetic correlations used in the existing INCWRD. This reviewed has resulted in notable changes in these correlations.
- The new 2005 data are based on a much broader set of test cases and plant configurations. Therefore the updated correlations for H<sub>2</sub>S, COS, CS<sub>2</sub> and H<sub>2</sub> will apply more accurately to a larger set of different plant types.
- The 2005 data set provided sufficient data to support an entirely new kinetic correlation for the oxidation of CO in thermal incinerators.
- The updated correlations have been implemented in a modern Windows based computer program which allow for fast and accurate evaluation of SRU thermal incinerators for opportunities to optimize for fuel gas consumption.

#### Application of New Technology for Incinerator Optimization

- Several new technologies have been investigated to further optimize SRU thermal incinerators for fuel gas consumption. These technologies are technically sound and could be implemented in virtually any existing plant. These technologies could also be implemented in new plant designs in order to realize significant fuel gas savings.
- The use of specialized Claus catalysts in order to achieve higher COS and CS<sub>2</sub> conversions and therefore lower TRS residuals in the SRU tail gas has been investigated. The results from this work indicate that these catalysts could be used effectively and economically in some plant situations. The advantage of these catalysts is sufficiently case sensitive to warrant and plant by plant review to determine the possible opportunity.
- The use of extended residence times in the incinerator/stack system is a very effective method for decreasing fuel gas demand in systems that are currently TRS limited. The predicted payout on these systems is less than 2 years for the case studies reviewed in this work.
- The use of high efficiency burners and incinerators in these incinerator/stack systems is also a very effective method for decreasing fuel gas demand in systems that are currently TRS limited. The predicted payout on these systems is less than 2 years for the case studies reviewed in this work.

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